Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:36 PM GMT

PDB ID	:	3ZZU
Title	:	Crystal structure of Staphylococcus aureus elongation factor G with mutations M16I and F88L
Authors	:	Koripella, R.K.; Chen, Y.; Selmer, M.; Sanyal, S.
Deposited on	:	2011-09-05
Resolution	:	2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

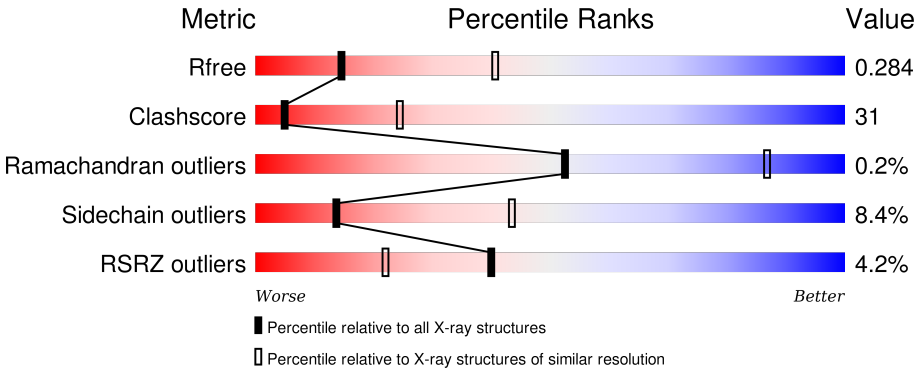
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	693	3% 49% 39% 5% 6%
1	B	693	5% 49% 41% · 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10039 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 ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	1
			5018	3151	841	1000	26			
1	B	649	Total	C	N	O	S	0	0	1
			5018	3151	841	1000	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ILE	MET	ENGINEERED MUTATION	UNP P68790
A	88	LEU	PHE	ENGINEERED MUTATION	UNP P68790
B	16	ILE	MET	ENGINEERED MUTATION	UNP P68790
B	88	LEU	PHE	ENGINEERED MUTATION	UNP P68790

- Molecule 2 is water.

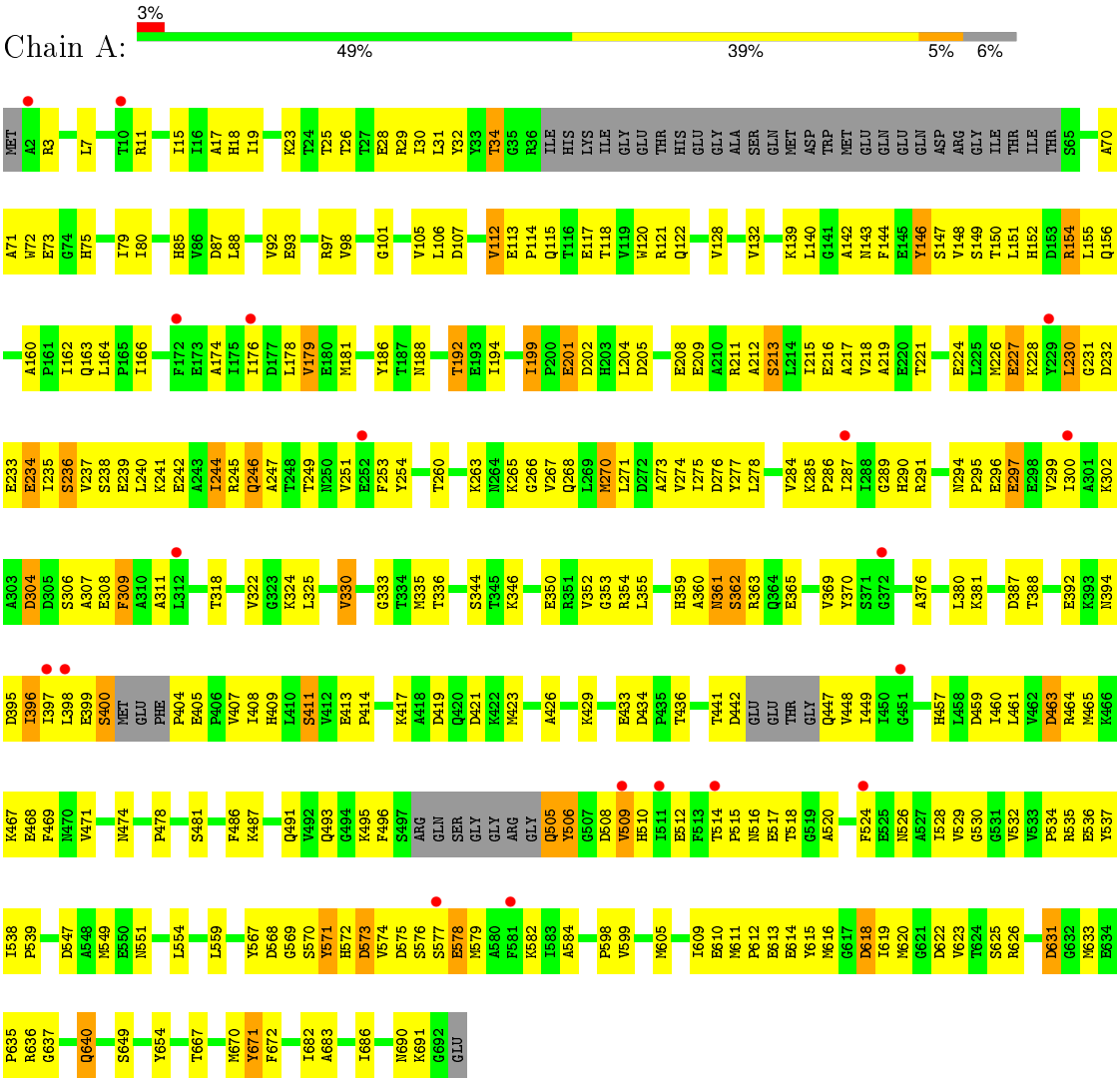
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

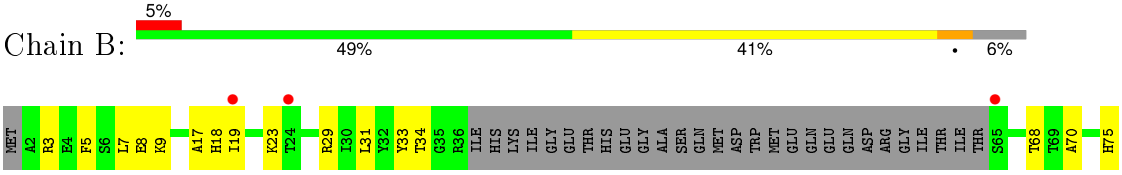
- Molecule 1: ELONGATION FACTOR G

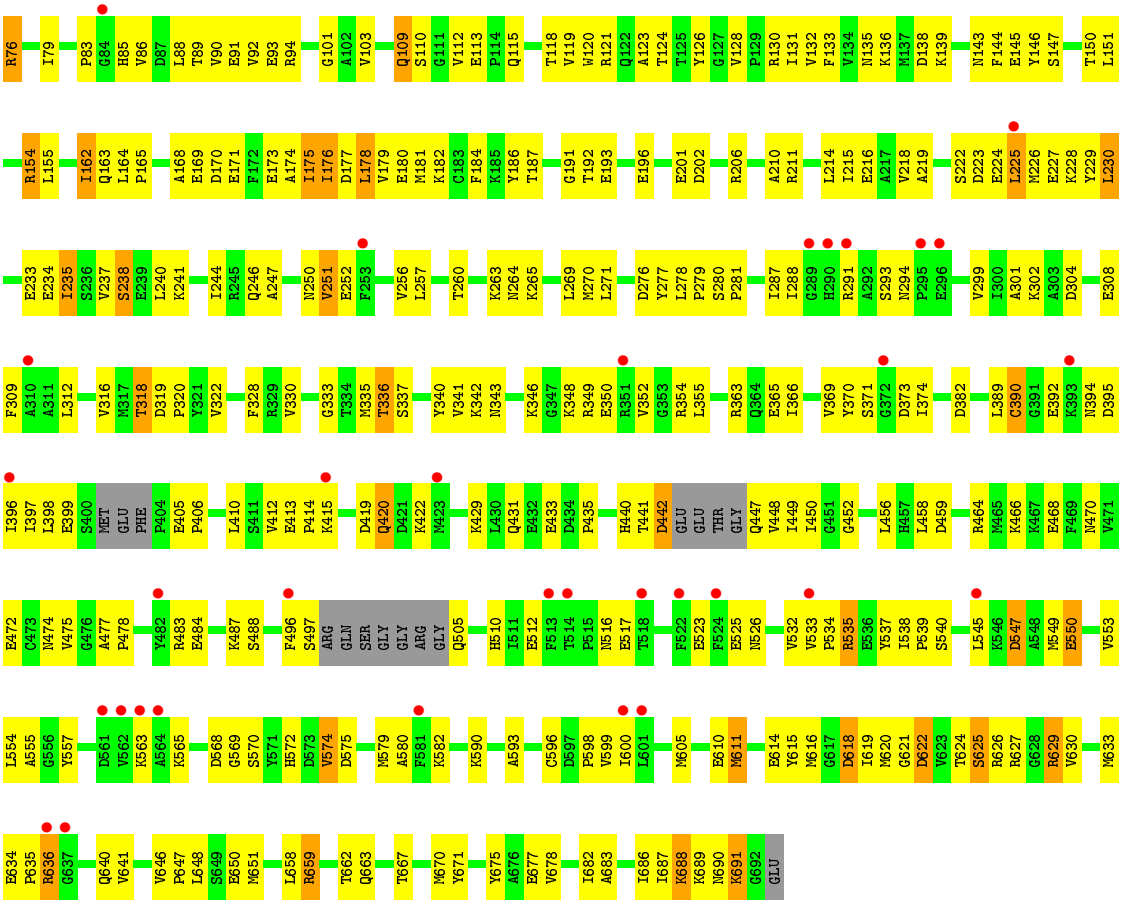
Chain A:



- Molecule 1: ELONGATION FACTOR G

Chain B:




R76 I79 P83 G84 H85 V86 D87 L88 T89 V90 E91 V92 E93 R94 G101 A102 V103 Q109 S110 G111 V112 E113 P114 Q115 T118 V119 W120 R121 Q122 A123 T124 T125 Y126 G127 V128 P129 R130 I131 V132 F133 V134 N135 K136 M137 D138 K139 N143 F144 E145 Y146 S147 T150 L151
R154 L155 I162 Q163 L164 P165 A168 E169 D170 E171 F172 E173 A174 I175 I176 D177 L178 V179 E180 M181 K182 C183 F184 K185 Y186 T187 G191 T192 E193 E196 E201 D202 R206 A210 R211 L214 I215 E216 A217 V218 A219 S222 D223 E224 L225 M226 E227 K228 Y229 L230
E233 E234 I235 S236 V237 S238 E239 L240 K241 I244 R245 Q246 A247 N250 V251 E252 F253 V256 L257 T260 K263 N264 K265 L269 M270 L271 D276 Y277 L278 P279 S280 P281 I287 I288 G289 H290 R291 A292 S293 N294 P295 E296 V299 I300 A301 K302 A303 D304 E308
F309 A310 A311 L312 V316 M317 T318 D319 P320 Y321 V322 F328 R329 V330 G333 T334 M335 T336 S337 Y340 V341 K342 N343 K346 G347 K348 R349 E350 R351 V352 G353 R354 L355 R363 Q364 E365 I366 V369 Y370 S371 G372 D373 I374 D382 L389 G390 G391 E392 K393 N394 D395
I396 I397 L398 E399 S400 MET GLU PHE P404 E405 P406 L410 S411 V412 E413 P414 K415 D419 Q420 D421 K422 M423 K429 L430 Q431 E432 E433 D434 P435 H440 T441 D442 GLU GLU THR GLY Q447 V448 I449 I450 G451 G452 L456 H457 L458 D459 R464 M465 K466 K467 E468 F469 N470 V471
E472 C473 N474 V475 G476 A477 P478 Y482 R483 E484 K487 S488 F496 S497 ARG GLN SER GLY GLY ARG GLY Q505 H510 I511 E512 F513 T514 P515 N516 E517 T518 F522 E523 F524 E525 N526 V532 V533 P534 R535 E536 Y537 I538 P539 S540 L545 K546 D547 A548 M549 E550 V553
L554 A555 G556 Y557 D561 V562 K563 A564 K565 D568 G569 S570 Y571 H572 D573 V574 D575 M579 A580 F581 K582 K590 A593 C596 D597 P598 V599 I600 L601 M605 E610 M611 E614 Y615 M616 G617 D618 I619 M620 G621 D622 V623 T624 S625 R626 R627 G628 R629 V630 M633
E634 P635 R636 G637 Q640 V641 V646 P647 L648 S649 E650 M651 L658 R659 T662 Q663 T667 M670 Y671 Y675 A676 E677 V678 I682 A683 I686 I687 K688 K689 N690 K691 G692 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.20Å 125.52Å 106.90Å 90.00° 108.21° 90.00°	Depositor
Resolution (Å)	47.15 – 2.98 47.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.15-2.98) 93.3 (47.15-2.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.294 0.228 , 0.284	Depositor DCC
R_{free} test set	1478 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	94.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 73.7	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 31218 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10039	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	1/5103 (0.0%)	0.50	0/6901
1	B	0.27	1/5103 (0.0%)	0.49	0/6901
All	All	0.27	2/10206 (0.0%)	0.50	0/13802

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-5.26	1.23	1.33
1	B	691	LYS	C-N	-5.17	1.23	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5018	0	4936	310	0
1	B	5018	0	4936	311	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
