Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:29 PM GMT

PDB ID	:	1FVF
Title	:	CRYSTAL STRUCTURE ANALYSIS OF NEURONAL SEC1 FROM THE SQUID L. PEALEI
Authors	:	Bracher, A.; Weissenhorn, W.
Deposited on	:	2000-09-19
Resolution	:	3.20 Å(reported)

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

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

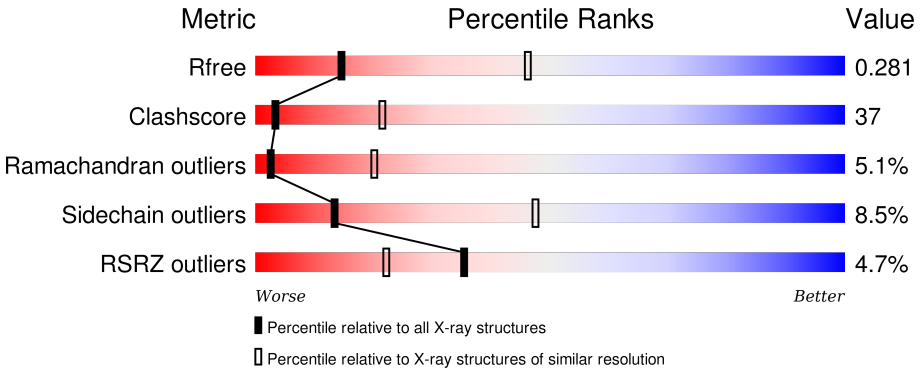
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	591	4% 42% 41% 8% 8%
1	B	591	5% 42% 41% 8% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8786 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 SEC1.

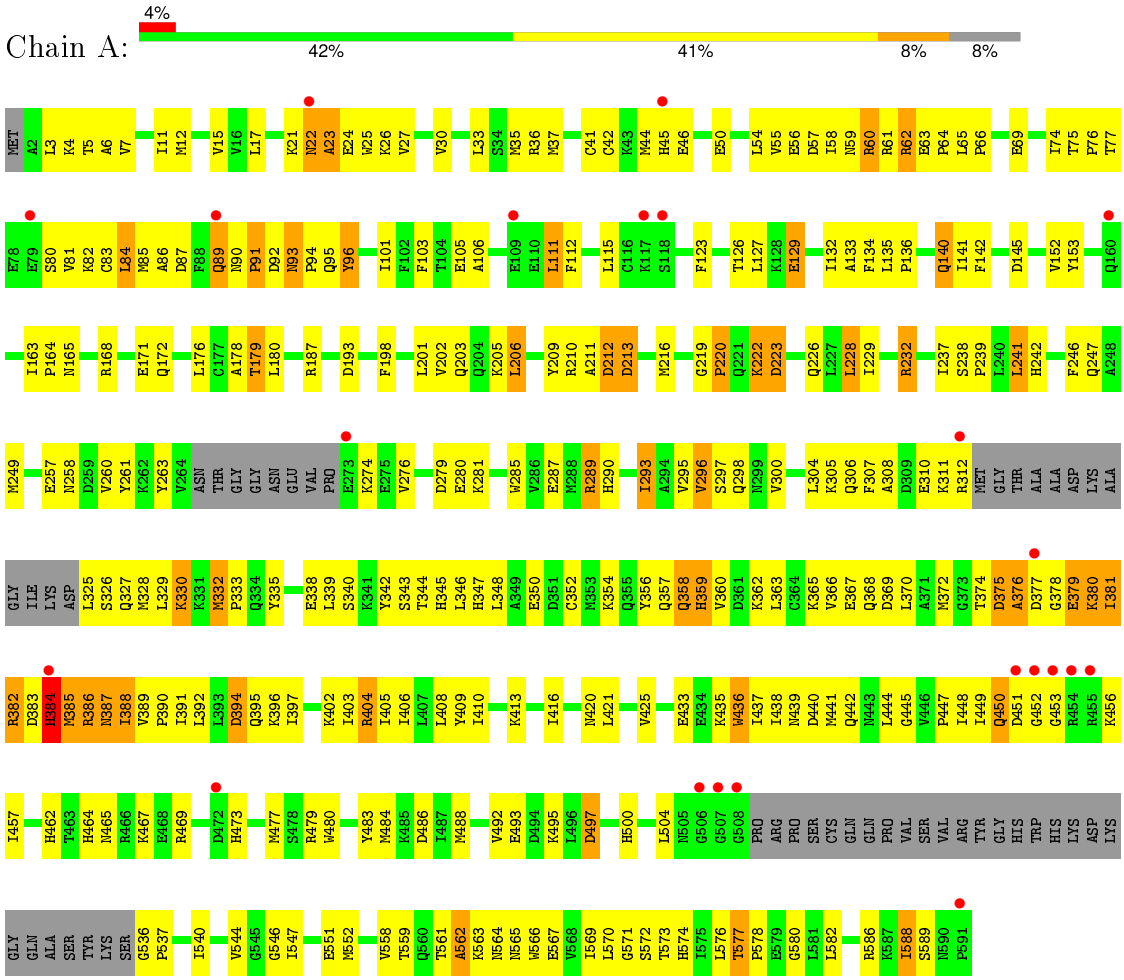
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4393	2783	759	823	28			
1	B	543	Total	C	N	O	S	0	0	0
			4393	2783	759	823	28			

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.

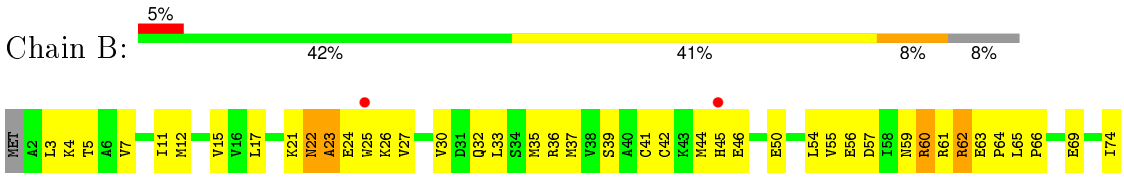
- Molecule 1: SEC1

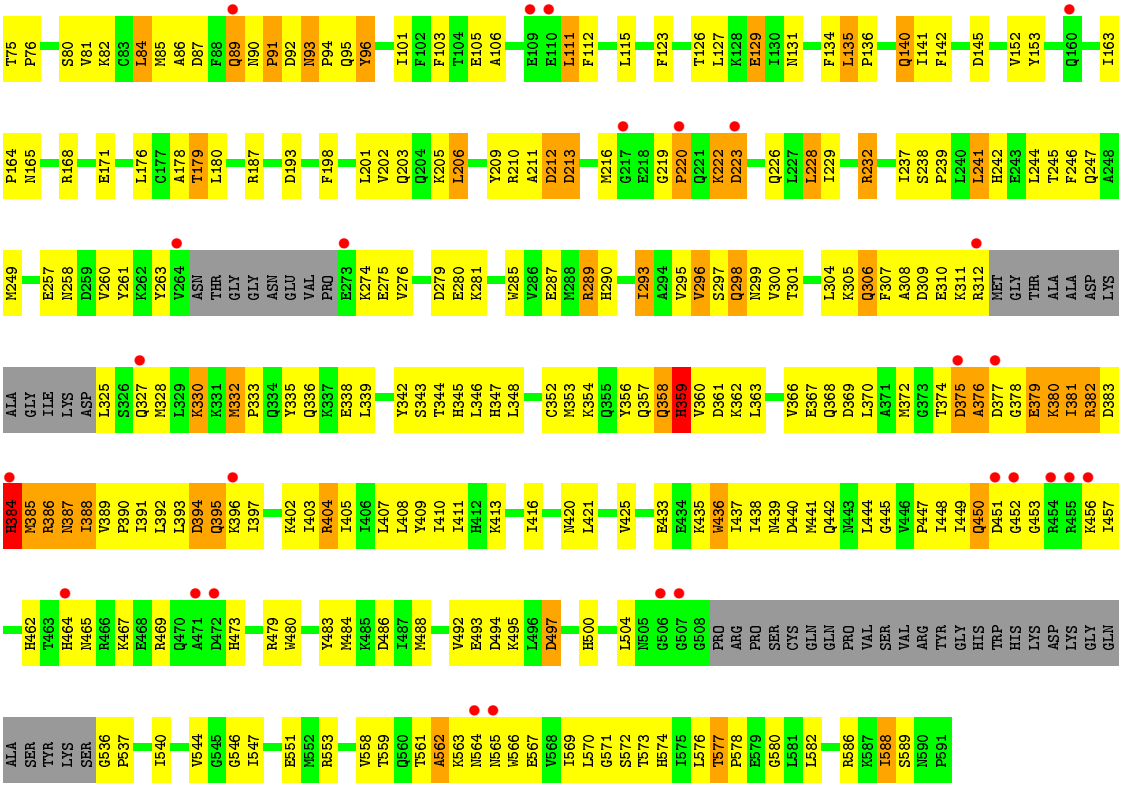
Chain A:



- Molecule 1: SEC1

Chain B:




T75 P76 S80 V81 K82 C83 L84 M85 A86 D87 F88 Q89 N90 P91 D92 N93 P94 Q95 Y96 I101 F102 F103 T104 E105 A106 E109 E110 L111 F112 L115 F123 T126 L127 K128 E129 I130 N131 F134 L135 P136 Q140 I141 F142 D145 V152 Y153 Q160 I163
P164 N165 R168 E171 L176 C177 A178 T179 L180 R187 D193 F198 L201 V202 Q203 Q204 K205 L206 Y209 R210 A211 D212 D213 M216 G217 E218 G219 P220 Q221 K222 D223 Q226 L227 L228 I229 R232 I237 S238 P239 L240 L241 H242 E243 L244 T245 F246 Q247 A248
M249 E257 N258 D259 V260 Y261 K262 Y263 V264 ASN THR GLY GLY ASN GLU VAL PRO E273 K274 E275 V276 D279 E280 K281 W285 V286 E287 M288 R289 H290 I293 A294 V295 V296 S297 Q298 N299 V300 T301 L304 K305 Q306 F307 A308 D309 E310 K311 R312 MET GLY THR ALA ALA ASP LYS
ALA GLY ILE LYS ASP L325 S326 Q327 H328 L329 K330 K331 M332 P333 Q334 Y335 Q336 K337 E338 L339 Y342 S343 T344 H345 L346 H347 L348 C352 M353 K354 Q355 Y356 Q357 Q358 H359 V360 D361 K362 L363 V366 E367 Q368 D369 L370 A371 H372 G373 T374 D375 A376 D377 G378 E379 K380 I381 R382 D383
B384 M385 R386 N387 I388 V389 P390 I391 L392 L393 D394 Q395 K396 I397 K402 I403 R404 I405 I406 L407 L408 Y409 I410 I411 H412 K413 I416 N420 L421 V425 E433 E434 K435 W436 I437 I438 N439 D440 M441 Q442 N443 L444 G445 V446 P447 I448 I449 Q450 D451 G452 G453 R454 R455 K456 I457
H462 T463 H464 N465 R466 K467 E468 R469 Q470 A471 D472 H473 R479 W480 Y483 M484 K485 D486 I487 M488 V492 E493 D494 K495 L496 D497 H500 L504 N505 G506 G507 G508 PRO ARG PRO SER CYS GLN GLN PRO VAL SER VAL ARG TYR GLY HIS TRP HIS LYS ASP LYS GLY GLN
ALA SER TYR LYS SER G536 P537 T540 V544 G545 G546 I547 E551 M552 R553 V558 T559 Q560 T561 A562 K563 N564 N565 W566 E567 V568 I569 L570 G571 S572 T573 H574 I575 L576 T577 P578 E579 G580 L581 L582 R586 K587 I588 S589 N590 P591

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.52Å 118.52Å 192.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.20 11.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (12.00-3.20) 95.8 (11.99-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 3.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.288 0.240 , 0.281	Depositor DCC
R_{free} test set	1202 reflections (4.85%)	DCC
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.0	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 24771 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8786	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.41	0/4481	0.69	2/6050 (0.0%)
1	B	0.40	0/4481	0.68	2/6050 (0.0%)
All	All	0.41	0/8962	0.69	4/12100 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	A	404	ARG	NE-CZ-NH2	-10.65	114.98	120.30
1	B	404	ARG	NE-CZ-NH1	-10.55	115.03	120.30
1	B	404	ARG	NE-CZ-NH2	9.76	125.18	120.30

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	4393	0	4393	330	0
1	B	4393	0	4393	338	0
All	All	8786	0	8786	646	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 37.