All	All	10039	0	9872	620	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (620) 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:B:610:GLU:OE2	1:B:636:ARG:NH1	1.78	1.14
1:B:33:TYR:OH	1:B:264:ASN:ND2	1.81	1.12
1:B:178:LEU:C	1:B:211:ARG:HH12	1.60	1.03
1:A:30:ILE:O	1:A:34:THR:OG1	1.76	1.03
1:B:18:HIS:CD2	1:B:19:ILE:H	1.76	1.02
1:A:179:VAL:HG21	1:A:241:LYS:HD3	1.02	1.02
1:B:113:GLU:OE1	1:B:115:GLN:N	1.93	1.01
1:B:659:ARG:HH11	1:B:659:ARG:HG3	1.20	1.00
1:B:222:SER:HB3	1:B:225:LEU:HD21	1.42	1.00
1:A:216:GLU:O	1:A:219:ALA:N	1.94	0.99
1:A:300:ILE:HG12	1:A:302:LYS:HD2	1.41	0.99
1:A:534:PRO:HD3	1:A:571:TYR:CD2	1.98	0.98
1:A:199:ILE:HD12	1:A:199:ILE:H	1.27	0.95
1:A:304:ASP:OD1	1:A:307:ALA:N	2.00	0.94
1:A:179:VAL:CG2	1:A:241:LYS:HD3	1.97	0.92
1:B:178:LEU:O	1:B:211:ARG:NH1	2.03	0.90
1:B:109:GLN:HG3	1:B:110:SER:N	1.86	0.89
1:A:622:ASP:OD1	1:A:626:ARG:NH1	2.04	0.89
1:B:33:TYR:HH	1:B:264:ASN:ND2	1.69	0.89
1:A:417:LYS:NZ	1:A:421:ASP:OD1	2.05	0.89
1:B:230:LEU:H	1:B:230:LEU:HD23	1.38	0.89
1:A:534:PRO:HD3	1:A:571:TYR:HD2	1.32	0.88
1:A:572:HIS:HD2	1:A:573:ASP:H	1.21	0.87
1:A:117:GLU:OE2	1:A:154:ARG:NH2	2.07	0.87
1:A:241:LYS:NZ	1:A:277:TYR:OH	2.06	0.87
1:A:409:HIS:HD2	1:A:481:SER:HB3	1.38	0.87
1:B:611:MET:SD	1:B:619:ILE:HG13	2.16	0.86
1:B:659:ARG:O	1:B:663:GLN:N	2.09	0.85
1:A:394:ASN:OD1	1:A:395:ASP:N	2.11	0.84
1:B:658:LEU:O	1:B:662:THR:HG22	1.77	0.84
1:B:90:VAL:HG23	1:B:91:GLU:H	1.42	0.83
1:B:342:LYS:NZ	1:B:394:ASN:O	2.11	0.83
1:B:164:LEU:HB2	1:B:176:ILE:HD11	1.61	0.83
1:B:112:VAL:HG21	1:B:155:LEU:HD11	1.61	0.83
1:A:392:GLU:N	1:A:392:GLU:OE1	2.12	0.82
1:A:287:ILE:HD13	1:A:398:LEU:HD23	1.61	0.82
1:A:413:GLU:HB3	1:A:474:ASN:HB2	1.60	0.82
1:B:633:MET:HE3	1:B:640:GLN:HG2	1.59	0.81
1:A:300:ILE:CG1	1:A:302:LYS:HD2	2.10	0.81
1:A:179:VAL:HG21	1:A:241:LYS:CD	1.99	0.81
1:B:534:PRO:HG2	1:B:537:TYR:HD2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLN:O	1:B:118:THR:OG1	1.99	0.80
1:A:495:LYS:HD3	1:A:508:ASP:HB2	1.64	0.80
1:A:286:PRO:HB3	1:A:302:LYS:HG3	1.64	0.79
1:B:488:SER:HB2	1:B:596:CYS:HA	1.63	0.79
1:A:268:GLN:OE1	1:A:268:GLN:N	2.15	0.78
1:A:686:ILE:O	1:A:690:ASN:ND2	2.16	0.78
1:B:651:MET:HG2	1:B:670:MET:CE	2.13	0.78
1:B:180:GLU:HG2	1:B:182:LYS:HE3	1.66	0.78
1:B:659:ARG:NH1	1:B:659:ARG:HG3	1.88	0.78
1:B:191:GLY:HA3	1:B:264:ASN:HD22	1.47	0.77
1:A:683:ALA:HA	1:A:686:ILE:HD12	1.65	0.77
1:B:219:ALA:HA	1:B:225:LEU:HD12	1.66	0.77
1:A:508:ASP:OD2	1:A:570:SER:N	2.18	0.77
1:A:166:ILE:HD12	1:A:174:ALA:HB3	1.66	0.76
1:A:308:GLU:OE1	1:A:394:ASN:HB2	1.85	0.76
1:B:18:HIS:HD2	1:B:19:ILE:H	1.27	0.76
1:A:260:THR:HG22	1:A:263:LYS:H	1.50	0.76
1:B:688:LYS:O	1:B:691:LYS:HG2	1.84	0.76
1:B:178:LEU:C	1:B:211:ARG:NH1	2.38	0.76
1:B:83:PRO:HG2	1:B:92:VAL:HG23	1.67	0.76
1:A:493:GLN:OE1	1:A:510:HIS:NE2	2.19	0.75
1:A:547:ASP:O	1:A:551:ASN:ND2	2.19	0.75
1:B:154:ARG:HD3	1:B:636:ARG:NH2	2.02	0.74
1:B:464:ARG:O	1:B:468:GLU:HB3	1.87	0.74
1:B:626:ARG:NH1	1:B:650:GLU:O	2.20	0.74
1:B:510:HIS:HB2	1:B:568:ASP:HB3	1.69	0.74
1:B:164:LEU:H	1:B:176:ILE:CD1	1.99	0.74
1:B:523:GLU:HB2	1:B:563:LYS:HE2	1.69	0.74
1:A:241:LYS:O	1:A:244:ILE:HG13	1.86	0.74
1:A:619:ILE:O	1:A:622:ASP:HB3	1.86	0.74
1:A:209:GLU:O	1:A:213:SER:OG	2.06	0.73
1:B:224:GLU:HG3	1:B:225:LEU:H	1.54	0.73
1:B:109:GLN:HG3	1:B:110:SER:H	1.52	0.72
1:B:124:THR:HG23	1:B:130:ARG:HH12	1.53	0.72
1:A:612:PRO:HG2	1:A:615:TYR:CD2	2.24	0.72
1:B:180:GLU:CG	1:B:182:LYS:HE3	2.20	0.72
1:A:538:ILE:CG2	1:A:539:PRO:HD3	2.20	0.71
1:A:335:MET:HE2	1:A:352:VAL:HG21	1.70	0.71
1:B:17:ALA:HB3	1:B:23:LYS:HD2	1.72	0.71
1:B:18:HIS:CD2	1:B:19:ILE:N	2.55	0.71
1:B:144:PHE:CD2	1:B:165:PRO:HD3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:MET:O	1:B:230:LEU:HD21	1.91	0.71
1:A:572:HIS:CD2	1:A:573:ASP:H	2.06	0.71
1:A:505:GLN:O	1:A:505:GLN:HG2	1.91	0.71
1:A:239:GLU:HA	1:A:242:GLU:OE1	1.90	0.71
1:A:612:PRO:HG2	1:A:615:TYR:HD2	1.56	0.71
1:A:572:HIS:NE2	1:A:574:VAL:HG12	2.06	0.70
1:A:274:VAL:HG13	1:A:278:LEU:HD12	1.72	0.70
1:B:163:GLN:CD	1:B:175:ILE:HD11	2.11	0.70
1:A:361:ASN:O	1:A:362:SER:HB3	1.91	0.70
1:B:419:ASP:HA	1:B:422:LYS:HE2	1.73	0.70
1:A:535:ARG:O	1:A:538:ILE:HG22	1.92	0.70
1:A:529:VAL:HG13	1:A:530:GLY:H	1.56	0.70
1:B:278:LEU:HB3	1:B:279:PRO:HD2	1.73	0.69
1:A:411:SER:HA	1:A:449:ILE:HD13	1.75	0.69