All (646) 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:89:GLN:HE21	1:A:89:GLN:HA	1.25	1.00
1:B:89:GLN:HA	1:B:89:GLN:HE21	1.27	0.98
1:A:577:THR:HG22	1:A:580:GLY:H	1.32	0.94
1:B:577:THR:HG22	1:B:580:GLY:H	1.33	0.94
1:B:305:LYS:HG3	1:B:306:GLN:H	1.35	0.90
1:A:305:LYS:HG3	1:A:306:GLN:N	1.85	0.90
1:B:305:LYS:HG3	1:B:306:GLN:N	1.87	0.90
1:A:330:LYS:HZ1	1:A:330:LYS:HA	1.36	0.89
1:A:305:LYS:HG3	1:A:306:GLN:H	1.36	0.89
1:B:163:ILE:HD12	1:B:163:ILE:H	1.39	0.87
1:B:54:LEU:HD23	1:B:55:VAL:N	1.89	0.87
1:A:163:ILE:HD12	1:A:163:ILE:H	1.40	0.86
1:B:54:LEU:HD23	1:B:55:VAL:H	1.41	0.84
1:B:439:ASN:HA	1:B:448:ILE:CD1	2.07	0.84
1:A:330:LYS:NZ	1:A:330:LYS:HA	1.92	0.84
1:A:308:ALA:HB1	1:B:305:LYS:HB3	1.60	0.83
1:A:54:LEU:HD23	1:A:55:VAL:N	1.94	0.83
1:A:439:ASN:HA	1:A:448:ILE:CD1	2.08	0.83
1:A:54:LEU:HD23	1:A:55:VAL:H	1.45	0.82
1:B:380:LYS:O	1:B:381:ILE:HG23	1.80	0.81
1:B:330:LYS:HA	1:B:330:LYS:NZ	1.95	0.81
1:B:540:ILE:HD13	1:B:569:ILE:HB	1.61	0.80
1:A:380:LYS:O	1:A:381:ILE:HG23	1.82	0.79
1:A:448:ILE:HG13	1:A:449:ILE:N	1.97	0.79
1:A:362:LYS:HE3	1:A:397:ILE:HD11	1.64	0.78
1:B:311:LYS:HG3	1:B:335:TYR:HE1	1.46	0.78
1:B:362:LYS:HE3	1:B:397:ILE:HD11	1.65	0.78
1:B:439:ASN:HA	1:B:448:ILE:HD13	1.65	0.77
1:A:311:LYS:HG3	1:A:335:TYR:HE1	1.50	0.77
1:A:93:ASN:H	1:A:94:PRO:CD	1.97	0.77
1:A:540:ILE:HD13	1:A:569:ILE:HB	1.66	0.77
1:A:439:ASN:HA	1:A:448:ILE:HD13	1.65	0.76
1:A:577:THR:HG22	1:A:580:GLY:N	2.01	0.76
1:B:201:LEU:HD22	1:B:201:LEU:H	1.51	0.76
1:A:89:GLN:NE2	1:A:89:GLN:HA	2.00	0.76
1:B:577:THR:HG22	1:B:580:GLY:N	2.01	0.75
1:B:433:GLU:CD	1:B:433:GLU:H	1.90	0.75
1:B:448:ILE:HG13	1:B:449:ILE:N	2.00	0.75
1:B:375:ASP:HA	1:B:479:ARG:NH1	2.02	0.75
1:B:89:GLN:HA	1:B:89:GLN:NE2	2.01	0.75
1:A:247:GLN:HB2	1:A:289:ARG:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASN:H	1:B:94:PRO:CD	2.01	0.74
1:B:86:ALA:HA	1:B:89:GLN:HB2	1.68	0.74
1:A:374:THR:HB	1:A:378:GLY:HA2	1.68	0.74
1:A:201:LEU:H	1:A:201:LEU:HD22	1.52	0.74
1:A:133:ALA:HB1	1:A:172:GLN:HG2	1.70	0.73
1:A:86:ALA:HA	1:A:89:GLN:HB2	1.71	0.73
1:A:93:ASN:H	1:A:94:PRO:HD3	1.54	0.73
1:A:305:LYS:HD2	1:B:312:ARG:HE	1.53	0.73
1:B:374:THR:HB	1:B:378:GLY:HA2	1.68	0.72
1:A:276:VAL:HG21	1:A:344:THR:HG21	1.69	0.72
1:A:435:LYS:HD2	1:A:436:TRP:CZ3	2.23	0.72
1:A:433:GLU:CD	1:A:433:GLU:H	1.93	0.72
1:A:263:TYR:OH	1:A:274:LYS:HE3	1.90	0.72
1:A:326:SER:HA	1:B:357:GLN:HE22	1.55	0.72
1:B:382:ARG:HB2	1:B:386:ARG:HD2	1.70	0.72
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.55	0.71
1:B:209:TYR:HB3	1:B:216:MET:HE1	1.73	0.71
1:B:263:TYR:OH	1:B:274:LYS:HE3	1.91	0.71
1:A:382:ARG:HB2	1:A:386:ARG:HD2	1.71	0.71
1:A:249:MET:CE	1:A:352:CYS:HB3	2.20	0.70
1:B:435:LYS:HD2	1:B:436:TRP:CZ3	2.27	0.70
1:A:350:GLU:OE2	1:B:332:MET:HG2	1.90	0.70
1:B:276:VAL:HG21	1:B:344:THR:HG21	1.71	0.70
1:B:379:GLU:HG3	1:B:380:LYS:H	1.56	0.70
1:A:558:VAL:O	1:A:561:THR:HG22	1.92	0.69
1:B:249:MET:CE	1:B:352:CYS:HB3	2.22	0.69
1:B:558:VAL:O	1:B:561:THR:HG22	1.93	0.69
1:B:247:GLN:HB2	1:B:289:ARG:HB2	1.72	0.69
1:A:379:GLU:HG3	1:A:380:LYS:H	1.58	0.69
1:B:93:ASN:H	1:B:94:PRO:HD3	1.57	0.69
1:B:134:PHE:CE1	1:B:176:LEU:HA	2.28	0.69
1:B:187:ARG:HD2	1:B:226:GLN:OE1	1.93	0.68
1:A:375:ASP:HA	1:A:479:ARG:NH1	2.08	0.68
1:B:564:ASN:HB3	1:B:566:TRP:HD1	1.59	0.68
1:B:210:ARG:HG3	1:B:210:ARG:HH11	1.59	0.68
1:A:279:ASP:OD2	1:A:281:LYS:HE2	1.95	0.67
1:A:62:ARG:HD3	1:A:62:ARG:N	2.08	0.67
1:A:187:ARG:HD2	1:A:226:GLN:OE1	1.95	0.67
1:B:62:ARG:N	1:B:62:ARG:HD3	2.09	0.67
1:A:577:THR:CG2	1:A:580:GLY:H	2.07	0.67
1:A:356:TYR:HA	1:A:360:VAL:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HD11	1:B:304:LEU:HD21	1.77	0.67
1:A:564:ASN:HB3	1:A:566:TRP:HD1	1.58	0.67
1:A:386:ARG:O	1:A:388:ILE:N	2.28	0.66
1:B:379:GLU:HG3	1:B:380:LYS:N	2.11	0.66
1:A:441:MET:CE	1:A:444:LEU:HD22	2.25	0.66
1:B:279:ASP:OD2	1:B:281:LYS:HE2	1.96	0.66
1:B:356:TYR:HA	1:B:360:VAL:HB	1.76	0.66
1:A:448:ILE:HG13	1:A:449:ILE:H	1.61	0.66
1:B:386:ARG:O	1:B:388:ILE:N	2.29	0.66
1:B:561:THR:C	1:B:563:LYS:H	2.00	0.66
1:A:132:ILE:HG22	1:A:132:ILE:O	1.97	0.65
1:A:232:ARG:O	1:A:232:ARG:HD3	1.96	0.65
1:B:546:GLY:HA3	1:B:576:LEU:HG	1.79	0.65
1:B:311:LYS:HG3	1:B:335:TYR:CE1	2.31	0.65
1:B:372:MET:HE1	1:B:480:TRP:HB2	1.78	0.65
1:B:561:THR:HG23	1:B:562:ALA:N	2.11	0.65
1:A:441:MET:HE1	1:A:444:LEU:HD22	1.77	0.65
1:B:441:MET:CE	1:B:444:LEU:HD22	2.27	0.65
1:B:163:ILE:CD1	1:B:163:ILE:H	2.09	0.65
1:B:577:THR:CG2	1:B:580:GLY:H	2.07	0.64
1:A:307:PHE:CE2	1:A:338:GLU:HG3	2.32	0.64
1:A:546:GLY:HA3	1:A:576:LEU:HG	1.79	0.64
1:B:441:MET:HE1	1:B:444:LEU:HD22	1.79	0.64
1:B:330:LYS:HZ1	1:B:330:LYS:HA	1.61	0.64
1:A:384:HIS:O	1:A:385:MET:HG2	1.98	0.64
1:A:84:LEU:HD11	1:A:101:ILE:CD1	2.28	0.64
1:B:112:PHE:HE1	1:B:127:LEU:HD21	1.62	0.64
1:B:81:VAL:HG21	1:B:111:LEU:HD13	1.80	0.64
1:B:22:ASN:O	1:B:24:GLU:HB2	1.98	0.63
1:A:249:MET:CE	1:A:293:ILE:HD12	2.28	0.63
1:A:62:ARG:HD3	1:A:62:ARG:H	1.64	0.63
1:A:561:THR:HG23	1:A:562:ALA:N	2.14	0.63
1:A:209:TYR:HB3	1:A:216:MET:CE	2.28	0.63
1:A:379:GLU:HG3	1:A:380:LYS:N	2.12	0.63
1:B:209:TYR:HB3	1:B:216:MET:CE	2.28	0.63
1:A:372:MET:HE1	1:A:480:TRP:HB2	1.79	0.63
1:B:84:LEU:HD11	1:B:101:ILE:CD1	2.29	0.63
1:A:308:ALA:HB1	1:B:305:LYS:CB	2.29	0.63
1:B:307:PHE:CE2	1:B:338:GLU:HG3	2.33	0.62
1:B:561:THR:HG23	1:B:562:ALA:H	1.64	0.62
1:B:380:LYS:O	1:B:381:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASN:HB3	1:A:566:TRP:CD1	2.34	0.62
1:B:366:VAL:HG21	1:B:391:ILE:HG13	1.81	0.62
1:A:202:VAL:HG21	1:A:229:ILE:HD11	1.81	0.62
1:A:312:ARG:HE	1:B:305:LYS:HD2	1.64	0.62
1:A:93:ASN:N	1:A:94:PRO:CD	2.62	0.62
1:B:22:ASN:O	1:B:24:GLU:N	2.32	0.62
1:A:112:PHE:HE1	1:A:127:LEU:HD21	1.64	0.62
1:A:163:ILE:H	1:A:163:ILE:CD1	2.09	0.62
1:A:81:VAL:HG21	1:A:111:LEU:HD13	1.79	0.62
1:B:202:VAL:HG21	1:B:229:ILE:HD11	1.80	0.62
1:B:232:ARG:O	1:B:232:ARG:HD3	1.98	0.62
1:A:22:ASN:O	1:A:24:GLU:HB2	2.00	0.62
1:B:448:ILE:HG13	1:B:449:ILE:H	1.64	0.62
1:B:564:ASN:HB3	1:B:566:TRP:CD1	2.34	0.61
1:A:375:ASP:O	1:A:377:ASP:N	2.34	0.61
1:A:22:ASN:O	1:A:24:GLU:N	2.33	0.61
1:B:152:VAL:HG21	1:B:165:ASN:ND2	2.15	0.61
1:B:201:LEU:H	1:B:201:LEU:CD2	2.13	0.61
1:A:33:LEU:H	1:A:33:LEU:HD22	1.66	0.61
1:A:64:PRO:O	1:A:65:LEU:HD23	2.01	0.61
1:B:375:ASP:O	1:B:377:ASP:N	2.33	0.61
1:A:561:THR:C	1:A:563:LYS:H	2.03	0.61
1:B:62:ARG:H	1:B:62:ARG:HD3	1.65	0.61
1:B:33:LEU:H	1:B:33:LEU:HD22	1.65	0.61
1:B:168:ARG:HH11	1:B:168:ARG:HG3	1.66	0.61
1:A:249:MET:HE3	1:A:352:CYS:HB3	1.82	0.61
1:A:201:LEU:H	1:A:201:LEU:CD2	2.14	0.60
1:B:384:HIS:O	1:B:385:MET:HG2	2.01	0.60
1:A:210:ARG:NH1	1:A:210:ARG:HG3	2.15	0.60
1:A:382:ARG:CB	1:A:386:ARG:HD2	2.31	0.60
1:A:380:LYS:O	1:A:381:ILE:HG12	2.02	0.60
1:B:263:TYR:CE2	1:B:344:THR:HG22	2.37	0.60
1:A:564:ASN:O	1:A:565:ASN:HB3	2.01	0.60
1:A:563:LYS:C	1:A:565:ASN:H	2.05	0.60
1:B:563:LYS:C	1:B:565:ASN:H	2.05	0.60
1:A:343:SER:OG	1:B:339:LEU:HD23	2.02	0.60
1:A:307:PHE:HE2	1:A:338:GLU:HG3	1.65	0.60
1:A:347:HIS:CD2	1:B:336:GLN:NE2	2.70	0.60
1:A:152:VAL:HG21	1:A:165:ASN:ND2	2.17	0.60
1:A:435:LYS:HD2	1:A:436:TRP:CE3	2.35	0.59
1:B:382:ARG:CB	1:B:386:ARG:HD2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ASN:O	1:B:565:ASN:HB3	2.02	0.59
1:B:261:TYR:CD2	1:B:348:LEU:HD13	2.37	0.59
1:A:347:HIS:HD2	1:B:336:GLN:NE2	2.00	0.59
1:A:62:ARG:NH2	1:A:87:ASP:OD2	2.35	0.59
1:A:368:GLN:NE2	1:A:479:ARG:HB2	2.17	0.59
1:A:329:LEU:HD13	1:B:353:MET:HB2	1.85	0.59
1:A:384:HIS:O	1:A:385:MET:CG	2.51	0.59
1:B:35:MET:O	1:B:35:MET:HE3	2.02	0.59