1:B:224:GLU:HG3	1:B:225:LEU:HD23	1.73	0.69
1:B:373:ASP:OD1	1:B:374:ILE:N	2.25	0.69
1:B:414:PRO:HG3	1:B:420:GLN:HG3	1.74	0.69
1:B:302:LYS:HE3	1:B:304:ASP:HB2	1.75	0.69
1:A:311:ALA:HB2	1:A:330:VAL:HG12	1.74	0.69
1:A:409:HIS:CD2	1:A:481:SER:HB3	2.26	0.69
1:A:276:ASP:HB3	1:A:277:TYR:CE1	2.29	0.68
1:A:304:ASP:OD1	1:A:306:SER:N	2.26	0.68
1:A:350:GLU:HG2	1:A:380:LEU:HG	1.74	0.68
1:B:8:GLU:OE1	1:B:8:GLU:N	2.21	0.68
1:B:223:ASP:O	1:B:226:MET:HG2	1.94	0.67
1:A:633:MET:SD	1:A:640:GLN:HG2	2.34	0.67
1:A:578:GLU:OE2	1:A:579:MET:HG2	1.94	0.67
1:A:3:ARG:HB3	1:A:370:TYR:CD2	2.29	0.67
1:B:260:THR:CG2	1:B:263:LYS:HB2	2.25	0.67
1:B:227:GLU:O	1:B:230:LEU:HG	1.93	0.67
1:B:433:GLU:OE1	1:B:464:ARG:NH2	2.25	0.67
1:A:354:ARG:HD2	1:A:365:GLU:OE1	1.93	0.67
1:B:176:ILE:HD12	1:B:176:ILE:H	1.59	0.67
1:A:218:VAL:O	1:A:221:THR:OG1	2.11	0.67
1:B:688:LYS:HA	1:B:691:LYS:HG2	1.77	0.67
1:B:319:ASP:OD1	1:B:320:PRO:HD2	1.95	0.66
1:B:162:ILE:HG13	1:B:163:GLN:HG3	1.77	0.66
1:A:201:GLU:H	1:A:201:GLU:CD	1.96	0.66
1:A:505:GLN:N	1:A:575:ASP:HB3	2.12	0.65
1:B:133:PHE:HD2	1:B:270:MET:HG3	1.61	0.65
1:A:181:MET:HG2	1:A:211:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH2	1:A:287:ILE:HD11	2.12	0.65
1:B:535:ARG:HG2	1:B:535:ARG:HH11	1.61	0.65
1:B:441:THR:O	1:B:442:ASP:HB3	1.95	0.65
1:A:516:ASN:OD1	1:A:517:GLU:N	2.27	0.65
1:A:414:PRO:HG3	1:A:423:MET:CE	2.27	0.65
1:A:117:GLU:HB3	1:A:155:LEU:HD11	1.79	0.65
1:B:651:MET:HG2	1:B:670:MET:HE1	1.77	0.65
1:A:309:PHE:HA	1:A:333:GLY:HA3	1.78	0.65
1:A:505:GLN:HE21	1:A:505:GLN:N	1.95	0.64
1:B:346:LYS:HG3	1:B:348:LYS:NZ	2.12	0.64
1:B:447:GLN:OE1	1:B:447:GLN:N	2.30	0.64
1:B:228:LYS:HE2	1:B:233:GLU:O	1.97	0.64
1:B:553:VAL:HG23	1:B:554:LEU:H	1.63	0.64
1:B:234:GLU:OE1	1:B:234:GLU:HA	1.98	0.64
1:B:316:VAL:HG23	1:B:433:GLU:HG2	1.79	0.64
1:B:257:LEU:HD22	1:B:270:MET:HA	1.80	0.64
1:A:188:ASN:ND2	1:A:192:THR:O	2.30	0.64
1:A:15:ILE:HD11	1:A:30:ILE:HD12	1.79	0.64
1:B:211:ARG:O	1:B:214:LEU:HB3	1.98	0.64
1:A:156:GLN:NE2	1:A:637:GLY:HA3	2.12	0.64
1:B:341:VAL:HG12	1:B:342:LYS:N	2.13	0.63
1:B:151:LEU:HA	1:B:155:LEU:HD13	1.80	0.63
1:B:83:PRO:HG3	1:B:91:GLU:HB3	1.79	0.63
1:B:346:LYS:HE2	1:B:348:LYS:HZ1	1.62	0.63
1:B:659:ARG:CG	1:B:659:ARG:HH11	2.01	0.63
1:A:622:ASP:O	1:A:625:SER:OG	2.09	0.63
1:A:572:HIS:CD2	1:A:573:ASP:N	2.66	0.63
1:A:284:VAL:HG22	1:A:285:LYS:N	2.14	0.63
1:A:234:GLU:OE1	1:A:234:GLU:HA	1.98	0.63
1:A:572:HIS:HD2	1:A:573:ASP:N	1.92	0.62
1:B:346:LYS:HG3	1:B:348:LYS:HZ3	1.63	0.62
1:B:90:VAL:HG23	1:B:91:GLU:N	2.13	0.62
1:A:434:ASP:OD1	1:A:436:THR:OG1	2.16	0.62
1:B:237:VAL:O	1:B:240:LEU:N	2.31	0.62
1:A:244:ILE:CD1	1:A:277:TYR:CE1	2.83	0.62
1:A:228:LYS:HA	1:A:233:GLU:HG3	1.82	0.62
1:B:179:VAL:HA	1:B:211:ARG:HH22	1.64	0.62
1:A:361:ASN:OD1	1:A:361:ASN:N	2.30	0.61
1:A:73:GLU:O	1:A:75:HIS:ND1	2.29	0.61
1:A:612:PRO:HB2	1:A:614:GLU:CD	2.20	0.61
1:A:291:ARG:HG3	1:A:297:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:OE1	1:A:297:GLU:N	2.19	0.61
1:A:414:PRO:HG3	1:A:423:MET:HE1	1.82	0.61
1:A:164:LEU:HD11	1:A:178:LEU:HD11	1.82	0.61
1:B:88:LEU:HD13	1:B:91:GLU:OE1	2.01	0.61
1:A:622:ASP:CG	1:A:626:ARG:HH12	2.04	0.61
1:A:318:THR:OG1	1:A:429:LYS:NZ	2.30	0.60
1:B:341:VAL:HG12	1:B:342:LYS:H	1.66	0.60
1:A:297:GLU:CD	1:A:297:GLU:H	2.03	0.60
1:B:335:MET:HG2	1:B:336:THR:N	2.15	0.60
1:B:620:MET:CE	1:B:630:VAL:HG21	2.32	0.60
1:B:276:ASP:HB3	1:B:277:TYR:CD1	2.37	0.60
1:B:201:GLU:HG2	1:B:202:ASP:N	2.15	0.60
1:A:26:THR:O	1:A:30:ILE:HG13	2.01	0.60
1:A:216:GLU:HA	1:A:219:ALA:HB3	1.83	0.60
1:B:291:ARG:HB3	1:B:395:ASP:OD2	2.02	0.60
1:B:276:ASP:HB3	1:B:277:TYR:CE1	2.36	0.60
1:B:614:GLU:HG2	1:B:615:TYR:CD1	2.36	0.60
1:A:201:GLU:N	1:A:201:GLU:OE1	2.35	0.60
1:B:144:PHE:HD2	1:B:165:PRO:CD	2.15	0.60
1:A:487:LYS:HD2	1:A:599:VAL:HG11	1.83	0.60
1:A:538:ILE:HG23	1:A:539:PRO:HD3	1.84	0.59
1:A:284:VAL:HG22	1:A:285:LYS:H	1.67	0.59
1:B:211:ARG:O	1:B:215:ILE:HG13	2.02	0.59
1:A:201:GLU:N	1:A:201:GLU:CD	2.55	0.59
1:A:491:GLN:HG2	1:A:512:GLU:HG3	1.85	0.59
1:B:85:HIS:O	1:B:88:LEU:HD12	2.02	0.59
1:B:171:GLU:O	1:B:173:GLU:HG3	2.02	0.59
1:B:224:GLU:HG3	1:B:225:LEU:N	2.18	0.59
1:B:633:MET:CE	1:B:640:GLN:HG2	2.32	0.59
1:A:3:ARG:HB3	1:A:370:TYR:CE2	2.37	0.59
1:B:237:VAL:HG23	1:B:238:SER:H	1.67	0.59
1:A:574:VAL:HG13	1:A:575:ASP:N	2.16	0.59
1:A:28:GLU:HG3	1:A:29:ARG:N	2.17	0.59
1:A:508:ASP:OD1	1:A:509:VAL:N	2.36	0.58
1:B:553:VAL:HG23	1:B:554:LEU:N	2.18	0.58
1:A:179:VAL:HG11	1:A:241:LYS:HZ3	1.67	0.58
1:B:164:LEU:H	1:B:176:ILE:HD12	1.68	0.58
1:B:222:SER:HB3	1:B:225:LEU:CD2	2.24	0.58
1:A:106:LEU:HD11	1:A:151:LEU:HD11	1.84	0.58
1:B:7:LEU:HD22	1:B:281:PRO:HG2	1.86	0.58
1:B:534:PRO:HG2	1:B:537:TYR:CD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:O	1:A:150:THR:OG1	2.22	0.57
1:A:244:ILE:O	1:A:247:ALA:N	2.38	0.57
1:A:107:ASP:OD2	1:A:139:LYS:NZ	2.38	0.57
1:A:88:LEU:O	1:A:92:VAL:HG23	2.05	0.57
1:A:631:ASP:HA	1:B:635:PRO:HD3	1.87	0.57
1:A:17:ALA:HB2	1:A:105:VAL:HB	1.87	0.57
1:A:251:VAL:HG22	1:A:251:VAL:O	2.04	0.57
1:A:144:PHE:O	1:A:148:VAL:HG23	2.05	0.57
1:B:574:VAL:HG22	1:B:575:ASP:N	2.20	0.57
1:B:120:TRP:CG	1:B:155:LEU:HD23	2.39	0.57
1:B:419:ASP:OD1	1:B:472:GLU:OE1	2.21	0.57
1:A:622:ASP:CG	1:A:626:ARG:NH1	2.57	0.56
1:B:164:LEU:CB	1:B:176:ILE:HD11	2.33	0.56
1:A:300:ILE:HG12	1:A:302:LYS:CD	2.28	0.56
1:B:343:ASN:N	1:B:348:LYS:O	2.34	0.56
1:B:447:GLN:HG2	1:B:447:GLN:O	2.05	0.56
1:B:94:ARG:HG3	1:B:399:GLU:OE2	2.05	0.56
1:A:146:TYR:CD1	1:A:146:TYR:C	2.76	0.56
1:B:132:VAL:HB	1:B:256:VAL:HG22	1.86	0.56
1:A:682:ILE:HG22	1:A:686:ILE:HD11	1.88	0.56
1:A:538:ILE:HG22	1:A:539:PRO:HD3	1.87	0.56
1:B:176:ILE:HG22	1:B:182:LYS:O	2.05	0.56
1:A:266:GLY:H	1:A:268:GLN:HE22	1.53	0.56
1:B:337:SER:HA	1:B:352:VAL:HG12	1.88	0.56
1:B:487:LYS:HE2	1:B:599:VAL:CG1	2.35	0.56
1:B:555:ALA:CB	1:B:557:TYR:HD2	2.19	0.56
1:A:686:ILE:HG22	1:A:690:ASN:HD21	1.71	0.56
1:A:199:ILE:H	1:A:199:ILE:CD1	2.03	0.56
1:B:342:LYS:HD3	1:B:392:GLU:HA	1.88	0.56
1:A:115:GLN:CD	1:A:115:GLN:H	2.08	0.56
1:B:646:VAL:HG11	1:B:651:MET:HE1	1.88	0.56
1:A:204:LEU:O	1:A:208:GLU:HG2	2.06	0.56
1:B:222:SER:CB	1:B:225:LEU:HD21	2.25	0.55
1:A:408:ILE:HD11	1:A:478:PRO:HB3	1.87	0.55
1:B:319:ASP:HB3	1:B:322:VAL:HG22	1.88	0.55
1:B:441:THR:HG23	1:B:442:ASP:N	2.21	0.55
1:A:11:ARG:NH2	1:A:275:ILE:O	2.28	0.55
1:B:143:ASN:ND2	1:B:146:TYR:HB2	2.21	0.55
1:B:177:ASP:O	1:B:181:MET:N	2.40	0.55
1:B:342:LYS:HA	1:B:349:ARG:HA	1.87	0.55
1:B:512:GLU:OE2	1:B:565:LYS:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:HG21	1:A:263:LYS:HG2	1.88	0.55
1:B:144:PHE:CD2	1:B:165:PRO:CD	2.88	0.55
1:B:431:GLN:NE2	1:B:435:PRO:HA	2.22	0.55
1:B:250:ASN:HB2	1:B:252:GLU:HG2	1.89	0.55
1:B:538:ILE:N	1:B:539:PRO:HD2	2.22	0.55
1:B:178:LEU:O	1:B:181:MET:N	2.40	0.54
1:A:620:MET:O	1:A:623:VAL:N	2.40	0.54
1:A:188:ASN:HD21	1:A:192:THR:C	2.08	0.54
1:A:143:ASN:HB3	1:A:146:TYR:HB3	1.88	0.54
1:A:117:GLU:O	1:A:121:ARG:HG3	2.08	0.54
1:B:688:LYS:CG	1:B:689:LYS:N	2.71	0.54
1:B:260:THR:HG23	1:B:263:LYS:HB2	1.89	0.54
1:B:164:LEU:N	1:B:176:ILE:CD1	2.70	0.54
1:A:529:VAL:HG13	1:A:530:GLY:N	2.20	0.54
1:A:164:LEU:CD1	1:A:178:LEU:HD21	2.37	0.54
1:B:237:VAL:O	1:B:240:LEU:HB3	2.08	0.54
1:A:227:GLU:HA	1:A:230:LEU:HD11	1.89	0.54
1:A:120:TRP:CD2	1:A:155:LEU:HD23	2.43	0.54
1:B:89:THR:O	1:B:93:GLU:HB2	2.07	0.54
1:A:276:ASP:CB	1:A:277:TYR:CE1	2.90	0.54
1:B:349:ARG:NH1	1:B:392:GLU:OE1	2.41	0.54
1:B:535:ARG:CG	1:B:535:ARG:HH11	2.21	0.54
1:B:247:ALA:HA	1:B:252:GLU:HG3	1.90	0.53
1:A:289:GLY:O	1:A:299:VAL:N	2.28	0.53
1:B:3:ARG:HD2	1:B:370:TYR:CD2	2.43	0.53
1:B:547:ASP:O	1:B:550:GLU:N	2.41	0.53
1:A:636:ARG:O	1:A:636:ARG:HG2	2.08	0.53
1:A:186:TYR:CE2	1:A:265:LYS:HA	2.43	0.53
1:A:346:LYS:NZ	1:A:387:ASP:OD2	2.34	0.53
1:B:615:TYR:CD2	1:B:662:THR:HA	2.44	0.53
1:A:335:MET:HE3	1:A:336:THR:O	2.09	0.53
1:A:362:SER:O	1:A:363:ARG:HG3	2.09	0.53
1:A:635:PRO:HB3	1:A:640:GLN:NE2	2.24	0.53
1:B:138:ASP:HA	1:B:169:GLU:O	2.08	0.53
1:B:31:LEU:HD23	1:B:79:ILE:HD12	1.91	0.53
1:A:212:ALA:O	1:A:215:ILE:HG12	2.09	0.53
1:B:120:TRP:CD1	1:B:155:LEU:HD23	2.43	0.53
1:A:537:TYR:OH	1:A:577:SER:HA	2.09	0.53
1:B:629:ARG:HG3	1:B:630:VAL:N	2.24	0.52
1:A:330:VAL:HG21	1:A:370:TYR:O	2.08	0.52
1:A:322:VAL:HG13	1:A:354:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LEU:O	1:B:549:MET:HG3	2.10	0.52
1:B:516:ASN:OD1	1:B:517:GLU:N	2.42	0.52
1:A:419:ASP:HB3	1:A:471:VAL:HG13	1.91	0.52
1:B:222:SER:HB3	1:B:225:LEU:HD11	1.91	0.52
1:A:505:GLN:NE2	1:A:505:GLN:N	2.57	0.52
1:B:101:GLY:HA2	1:B:128:VAL:HG13	1.91	0.52
1:A:290:HIS:HA	1:A:297:GLU:O	2.09	0.52
1:A:216:GLU:OE1	1:A:216:GLU:N	2.33	0.52
1:A:505:GLN:CG	1:A:505:GLN:O	2.57	0.52