1:B:307:PHE:HE2	1:B:338:GLU:HG3	1.67	0.59
1:A:362:LYS:NZ	1:A:396:LYS:HD2	2.18	0.59
1:B:362:LYS:NZ	1:B:396:LYS:HD2	2.17	0.58
1:A:263:TYR:CE2	1:A:344:THR:HG22	2.37	0.58
1:B:467:LYS:HE3	1:B:469:ARG:NH1	2.18	0.58
1:B:421:LEU:O	1:B:425:VAL:HG23	2.03	0.58
1:A:35:MET:HE3	1:A:35:MET:O	2.02	0.58
1:A:561:THR:HG23	1:A:562:ALA:H	1.66	0.58
1:A:366:VAL:HG21	1:A:391:ILE:HG13	1.85	0.58
1:A:330:LYS:O	1:A:333:PRO:HD2	2.04	0.58
1:B:163:ILE:HD12	1:B:163:ILE:N	2.13	0.58
1:A:163:ILE:HD12	1:A:163:ILE:N	2.13	0.58
1:B:30:VAL:O	1:B:57:ASP:HA	2.04	0.58
1:A:357:GLN:HE21	1:B:325:LEU:CD2	2.16	0.58
1:B:62:ARG:NH2	1:B:87:ASP:OD2	2.37	0.58
1:A:209:TYR:HB3	1:A:216:MET:HE1	1.85	0.57
1:B:464:HIS:CD2	1:B:465:ASN:HD21	2.22	0.57
1:A:311:LYS:HG3	1:A:335:TYR:CE1	2.34	0.57
1:A:103:PHE:O	1:A:129:GLU:HA	2.04	0.57
1:B:64:PRO:O	1:B:65:LEU:HD23	2.03	0.57
1:A:473:HIS:ND1	1:A:479:ARG:HG2	2.19	0.57
1:B:210:ARG:NH1	1:B:210:ARG:HG3	2.17	0.57
1:B:464:HIS:CD2	1:B:465:ASN:ND2	2.73	0.57
1:A:483:TYR:O	1:A:486:ASP:HB2	2.05	0.57
1:B:61:ARG:HH21	1:B:95:GLN:HE22	1.52	0.57
1:B:403:ILE:HG23	1:B:438:ILE:CD1	2.34	0.57
1:B:103:PHE:O	1:B:129:GLU:HA	2.05	0.57
1:A:421:LEU:O	1:A:425:VAL:HG23	2.05	0.57
1:B:202:VAL:O	1:B:206:LEU:HG	2.05	0.57
1:A:403:ILE:HG23	1:A:438:ILE:CD1	2.33	0.57
1:A:328:MET:C	1:A:330:LYS:H	2.08	0.56
1:B:435:LYS:HD2	1:B:436:TRP:CE3	2.39	0.56
1:B:368:GLN:NE2	1:B:479:ARG:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LYS:O	1:B:333:PRO:HD2	2.05	0.56
1:A:82:LYS:HA	1:A:85:MET:HE2	1.85	0.56
1:B:483:TYR:O	1:B:486:ASP:HB2	2.05	0.56
1:A:346:LEU:HD11	1:B:335:TYR:CE2	2.39	0.56
1:A:249:MET:SD	1:A:293:ILE:HD12	2.46	0.56
1:A:444:LEU:N	1:A:444:LEU:HD12	2.20	0.56
1:A:357:GLN:NE2	1:B:325:LEU:HD23	2.20	0.56
1:A:464:HIS:CD2	1:A:465:ASN:ND2	2.74	0.56
1:B:93:ASN:N	1:B:94:PRO:CD	2.64	0.56
1:A:261:TYR:CD2	1:A:348:LEU:HD13	2.41	0.56
1:A:90:ASN:OD1	1:A:91:PRO:O	2.23	0.56
1:B:90:ASN:OD1	1:B:91:PRO:O	2.24	0.56
1:A:36:ARG:HD3	1:A:135:LEU:HD11	1.88	0.56
1:A:61:ARG:NH2	1:A:95:GLN:HE22	2.03	0.56
1:B:439:ASN:HA	1:B:448:ILE:HD11	1.87	0.56
1:B:330:LYS:HZ2	1:B:330:LYS:HA	1.71	0.56
1:B:4:LYS:NZ	1:B:280:GLU:HG3	2.21	0.56
1:A:168:ARG:HG3	1:A:168:ARG:HH11	1.70	0.56
1:B:241:LEU:HD12	1:B:408:LEU:HD11	1.88	0.56
1:A:464:HIS:CD2	1:A:465:ASN:HD21	2.24	0.55
1:B:367:GLU:HG2	1:B:408:LEU:HD12	1.88	0.55
1:A:547:ILE:HG23	1:A:572:SER:HB2	1.88	0.55
1:A:394:ASP:CG	1:A:397:ILE:HG12	2.26	0.55
1:B:384:HIS:O	1:B:385:MET:CG	2.54	0.55
1:A:339:LEU:HD11	1:B:304:LEU:CD2	2.36	0.55
1:A:257:GLU:O	1:A:260:VAL:HG12	2.07	0.55
1:B:249:MET:HE3	1:B:352:CYS:HB3	1.89	0.55
1:B:61:ARG:NH2	1:B:95:GLN:HE22	2.05	0.55
1:B:473:HIS:ND1	1:B:479:ARG:HG2	2.21	0.55
1:B:451:ASP:C	1:B:453:GLY:H	2.10	0.55
1:B:368:GLN:NE2	1:B:479:ARG:H	2.05	0.55
1:A:61:ARG:HH21	1:A:95:GLN:HE22	1.52	0.55
1:B:328:MET:C	1:B:330:LYS:H	2.08	0.55
1:A:247:GLN:HG3	1:A:285:TRP:HZ2	1.72	0.55
1:B:263:TYR:CZ	1:B:344:THR:HG22	2.42	0.54
1:A:467:LYS:HE3	1:A:469:ARG:NH1	2.22	0.54
1:A:238:SER:N	1:A:239:PRO:HD2	2.22	0.54
1:A:105:GLU:OE1	1:A:168:ARG:NH2	2.41	0.54
1:A:382:ARG:HH11	1:A:382:ARG:HG3	1.73	0.54
1:B:385:MET:O	1:B:389:VAL:HG23	2.07	0.54
1:B:444:LEU:N	1:B:444:LEU:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASP:C	1:A:453:GLY:H	2.10	0.54
1:A:95:GLN:O	1:A:96:TYR:HB2	2.07	0.54
1:B:433:GLU:CD	1:B:433:GLU:N	2.58	0.54
1:A:296:VAL:O	1:A:300:VAL:HG23	2.07	0.54
1:A:263:TYR:CZ	1:A:344:THR:HG22	2.43	0.54
1:A:385:MET:O	1:A:389:VAL:HG23	2.08	0.54
1:B:370:LEU:HD11	1:B:388:ILE:HD11	1.90	0.54
1:A:279:ASP:OD1	1:A:280:GLU:N	2.41	0.53
1:B:95:GLN:O	1:B:96:TYR:HB2	2.09	0.53
1:A:439:ASN:HA	1:A:448:ILE:HD11	1.89	0.53
1:B:279:ASP:OD1	1:B:280:GLU:N	2.42	0.53
1:B:203:GLN:O	1:B:206:LEU:HD12	2.07	0.53
1:A:249:MET:HE1	1:A:293:ILE:HG21	1.91	0.53