1:B:687:ILE:C	1:B:691:LYS:HZ2	2.14	0.52
1:B:535:ARG:HB2	1:B:535:ARG:CZ	2.39	0.52
1:B:525:GLU:CD	1:B:565:LYS:HE2	2.31	0.52
1:B:103:VAL:HG22	1:B:131:ILE:HG12	1.92	0.52
1:A:620:MET:C	1:A:622:ASP:N	2.63	0.52
1:A:231:GLY:O	1:A:232:ASP:HB3	2.10	0.52
1:B:225:LEU:O	1:B:228:LYS:N	2.43	0.51
1:A:325:LEU:HD22	1:A:376:ALA:HB1	1.91	0.51
1:B:488:SER:HB2	1:B:596:CYS:CA	2.38	0.51
1:A:622:ASP:OD2	1:A:654:TYR:HE1	1.92	0.51
1:B:31:LEU:HD22	1:B:68:THR:HG21	1.92	0.51
1:B:618:ASP:OD1	1:B:618:ASP:N	2.38	0.51
1:A:284:VAL:CG2	1:A:285:LYS:H	2.23	0.51
1:B:572:HIS:CE1	1:B:574:VAL:HG13	2.45	0.51
1:A:404:PRO:O	1:A:405:GLU:HB2	2.10	0.51
1:A:236:SER:HB3	1:A:239:GLU:HG2	1.91	0.51
1:B:620:MET:HE3	1:B:630:VAL:HG21	1.92	0.51
1:A:106:LEU:HD22	1:A:112:VAL:HA	1.93	0.51
1:B:440:HIS:O	1:B:448:VAL:HG23	2.10	0.51
1:A:609:ILE:HG22	1:A:610:GLU:N	2.26	0.51
1:B:163:GLN:O	1:B:164:LEU:HD12	2.10	0.51
1:A:352:VAL:CG1	1:A:355:LEU:HD21	2.41	0.51
1:A:18:HIS:CG	1:A:19:ILE:H	2.28	0.51
1:A:304:ASP:C	1:A:304:ASP:OD1	2.48	0.51
1:A:117:GLU:OE2	1:A:154:ARG:CZ	2.58	0.51
1:B:86:VAL:O	1:B:86:VAL:HG12	2.11	0.51
1:A:294:ASN:O	1:A:297:GLU:OE1	2.29	0.51
1:A:496:PHE:O	1:A:506:TYR:HA	2.11	0.51
1:A:294:ASN:O	1:A:297:GLU:CD	2.50	0.51
1:A:463:ASP:O	1:A:467:LYS:HD2	2.11	0.50
1:A:244:ILE:HD13	1:A:277:TYR:CE1	2.45	0.50
1:B:688:LYS:HA	1:B:691:LYS:CG	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:HA2	1:B:128:VAL:CG1	2.42	0.50
1:A:31:LEU:HD23	1:A:79:ILE:HD12	1.92	0.50
1:A:246:GLN:HA	1:A:246:GLN:NE2	2.26	0.50
1:A:626:ARG:HH11	1:A:626:ARG:HG3	1.76	0.50
1:A:181:MET:HG2	1:A:211:ARG:NH1	2.24	0.50
1:B:555:ALA:HB3	1:B:557:TYR:HD2	1.76	0.50
1:A:18:HIS:O	1:A:23:LYS:HB2	2.12	0.50
1:A:605:MET:HB3	1:A:670:MET:HG3	1.93	0.50
1:B:308:GLU:OE2	1:B:394:ASN:ND2	2.45	0.50
1:A:352:VAL:HG12	1:A:353:GLY:O	2.12	0.50
1:B:554:LEU:HD23	1:B:600:ILE:HG13	1.92	0.50
1:A:270:MET:O	1:A:273:ALA:HB3	2.12	0.50
1:A:120:TRP:CG	1:A:155:LEU:HD23	2.47	0.50
1:B:112:VAL:HG11	1:B:155:LEU:CD1	2.42	0.49
1:B:138:ASP:O	1:B:139:LYS:HB2	2.12	0.49
1:A:18:HIS:CG	1:A:19:ILE:N	2.80	0.49
1:A:460:ILE:HA	1:A:463:ASP:HB3	1.95	0.49
1:A:224:GLU:O	1:A:228:LYS:HG3	2.13	0.49
1:B:343:ASN:HA	1:B:389:LEU:HD23	1.95	0.49
1:B:550:GLU:OE1	1:B:550:GLU:N	2.46	0.49
1:A:114:PRO:O	1:A:118:THR:HG23	2.13	0.49
1:B:662:THR:O	1:B:663:GLN:HB2	2.12	0.49
1:A:227:GLU:C	1:A:227:GLU:OE1	2.51	0.49
1:A:671:TYR:N	1:A:671:TYR:CD1	2.81	0.49
1:B:191:GLY:CA	1:B:264:ASN:HD22	2.23	0.49
1:B:523:GLU:CB	1:B:563:LYS:HE2	2.42	0.48
1:A:284:VAL:CG2	1:A:285:LYS:N	2.76	0.48
1:A:294:ASN:O	1:A:297:GLU:OE2	2.31	0.48
1:A:226:MET:O	1:A:230:LEU:HG	2.12	0.48
1:A:463:ASP:OD2	1:A:467:LYS:NZ	2.32	0.48
1:A:426:ALA:HB2	1:A:469:PHE:CD2	2.47	0.48
1:A:574:VAL:CG1	1:A:575:ASP:N	2.76	0.48
1:A:532:VAL:HG12	1:A:570:SER:HA	1.96	0.48
1:A:268:GLN:H	1:A:268:GLN:CD	2.10	0.48
1:B:441:THR:HG23	1:B:442:ASP:H	1.78	0.48
1:B:677:GLU:HG2	1:B:678:VAL:H	1.79	0.48
1:B:413:GLU:HB3	1:B:474:ASN:OD1	2.13	0.48
1:A:532:VAL:HG11	1:A:569:GLY:O	2.13	0.48
1:A:286:PRO:CG	1:A:300:ILE:HD11	2.44	0.48
1:B:164:LEU:HD11	1:B:210:ALA:HB1	1.94	0.48
1:B:633:MET:HE3	1:B:640:GLN:CG	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:MET:HG2	1:B:670:MET:HE3	1.93	0.48
1:B:621:GLY:O	1:B:625:SER:OG	2.31	0.48
1:B:683:ALA:O	1:B:687:ILE:HG13	2.14	0.48
1:B:119:VAL:O	1:B:123:ALA:N	2.44	0.48
1:B:688:LYS:CA	1:B:691:LYS:HG2	2.43	0.48
1:B:505:GLN:HG2	1:B:505:GLN:O	2.13	0.48
1:A:407:VAL:HG11	1:A:672:PHE:CD1	2.49	0.48
1:A:532:VAL:CG1	1:A:569:GLY:O	2.62	0.48
1:B:452:GLY:HA3	1:B:458:LEU:HD21	1.96	0.48
1:B:174:ALA:HB1	1:B:184:PHE:O	2.14	0.48
1:A:457:HIS:O	1:A:460:ILE:HG13	2.13	0.47
1:B:413:GLU:O	1:B:474:ASN:OD1	2.32	0.47
1:A:194:ILE:HG13	1:A:194:ILE:O	2.14	0.47
1:A:205:ASP:O	1:A:209:GLU:OE1	2.32	0.47
1:A:618:ASP:OD1	1:A:618:ASP:N	2.47	0.47
1:B:168:ALA:O	1:B:171:GLU:N	2.46	0.47
1:B:337:SER:HA	1:B:352:VAL:CG1	2.44	0.47
1:B:186:TYR:CD2	1:B:265:LYS:HG2	2.49	0.47
1:A:433:GLU:OE1	1:A:464:ARG:NH1	2.46	0.47
1:B:146:TYR:O	1:B:150:THR:HG23	2.14	0.47
1:B:214:LEU:O	1:B:218:VAL:HG23	2.15	0.47
1:A:572:HIS:CE1	1:A:574:VAL:HG12	2.49	0.47
1:B:121:ARG:HA	1:B:124:THR:OG1	2.14	0.47
1:A:3:ARG:HH22	1:A:7:LEU:HD23	1.79	0.47
1:A:613:GLU:HB2	1:A:616:MET:HE2	1.96	0.47
1:A:509:VAL:HG22	1:A:584:ALA:HB1	1.96	0.47
1:A:324:LYS:CE	1:A:380:LEU:O	2.61	0.47
1:B:7:LEU:HD22	1:B:281:PRO:CG	2.44	0.47
1:A:468:GLU:CD	1:A:469:PHE:HE1	2.18	0.47
1:A:146:TYR:O	1:A:149:SER:N	2.45	0.47
1:A:101:GLY:HA2	1:A:128:VAL:HG13	1.96	0.47
1:B:240:LEU:O	1:B:244:ILE:HG13	2.15	0.47
1:B:241:LYS:HA	1:B:244:ILE:HD12	1.97	0.47
1:A:251:VAL:HG23	1:A:254:TYR:CE1	2.50	0.47
1:A:163:GLN:HA	1:A:176:ILE:O	2.15	0.47
1:A:34:THR:HG22	1:A:71:ALA:O	2.15	0.47
1:B:83:PRO:HG3	1:B:91:GLU:CB	2.44	0.47
1:A:549:MET:HB3	1:A:559:LEU:HB3	1.96	0.47
1:B:309:PHE:O	1:B:390:CYS:HA	2.14	0.47
1:B:450:ILE:HG13	1:B:450:ILE:O	2.14	0.47
1:A:85:HIS:HE1	1:A:87:ASP:CG	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HG23	1:B:238:SER:N	2.30	0.46
1:A:538:ILE:HG23	1:A:539:PRO:CD	2.45	0.46
1:B:484:GLU:OE2	1:B:555:ALA:HB3	2.15	0.46
1:A:426:ALA:HB2	1:A:469:PHE:HD2	1.80	0.46
1:B:677:GLU:HG2	1:B:678:VAL:N	2.30	0.46
1:A:25:THR:O	1:A:29:ARG:HG2	2.14	0.46
1:B:287:ILE:HG22	1:B:301:ALA:HB3	1.98	0.46
1:A:554:LEU:HD22	1:A:598:PRO:HB2	1.98	0.46
1:A:146:TYR:O	1:A:149:SER:OG	2.26	0.46
1:B:405:GLU:HG3	1:B:406:PRO:HD2	1.96	0.46
1:B:112:VAL:HG11	1:B:155:LEU:HD11	1.97	0.46
1:A:487:LYS:CD	1:A:599:VAL:HG11	2.46	0.46
1:B:34:THR:HB	1:B:70:ALA:HB1	1.98	0.46
1:A:216:GLU:O	1:A:217:ALA:C	2.54	0.46
1:A:201:GLU:O	1:A:204:LEU:HB2	2.16	0.46
1:B:202:ASP:OD1	1:B:202:ASP:N	2.41	0.46
1:A:149:SER:O	1:A:152:HIS:HB2	2.15	0.46
1:B:154:ARG:HB3	1:B:155:LEU:HD12	1.96	0.46
1:A:330:VAL:HG21	1:A:369:VAL:CG1	2.46	0.46
1:B:397:ILE:HG22	1:B:398:LEU:N	2.31	0.46
1:A:396:ILE:HG12	1:A:397:ILE:N	2.31	0.46
1:B:688:LYS:C	1:B:690:ASN:N	2.70	0.46
1:B:626:ARG:O	1:B:627:ARG:HB2	2.15	0.46
1:B:278:LEU:HB3	1:B:279:PRO:CD	2.42	0.46
1:A:113:GLU:HB3	1:A:114:PRO:HD2	1.98	0.46
1:A:423:MET:SD	1:A:465:MET:HE1	2.55	0.45
1:B:477:ALA:HA	1:B:478:PRO:HD3	1.75	0.45
1:A:205:ASP:O	1:A:208:GLU:N	2.49	0.45
1:A:85:HIS:CE1	1:A:87:ASP:CG	2.89	0.45
1:B:540:SER:O	1:B:582:LYS:HG3	2.15	0.45
1:B:179:VAL:CA	1:B:211:ARG:HH22	2.28	0.45
1:B:343:ASN:HA	1:B:389:LEU:CD2	2.46	0.45
1:A:291:ARG:HG2	1:A:299:VAL:HG21	1.97	0.45
1:A:230:LEU:H	1:A:230:LEU:HG	1.52	0.45
1:B:154:ARG:HD3	1:B:636:ARG:CZ	2.46	0.45
1:A:517:GLU:HB3	1:A:520:ALA:HB2	1.99	0.45
1:B:3:ARG:HH12	1:B:7:LEU:N	2.15	0.45
1:B:230:LEU:H	1:B:230:LEU:CD2	2.08	0.45
1:B:633:MET:O	1:B:634:GLU:HB3	2.15	0.45
1:B:235:ILE:HD13	1:B:235:ILE:N	2.31	0.45
1:B:496:PHE:CD1	1:B:497:SER:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:CD1	1:A:30:ILE:HD12	2.46	0.45
1:B:651:MET:HE2	1:B:651:MET:HA	1.98	0.45
1:B:18:HIS:CD2	1:B:19:ILE:HG22	2.52	0.45
1:B:225:LEU:O	1:B:226:MET:C	2.53	0.45
1:B:17:ALA:HB1	1:B:23:LYS:HB2	1.99	0.45
1:B:318:THR:O	1:B:318:THR:HG22	2.17	0.45
1:B:112:VAL:HG12	1:B:150:THR:OG1	2.17	0.45
1:A:296:GLU:N	1:A:297:GLU:OE1	2.49	0.45
1:A:244:ILE:HG13	1:A:245:ARG:H	1.80	0.45
1:B:175:ILE:HG12	1:B:176:ILE:N	2.32	0.45
1:A:201:GLU:HA	1:A:204:LEU:HD12	1.99	0.45
1:A:201:GLU:HA	1:A:204:LEU:HG	1.98	0.45
1:B:187:THR:HG23	1:B:193:GLU:O	2.16	0.45
1:B:308:GLU:O	1:B:333:GLY:HA3	2.17	0.44
1:A:335:MET:CE	1:A:352:VAL:HG21	2.43	0.44
1:A:238:SER:OG	1:A:239:GLU:N	2.50	0.44
1:B:593:ALA:O	1:B:598:PRO:HD3	2.17	0.44
1:A:277:TYR:N	1:A:277:TYR:CD1	2.82	0.44
1:A:93:GLU:O	1:A:97:ARG:HG3	2.17	0.44
1:A:230:LEU:C	1:A:232:ASP:N	2.70	0.44
1:A:506:TYR:HD1	1:A:576:SER:OG	1.99	0.44
1:B:682:ILE:O	1:B:686:ILE:HG13	2.16	0.44
1:B:182:LYS:HD3	1:B:196:GLU:OE2	2.17	0.44
1:A:146:TYR:HD1	1:A:146:TYR:C	2.19	0.44
1:A:160:ALA:N	1:A:253:PHE:HE1	2.16	0.44
1:A:34:THR:HB	1:A:70:ALA:HB1	2.00	0.44
1:B:659:ARG:O	1:B:662:THR:N	2.44	0.44
1:A:417:LYS:HA	1:A:417:LYS:HD2	1.77	0.44
1:A:388:THR:CG2	1:A:398:LEU:HD13	2.46	0.44
1:A:508:ASP:O	1:A:509:VAL:HG13	2.18	0.44
1:B:526:ASN:OD1	1:B:538:ILE:HD13	2.18	0.44
1:B:410:LEU:HD12	1:B:410:LEU:O	2.18	0.44
1:B:396:ILE:C	1:B:397:ILE:HG12	2.37	0.44
1:A:179:VAL:HG11	1:A:241:LYS:NZ	2.32	0.44
1:B:662:THR:C	1:B:663:GLN:OE1	2.56	0.44
1:A:201:GLU:OE1	1:A:202:ASP:OD1	2.36	0.44
1:A:118:THR:O	1:A:122:GLN:HG3	2.16	0.44
1:A:276:ASP:CB	1:A:277:TYR:CD1	3.01	0.44
1:A:276:ASP:C	1:A:277:TYR:CD1	2.90	0.44
1:A:359:HIS:HB2	1:A:362:SER:OG	2.16	0.44
1:A:469:PHE:CD1	1:A:469:PHE:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASP:HA	1:B:226:MET:CE	2.48	0.44
1:B:175:ILE:HD13	1:B:269:LEU:HD12	1.99	0.44
1:A:324:LYS:NZ	1:A:380:LEU:O	2.50	0.44