1:A:201:LEU:N	1:A:201:LEU:HD22	2.22	0.53
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.73	0.53
1:A:202:VAL:O	1:A:206:LEU:HG	2.09	0.53
1:B:462:HIS:HB3	1:B:464:HIS:CE1	2.43	0.53
1:A:84:LEU:HD11	1:A:101:ILE:HD13	1.90	0.53
1:A:332:MET:HB3	1:A:333:PRO:HD3	1.91	0.53
1:B:249:MET:CE	1:B:293:ILE:HD12	2.38	0.53
1:B:394:ASP:CG	1:B:397:ILE:HG12	2.29	0.53
1:A:368:GLN:NE2	1:A:479:ARG:H	2.06	0.53
1:B:4:LYS:HZ3	1:B:280:GLU:HG3	1.73	0.53
1:B:451:ASP:O	1:B:453:GLY:N	2.42	0.53
1:A:451:ASP:O	1:A:453:GLY:N	2.42	0.53
1:B:82:LYS:HA	1:B:85:MET:HE2	1.90	0.53
1:A:456:LYS:HD3	1:A:457:ILE:N	2.24	0.53
1:B:134:PHE:HE1	1:B:176:LEU:HA	1.71	0.53
1:A:440:ASP:C	1:A:442:GLN:N	2.61	0.53
1:A:347:HIS:CD2	1:B:336:GLN:HE21	2.26	0.53
1:B:95:GLN:O	1:B:96:TYR:CB	2.57	0.52
1:A:95:GLN:O	1:A:96:TYR:CB	2.57	0.52
1:A:433:GLU:CD	1:A:433:GLU:N	2.62	0.52
1:B:416:ILE:C	1:B:450:GLN:HB2	2.29	0.52
1:B:249:MET:SD	1:B:293:ILE:HD12	2.50	0.52
1:A:36:ARG:HD3	1:A:135:LEU:CD1	2.39	0.52
1:B:456:LYS:HD3	1:B:457:ILE:N	2.24	0.52
1:B:447:PRO:HG3	1:B:457:ILE:HB	1.91	0.52
1:A:416:ILE:C	1:A:450:GLN:HB2	2.30	0.52
1:A:304:LEU:O	1:A:307:PHE:HB3	2.10	0.52
1:B:249:MET:HE2	1:B:352:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:O	1:A:57:ASP:HA	2.10	0.52
1:B:332:MET:HB3	1:B:333:PRO:HD3	1.92	0.52
1:B:242:HIS:ND1	1:B:404:ARG:NH1	2.58	0.52
1:A:232:ARG:NH2	1:A:551:GLU:OE1	2.43	0.52
1:B:84:LEU:HD11	1:B:101:ILE:HD11	1.92	0.52
1:A:76:PRO:HG2	1:A:105:GLU:O	2.09	0.52
1:A:447:PRO:HG3	1:A:457:ILE:HB	1.92	0.52
1:B:201:LEU:HD22	1:B:201:LEU:N	2.22	0.52
1:B:46:GLU:O	1:B:50:GLU:HG2	2.10	0.51
1:A:203:GLN:O	1:A:206:LEU:HD12	2.10	0.51
1:A:416:ILE:HG13	1:A:420:ASN:HB2	1.93	0.51
1:A:247:GLN:HG3	1:A:285:TRP:CZ2	2.44	0.51
1:B:561:THR:C	1:B:563:LYS:N	2.63	0.51
1:A:84:LEU:HD11	1:A:101:ILE:HD11	1.93	0.51
1:B:54:LEU:CD2	1:B:55:VAL:N	2.69	0.51
1:A:198:PHE:CD1	1:A:229:ILE:HD13	2.45	0.51
1:B:198:PHE:CD1	1:B:229:ILE:HD13	2.44	0.51
1:B:421:LEU:C	1:B:421:LEU:HD13	2.31	0.51
1:A:33:LEU:O	1:A:36:ARG:HB2	2.11	0.51
1:B:297:SER:OG	1:B:353:MET:HE1	2.11	0.51
1:B:547:ILE:HG23	1:B:572:SER:HB2	1.91	0.51
1:B:7:VAL:HB	1:B:41:CYS:SG	2.51	0.51
1:B:380:LYS:O	1:B:381:ILE:CG2	2.56	0.51
1:B:123:PHE:H	1:B:123:PHE:HD1	1.58	0.51
1:B:247:GLN:HG3	1:B:285:TRP:HZ2	1.74	0.51
1:A:241:LEU:HD12	1:A:408:LEU:HD11	1.92	0.51
1:A:462:HIS:HB3	1:A:464:HIS:CE1	2.45	0.51
1:B:26:LYS:HD3	1:B:69:GLU:HB2	1.92	0.51
1:B:263:TYR:OH	1:B:344:THR:HG22	2.10	0.51
1:B:238:SER:N	1:B:239:PRO:HD2	2.25	0.51
1:A:11:ILE:HD11	1:A:37:MET:HE1	1.93	0.51
1:B:304:LEU:O	1:B:307:PHE:HB3	2.10	0.51
1:A:362:LYS:HZ2	1:A:396:LYS:HD2	1.76	0.51
1:A:372:MET:CE	1:A:480:TRP:HB2	2.40	0.51
1:B:289:ARG:HG2	1:B:290:HIS:N	2.25	0.51
1:B:440:ASP:C	1:B:442:GLN:N	2.64	0.51
1:B:437:ILE:HD11	1:B:586:ARG:HD2	1.93	0.50
1:A:379:GLU:CG	1:A:380:LYS:H	2.19	0.50
1:A:46:GLU:O	1:A:50:GLU:HG2	2.11	0.50
1:B:89:GLN:CA	1:B:89:GLN:HE21	2.04	0.50
1:A:54:LEU:CD2	1:A:55:VAL:N	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TRP:CE3	1:A:436:TRP:HA	2.46	0.50
1:A:335:TYR:CE2	1:B:346:LEU:HD11	2.46	0.50
1:A:123:PHE:CD1	1:A:123:PHE:N	2.78	0.50
1:B:84:LEU:HD11	1:B:101:ILE:HD13	1.93	0.50
1:B:372:MET:CE	1:B:480:TRP:HB2	2.40	0.50
1:A:370:LEU:HD11	1:A:388:ILE:HD11	1.93	0.50
1:B:559:THR:HG23	1:B:567:GLU:HA	1.93	0.50
1:A:237:ILE:C	1:A:239:PRO:HD2	2.32	0.50
1:B:379:GLU:CG	1:B:380:LYS:H	2.17	0.50
1:B:380:LYS:C	1:B:381:ILE:HG12	2.31	0.50
1:B:123:PHE:N	1:B:123:PHE:CD1	2.78	0.50
1:A:263:TYR:OH	1:A:344:THR:HG22	2.12	0.50
1:A:437:ILE:HD11	1:A:586:ARG:HD2	1.93	0.50
1:A:176:LEU:C	1:A:176:LEU:HD13	2.30	0.50
1:A:74:ILE:HD12	1:A:80:SER:HB3	1.94	0.50
1:B:232:ARG:NH2	1:B:551:GLU:OE1	2.45	0.50
1:B:168:ARG:NH1	1:B:168:ARG:HG3	2.27	0.50
1:A:363:LEU:HD23	1:A:391:ILE:HD12	1.94	0.50
1:B:257:GLU:O	1:B:260:VAL:HG12	2.11	0.50
1:B:436:TRP:HA	1:B:436:TRP:CE3	2.47	0.49
1:A:310:GLU:O	1:A:311:LYS:HD2	2.12	0.49
1:A:289:ARG:HG2	1:A:290:HIS:N	2.25	0.49
1:B:386:ARG:HG2	1:B:387:ASN:N	2.27	0.49
1:A:56:GLU:OE1	1:A:62:ARG:HG3	2.12	0.49
1:B:22:ASN:O	1:B:23:ALA:C	2.50	0.49
1:B:416:ILE:HG13	1:B:420:ASN:HB2	1.92	0.49
1:B:142:PHE:CE1	1:B:571:GLY:HA3	2.46	0.49
1:B:176:LEU:C	1:B:176:LEU:HD13	2.32	0.49
1:B:540:ILE:CD1	1:B:569:ILE:HB	2.38	0.49
1:A:380:LYS:C	1:A:381:ILE:HG12	2.33	0.49
1:B:310:GLU:O	1:B:311:LYS:HD2	2.12	0.49
1:A:82:LYS:HA	1:A:85:MET:CE	2.42	0.49
1:A:30:VAL:HG21	1:A:35:MET:SD	2.52	0.49
1:A:163:ILE:HB	1:A:164:PRO:HD3	1.94	0.49
1:B:375:ASP:HA	1:B:479:ARG:HH12	1.77	0.49
1:B:375:ASP:CG	1:B:376:ALA:N	2.65	0.49
1:A:386:ARG:HG2	1:A:387:ASN:N	2.28	0.49
1:A:135:LEU:HD23	1:A:136:PRO:N	2.28	0.49
1:A:22:ASN:O	1:A:23:ALA:C	2.51	0.49
1:A:561:THR:C	1:A:563:LYS:N	2.66	0.49
1:B:163:ILE:HB	1:B:164:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:CE1	1:A:571:GLY:HA3	2.47	0.49
1:A:440:ASP:O	1:A:442:GLN:N	2.45	0.49
1:B:249:MET:HE1	1:B:293:ILE:HG21	1.94	0.48
1:B:222:LYS:O	1:B:223:ASP:HB3	2.13	0.48
1:A:287:GLU:HG2	1:A:287:GLU:O	2.14	0.48
1:B:497:ASP:OD2	1:B:500:HIS:HB2	2.12	0.48
1:B:389:VAL:HB	1:B:390:PRO:HD3	1.96	0.48
1:A:488:MET:O	1:A:492:VAL:HG23	2.13	0.48
1:A:421:LEU:C	1:A:421:LEU:HD13	2.34	0.48
1:A:123:PHE:H	1:A:123:PHE:HD1	1.58	0.48
1:A:389:VAL:HB	1:A:390:PRO:HD3	1.96	0.48
1:B:30:VAL:HG21	1:B:35:MET:SD	2.53	0.48
1:A:357:GLN:HE21	1:B:325:LEU:HD23	1.78	0.48
1:B:141:ILE:HA	1:B:570:LEU:O	2.14	0.48
1:A:375:ASP:CG	1:A:376:ALA:N	2.66	0.48
1:B:368:GLN:HE21	1:B:479:ARG:HB2	1.77	0.48
1:B:403:ILE:HG23	1:B:438:ILE:HD11	1.95	0.48
1:A:367:GLU:HG2	1:A:408:LEU:HD12	1.95	0.48
1:B:436:TRP:HA	1:B:436:TRP:HE3	1.79	0.48
1:A:368:GLN:HE21	1:A:479:ARG:HB2	1.78	0.48
1:A:559:THR:HG23	1:A:567:GLU:HA	1.95	0.48
1:B:561:THR:O	1:B:563:LYS:HG3	2.13	0.48
1:B:383:ASP:O	1:B:384:HIS:HB2	2.14	0.48
1:A:369:ASP:CG	1:A:375:ASP:HB2	2.34	0.48
1:A:564:ASN:O	1:A:565:ASN:CB	2.61	0.48
1:B:171:GLU:HA	1:B:205:LYS:HG2	1.95	0.48
1:A:436:TRP:HE3	1:A:436:TRP:HA	1.79	0.48
1:B:536:GLY:HA3	1:B:537:PRO:C	2.34	0.48
1:B:344:THR:O	1:B:348:LEU:N	2.47	0.48
1:B:134:PHE:C	1:B:134:PHE:CD2	2.87	0.48
1:B:363:LEU:HD23	1:B:391:ILE:HD12	1.96	0.48
1:B:228:LEU:HD23	1:B:229:ILE:N	2.29	0.47
1:B:26:LYS:HG2	1:B:69:GLU:HB2	1.96	0.47
1:A:242:HIS:CE1	1:A:404:ARG:CZ	2.96	0.47
1:B:564:ASN:O	1:B:565:ASN:CB	2.62	0.47
1:A:403:ILE:HG23	1:A:438:ILE:HD11	1.96	0.47
1:A:367:GLU:HG3	1:A:405:ILE:CD1	2.45	0.47
1:A:344:THR:O	1:A:348:LEU:N	2.45	0.47
1:B:484:MET:O	1:B:488:MET:HG3	2.13	0.47
1:B:33:LEU:HD12	1:B:135:LEU:HD11	1.97	0.47
1:A:3:LEU:HD11	1:A:134:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:HA	1:A:205:LYS:HG2	1.95	0.47
1:A:484:MET:O	1:A:488:MET:HG3	2.14	0.47
1:B:425:VAL:HG11	1:B:435:LYS:HG2	1.96	0.47
1:B:369:ASP:CG	1:B:375:ASP:HB2	2.35	0.47
1:A:380:LYS:HB2	1:A:381:ILE:H	1.56	0.47
1:A:249:MET:HE2	1:A:352:CYS:HB3	1.94	0.47
1:A:561:THR:CG2	1:A:562:ALA:H	2.26	0.47
1:B:56:GLU:OE1	1:B:62:ARG:HG3	2.15	0.47
1:A:232:ARG:HH22	1:A:551:GLU:CD	2.17	0.47
1:B:383:ASP:OD1	1:B:413:LYS:NZ	2.47	0.47
1:A:403:ILE:HG23	1:A:438:ILE:HD13	1.96	0.47
1:B:11:ILE:HD11	1:B:37:MET:HE1	1.97	0.47
1:A:588:ILE:HD12	1:A:588:ILE:C	2.35	0.47
1:A:222:LYS:O	1:A:223:ASP:HB3	2.15	0.47
1:B:586:ARG:HG2	1:B:586:ARG:HH11	1.80	0.47
1:B:285:TRP:O	1:B:289:ARG:HD2	2.14	0.47
1:B:27:VAL:HG11	1:B:65:LEU:HD12	1.97	0.47
1:A:26:LYS:HD3	1:A:69:GLU:HB2	1.96	0.47
1:B:82:LYS:HA	1:B:85:MET:CE	2.45	0.47
1:A:152:VAL:HG11	1:A:165:ASN:HD22	1.80	0.47
1:A:263:TYR:CZ	1:A:274:LYS:HG2	2.50	0.46
1:B:76:PRO:HG2	1:B:105:GLU:O	2.15	0.46
1:A:346:LEU:HD11	1:B:335:TYR:HE2	1.81	0.46