1:A:572:HIS:CD2	1:A:574:VAL:H	2.35	0.44
1:B:17:ALA:HB3	1:B:23:LYS:CD	2.43	0.44
1:B:93:GLU:HG2	1:B:126:TYR:OH	2.18	0.44
1:B:178:LEU:O	1:B:179:VAL:C	2.56	0.44
1:A:549:MET:CE	1:A:559:LEU:HD23	2.48	0.44
1:B:456:LEU:O	1:B:459:ASP:N	2.51	0.44
1:A:236:SER:CB	1:A:239:GLU:HG2	2.48	0.43
1:B:341:VAL:CG1	1:B:342:LYS:N	2.80	0.43
1:A:72:TRP:O	1:A:75:HIS:HB2	2.18	0.43
1:B:341:VAL:CG1	1:B:342:LYS:H	2.31	0.43
1:B:533:VAL:HA	1:B:534:PRO:HD2	1.88	0.43
1:B:410:LEU:HG	1:B:458:LEU:HD13	2.00	0.43
1:B:5:PHE:CD2	1:B:76:ARG:HB2	2.53	0.43
1:B:333:GLY:N	1:B:371:SER:OG	2.51	0.43
1:B:260:THR:HG21	1:B:263:LYS:HB2	1.96	0.43
1:A:309:PHE:CD1	1:A:309:PHE:C	2.91	0.43
1:B:251:VAL:O	1:B:251:VAL:HG12	2.17	0.43
1:A:571:TYR:C	1:A:571:TYR:CD1	2.92	0.43
1:A:308:GLU:CD	1:A:394:ASN:HB2	2.39	0.43
1:B:555:ALA:CB	1:B:557:TYR:CD2	2.99	0.43
1:B:135:ASN:OD1	1:B:136:LYS:N	2.49	0.43
1:B:370:TYR:N	1:B:370:TYR:CD1	2.86	0.43
1:A:267:VAL:O	1:A:270:MET:HG3	2.18	0.43
1:A:113:GLU:HB3	1:A:114:PRO:CD	2.48	0.43
1:A:202:ASP:OD1	1:A:202:ASP:N	2.51	0.43
1:B:244:ILE:HG13	1:B:244:ILE:H	1.60	0.43
1:A:491:GLN:CG	1:A:512:GLU:HG3	2.48	0.43
1:A:115:GLN:OE1	1:A:115:GLN:N	2.31	0.43
1:A:505:GLN:N	1:A:575:ASP:CB	2.80	0.43
1:A:112:VAL:HG13	1:A:150:THR:CB	2.49	0.43
1:B:574:VAL:CG2	1:B:575:ASP:N	2.81	0.43
1:B:415:LYS:HZ2	1:B:474:ASN:N	2.16	0.43
1:B:9:LYS:HD2	1:B:75:HIS:CD2	2.54	0.43
1:A:241:LYS:O	1:A:244:ILE:CG1	2.64	0.43
1:A:574:VAL:CG1	1:A:575:ASP:H	2.32	0.43
1:B:646:VAL:HG12	1:B:647:PRO:HD2	2.00	0.43
1:A:140:LEU:O	1:A:142:ALA:N	2.52	0.43
1:A:241:LYS:HD2	1:A:241:LYS:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:HIS:HB3	1:A:567:TYR:CE1	2.53	0.42
1:A:579:MET:O	1:A:582:LYS:HB2	2.19	0.42
1:A:270:MET:HG3	1:A:271:LEU:N	2.33	0.42
1:B:355:LEU:HB3	1:B:366:ILE:HG13	2.01	0.42
1:A:201:GLU:OE1	1:A:202:ASP:N	2.46	0.42
1:A:615:TYR:HB3	1:A:618:ASP:OD2	2.18	0.42
1:B:590:LYS:O	1:B:593:ALA:N	2.52	0.42
1:B:448:VAL:HG22	1:B:449:ILE:N	2.34	0.42
1:B:405:GLU:CG	1:B:406:PRO:HD2	2.49	0.42
1:B:412:VAL:O	1:B:412:VAL:HG13	2.18	0.42
1:B:633:MET:HG2	1:B:634:GLU:N	2.35	0.42
1:A:156:GLN:HE21	1:A:637:GLY:HA3	1.84	0.42
1:A:290:HIS:HB2	1:A:295:PRO:HA	2.01	0.42
1:A:441:THR:HG22	1:A:441:THR:O	2.19	0.42
1:A:17:ALA:CB	1:A:105:VAL:HB	2.47	0.42
1:B:9:LYS:HA	1:B:75:HIS:CD2	2.55	0.42
1:B:163:GLN:OE1	1:B:175:ILE:HD11	2.19	0.42
1:A:567:TYR:HD1	1:A:568:ASP:HB2	1.83	0.42
1:A:469:PHE:HD1	1:A:469:PHE:N	2.16	0.42
1:B:128:VAL:O	1:B:130:ARG:NH2	2.49	0.42
1:A:369:VAL:HG12	1:A:369:VAL:O	2.18	0.42
1:B:145:GLU:OE1	1:B:145:GLU:HA	2.20	0.42
1:A:461:LEU:HA	1:A:461:LEU:HD23	1.83	0.42
1:B:180:GLU:HG3	1:B:182:LYS:HG3	2.01	0.42
1:A:614:GLU:OE1	1:A:614:GLU:N	2.48	0.42
1:A:112:VAL:HG13	1:A:150:THR:HB	2.02	0.42
1:B:429:LYS:HA	1:B:429:LYS:HD3	1.75	0.42
1:B:216:GLU:HG3	1:B:229:TYR:CE2	2.55	0.42
1:B:90:VAL:CG2	1:B:91:GLU:H	2.20	0.42
1:B:330:VAL:HG22	1:B:373:ASP:O	2.19	0.42
1:B:590:LYS:N	1:B:590:LYS:HD2	2.34	0.42
1:A:245:ARG:O	1:A:249:THR:OG1	2.25	0.42
1:B:133:PHE:CD2	1:B:270:MET:HG3	2.48	0.42
1:A:132:VAL:HG21	1:A:151:LEU:HD21	2.02	0.42
1:A:486:PHE:O	1:A:515:PRO:HB3	2.20	0.42
1:A:524:PHE:HE1	1:A:526:ASN:HB2	1.85	0.42
1:A:441:THR:O	1:A:442:ASP:C	2.58	0.41
1:B:535:ARG:NH1	1:B:535:ARG:CG	2.80	0.41
1:B:350:GLU:OE1	1:B:382:ASP:HB2	2.20	0.41
1:B:579:MET:HG3	1:B:580:ALA:N	2.35	0.41
1:B:312:LEU:O	1:B:328:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HB2	1:B:176:ILE:CD1	2.42	0.41
1:A:235:ILE:HG23	1:A:239:GLU:OE2	2.21	0.41
1:B:555:ALA:HB1	1:B:557:TYR:CD2	2.54	0.41
1:B:354:ARG:HE	1:B:365:GLU:CD	2.23	0.41
1:A:237:VAL:O	1:A:240:LEU:HB3	2.20	0.41
1:A:120:TRP:CD1	1:A:120:TRP:C	2.93	0.41
1:B:670:MET:HB2	1:B:670:MET:HE2	1.74	0.41
1:A:309:PHE:CA	1:A:333:GLY:HA3	2.48	0.41
1:A:162:ILE:HG13	1:A:163:GLN:HG3	2.02	0.41
1:B:164:LEU:HD11	1:B:210:ALA:CB	2.51	0.41
1:B:299:VAL:HG13	1:B:299:VAL:O	2.21	0.41
1:B:340:TYR:CD2	1:B:349:ARG:NH2	2.82	0.41
1:B:523:GLU:HB2	1:B:563:LYS:CE	2.44	0.41
1:B:278:LEU:CB	1:B:279:PRO:HD2	2.47	0.41
1:A:549:MET:HE3	1:A:559:LEU:HD23	2.02	0.41
1:A:524:PHE:CD1	1:A:524:PHE:C	2.93	0.41
1:B:340:TYR:HB3	1:B:392:GLU:OE2	2.21	0.41
1:A:528:ILE:HD11	1:A:568:ASP:N	2.35	0.41
1:B:103:VAL:HG22	1:B:131:ILE:CG1	2.51	0.41
1:B:605:MET:SD	1:B:648:LEU:HD13	2.60	0.41
1:A:201:GLU:HA	1:A:204:LEU:CD1	2.50	0.41
1:B:554:LEU:HD13	1:B:598:PRO:HG2	2.02	0.41
1:A:408:ILE:HD11	1:A:478:PRO:CB	2.50	0.41
1:A:381:LYS:HE3	1:A:381:LYS:HB2	1.90	0.41
1:B:483:ARG:HG3	1:B:675:TYR:CE1	2.56	0.41
1:A:32:TYR:CD1	1:A:32:TYR:C	2.94	0.41
1:A:268:GLN:CD	1:A:268:GLN:N	2.73	0.41
1:B:410:LEU:HD21	1:B:458:LEU:HB3	2.03	0.41
1:B:670:MET:O	1:B:671:TYR:HD1	2.05	0.40
1:A:112:VAL:HG13	1:A:150:THR:OG1	2.20	0.40
1:B:569:GLY:O	1:B:570:SER:HB3	2.21	0.40
1:B:619:ILE:O	1:B:622:ASP:HB3	2.21	0.40
1:B:17:ALA:CB	1:B:23:LYS:HB2	2.51	0.40
1:B:330:VAL:O	1:B:330:VAL:HG23	2.21	0.40
1:B:620:MET:HE1	1:B:630:VAL:HG21	2.03	0.40
1:B:466:LYS:O	1:B:470:ASN:HA	2.21	0.40
1:B:138:ASP:OD2	1:B:263:LYS:HG3	2.21	0.40
1:A:414:PRO:HG3	1:A:423:MET:HE2	2.01	0.40
1:B:512:GLU:HG2	1:B:565:LYS:HB3	2.03	0.40
1:A:140:LEU:C	1:A:142:ALA:N	2.74	0.40
1:A:80:ILE:HG12	1:A:98:VAL:CG1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:SER:O	1:B:150:THR:OG1	2.21	0.40
1:B:219:ALA:HA	1:B:225:LEU:CD1	2.43	0.40
1:B:688:LYS:HA	1:B:691:LYS:NZ	2.36	0.40
1:B:487:LYS:HE2	1:B:599:VAL:HG13	2.03	0.40
1:A:399:GLU:CG	1:A:400:SER:N	2.85	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	639/693 (92%)	593 (93%)	44 (7%)	2 (0%)	46	82
1	B	639/693 (92%)	580 (91%)	58 (9%)	1 (0%)	52	87
All	All	1278/1386 (92%)	1173 (92%)	102 (8%)	3 (0%)	52	87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	360	ALA
1	B	251	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	543/579 (94%)	498 (92%)	45 (8%)	14 44
1	B	543/579 (94%)	497 (92%)	46 (8%)	13 43
All	All	1086/1158 (94%)	995 (92%)	91 (8%)	14 43

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	112	VAL
1	A	146	TYR
1	A	154	ARG
1	A	179	VAL
1	A	192	THR
1	A	199	ILE
1	A	201	GLU
1	A	213	SER
1	A	227	GLU
1	A	230	LEU
1	A	234	GLU
1	A	236	SER
1	A	244	ILE
1	A	246	GLN
1	A	270	MET
1	A	297	GLU
1	A	304	ASP
1	A	309	PHE
1	A	330	VAL
1	A	344	SER
1	A	361	ASN
1	A	396	ILE
1	A	400	SER
1	A	411	SER
1	A	447	GLN
1	A	448	VAL
1	A	459	ASP
1	A	463	ASP
1	A	505	GLN
1	A	506	TYR
1	A	509	VAL
1	A	514	THR
1	A	518	THR
1	A	536	GLU

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Mol	Chain	Res	Type
1	A	571	TYR
1	A	573	ASP
1	A	578	GLU
1	A	611	MET
1	A	618	ASP
1	A	631	ASP
1	A	640	GLN
1	A	649	SER
1	A	667	THR
1	A	671	TYR
1	B	29	ARG
1	B	76	ARG
1	B	109	GLN
1	B	154	ARG
1	B	162	ILE
1	B	170	ASP
1	B	175	ILE
1	B	176	ILE
1	B	178	LEU
1	B	192	THR
1	B	206	ARG
1	B	225	LEU
1	B	230	LEU
1	B	235	ILE
1	B	238	SER
1	B	246	GLN
1	B	271	LEU
1	B	280	SER
1	B	288	ILE
1	B	293	SER
1	B	294	ASN
1	B	318	THR
1	B	336	THR
1	B	363	ARG
1	B	369	VAL
1	B	390	CYS
1	B	420	GLN
1	B	442	ASP
1	B	475	VAL
1	B	532	VAL
1	B	535	ARG
1	B	547	ASP

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Mol	Chain	Res	Type
1	B	550	GLU
1	B	574	VAL
1	B	611	MET
1	B	616	MET
1	B	618	ASP
1	B	622	ASP
1	B	624	THR
1	B	625	SER
1	B	629	ARG
1	B	636	ARG
1	B	641	VAL
1	B	659	ARG
1	B	667	THR
1	B	688	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	246	GLN
1	A	409	HIS
1	A	572	HIS
1	A	690	ASN
1	B	18	HIS
1	B	75	HIS
1	B	115	GLN
1	B	264	ASN
1	B	431	GLN
1	B	447	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	649/693 (93%)	0.10	19 (2%)	55	33	55, 104, 163, 250	0
1	B	649/693 (93%)	0.33	36 (5%)	29	15	68, 115, 175, 278	0
All	All	1298/1386 (93%)	0.22	55 (4%)	40	22	55, 109, 168, 278	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	ARG	5.2
1	B	518	THR	4.1
1	B	563	LYS	3.9
1	B	310	ALA	3.7
1	B	393	LYS	3.7
1	B	290	HIS	3.6
1	B	296	GLU	3.5
1	A	398	LEU	3.4
1	B	581	PHE	3.3
1	B	564	ALA	3.3
1	B	514	THR	3.1
1	B	396	ILE	3.0
1	B	295	PRO	2.9
1	B	253	PHE	2.8
1	A	287	ILE	2.8
1	B	513	PHE	2.8
1	B	496	PHE	2.7
1	A	252	GLU	2.7
1	A	10	THR	2.7
1	B	482	TYR	2.6
1	A	451	GLY	2.6
1	B	351	ARG	2.6
1	B	423	MET	2.6
1	B	533	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	561	ASP	2.5
1	A	300	ILE	2.5
1	B	601	LEU	2.4
1	B	289	GLY	2.4
1	B	545	LEU	2.4
1	A	2	ALA	2.4
1	A	581	PHE	2.4
1	B	65	SER	2.4
1	A	176	ILE	2.3
1	A	372	GLY	2.3
1	A	524	PHE	2.3
1	B	415	LYS	2.3
1	B	524	PHE	2.3
1	A	172	PHE	2.2
1	B	637	GLY	2.2
1	B	225	LEU	2.2
1	A	577	SER	2.2
1	B	562	VAL	2.2
1	A	312	LEU	2.2
1	A	397	ILE	2.2
1	B	84	GLY	2.2
1	A	509	VAL	2.2
1	B	19	ILE	2.1
1	A	511	ILE	2.1
1	B	24	THR	2.1
1	B	372	GLY	2.1
1	A	514	THR	2.1
1	A	229	TYR	2.1
1	B	291	ARG	2.0
1	B	522	PHE	2.0
1	B	600	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.