1:B:39:SER:HB2	1:B:281:LYS:NZ	2.30	0.46
1:A:135:LEU:C	1:A:135:LEU:HD23	2.35	0.46
1:B:287:GLU:O	1:B:287:GLU:HG2	2.15	0.46
1:B:92:ASP:O	1:B:93:ASN:HB2	2.15	0.46
1:A:383:ASP:O	1:A:384:HIS:HB2	2.15	0.46
1:B:247:GLN:HG3	1:B:285:TRP:CZ2	2.49	0.46
1:A:279:ASP:HB3	1:A:281:LYS:HG2	1.98	0.46
1:A:81:VAL:O	1:A:85:MET:HG3	2.15	0.46
1:B:33:LEU:O	1:B:36:ARG:HB2	2.15	0.46
1:B:140:GLN:C	1:B:141:ILE:HD12	2.36	0.46
1:A:180:LEU:O	1:A:222:LYS:NZ	2.48	0.46
1:B:81:VAL:O	1:B:85:MET:HG3	2.16	0.46
1:A:536:GLY:HA3	1:A:537:PRO:C	2.34	0.46
1:A:425:VAL:HG11	1:A:435:LYS:HG2	1.98	0.46
1:A:7:VAL:HB	1:A:41:CYS:SG	2.56	0.46
1:B:74:ILE:HD12	1:B:80:SER:HB3	1.97	0.46
1:A:312:ARG:NH1	1:A:312:ARG:HB2	2.31	0.46
1:A:94:PRO:HG3	1:A:123:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:TYR:CE2	1:B:348:LEU:HD13	2.50	0.46
1:A:383:ASP:OD1	1:A:383:ASP:O	2.34	0.46
1:A:384:HIS:O	1:A:385:MET:SD	2.74	0.46
1:A:105:GLU:O	1:A:106:ALA:C	2.54	0.46
1:B:305:LYS:O	1:B:307:PHE:N	2.49	0.46
1:B:362:LYS:HZ2	1:B:396:LYS:HD2	1.80	0.46
1:B:388:ILE:O	1:B:392:LEU:HD13	2.16	0.46
1:A:168:ARG:HG3	1:A:168:ARG:NH1	2.29	0.46
1:A:295:VAL:O	1:A:298:GLN:HB3	2.16	0.46
1:B:588:ILE:HD12	1:B:588:ILE:C	2.36	0.46
1:A:577:THR:HG22	1:A:580:GLY:CA	2.46	0.46
1:A:440:ASP:C	1:A:442:GLN:H	2.18	0.46
1:B:232:ARG:HH22	1:B:551:GLU:CD	2.20	0.45
1:A:394:ASP:OD1	1:A:396:LYS:HB3	2.17	0.45
1:B:178:ALA:O	1:B:180:LEU:N	2.49	0.45
1:B:577:THR:HG22	1:B:580:GLY:CA	2.46	0.45
1:A:388:ILE:O	1:A:392:LEU:HD13	2.17	0.45
1:B:180:LEU:O	1:B:222:LYS:NZ	2.50	0.45
1:B:394:ASP:OD1	1:B:396:LYS:HB3	2.15	0.45
1:A:92:ASP:O	1:A:93:ASN:HB2	2.16	0.45
1:A:383:ASP:OD1	1:A:413:LYS:NZ	2.48	0.45
1:A:249:MET:SD	1:A:293:ILE:CD1	3.05	0.45
1:B:563:LYS:C	1:B:565:ASN:N	2.69	0.45
1:B:242:HIS:CE1	1:B:404:ARG:CZ	2.99	0.45
1:A:3:LEU:HD11	1:A:134:PHE:CE2	2.52	0.45
1:B:105:GLU:O	1:B:106:ALA:C	2.53	0.45
1:B:59:ASN:O	1:B:60:ARG:C	2.55	0.45
1:A:103:PHE:HB2	1:A:129:GLU:HB3	1.99	0.45
1:A:242:HIS:ND1	1:A:404:ARG:NH1	2.64	0.45
1:A:285:TRP:O	1:A:289:ARG:HD2	2.15	0.45
1:A:561:THR:O	1:A:563:LYS:HG3	2.16	0.45
1:A:232:ARG:C	1:A:232:ARG:HD3	2.36	0.45
1:B:384:HIS:HA	1:B:409:TYR:OH	2.17	0.45
1:A:573:THR:OG1	1:A:574:HIS:HD2	2.00	0.45
1:A:212:ASP:O	1:A:213:ASP:HB2	2.17	0.45
1:B:403:ILE:HG23	1:B:438:ILE:HD13	1.98	0.45
1:B:445:GLY:O	1:B:457:ILE:HG21	2.17	0.45
1:A:145:ASP:O	1:A:145:ASP:OD1	2.35	0.45
1:B:293:ILE:HD13	1:B:293:ILE:H	1.81	0.45
1:B:152:VAL:HG11	1:B:165:ASN:HD22	1.82	0.45
1:B:383:ASP:O	1:B:383:ASP:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASP:HB3	1:B:281:LYS:HG2	1.99	0.45
1:A:228:LEU:HD23	1:A:229:ILE:N	2.32	0.45
1:A:588:ILE:HG13	1:A:589:SER:N	2.31	0.45
1:B:588:ILE:HG13	1:B:589:SER:N	2.32	0.45
1:B:299:ASN:N	1:B:299:ASN:HD22	2.14	0.45
1:B:451:ASP:C	1:B:453:GLY:N	2.70	0.44
1:B:440:ASP:O	1:B:442:GLN:N	2.51	0.44
1:A:451:ASP:C	1:A:453:GLY:N	2.70	0.44
1:B:573:THR:OG1	1:B:574:HIS:HD2	2.00	0.44
1:A:380:LYS:O	1:A:381:ILE:CG2	2.58	0.44
1:A:384:HIS:HA	1:A:409:TYR:OH	2.17	0.44
1:A:563:LYS:C	1:A:565:ASN:N	2.69	0.44
1:B:7:VAL:HG13	1:B:37:MET:HE3	2.00	0.44
1:B:12:MET:O	1:B:17:LEU:HD23	2.18	0.44
1:B:312:ARG:HB2	1:B:312:ARG:NH1	2.33	0.44
1:A:375:ASP:O	1:A:378:GLY:N	2.51	0.44
1:B:561:THR:CG2	1:B:562:ALA:H	2.24	0.44
1:B:11:ILE:O	1:B:15:VAL:HB	2.18	0.44
1:A:7:VAL:HG13	1:A:37:MET:HE3	1.99	0.44
1:A:12:MET:O	1:A:17:LEU:HD23	2.18	0.44
1:A:358:GLN:O	1:A:396:LYS:HD3	2.18	0.44
1:A:368:GLN:O	1:A:372:MET:HB2	2.18	0.44
1:A:279:ASP:CG	1:A:281:LYS:HE2	2.38	0.44
1:B:367:GLU:HG3	1:B:405:ILE:CD1	2.48	0.44
1:B:343:SER:O	1:B:347:HIS:HB2	2.17	0.44
1:A:305:LYS:HB3	1:B:308:ALA:HB1	1.99	0.44
1:B:358:GLN:O	1:B:396:LYS:HD3	2.18	0.44
1:B:237:ILE:C	1:B:239:PRO:HD2	2.38	0.44
1:B:577:THR:O	1:B:578:PRO:C	2.55	0.44
1:A:305:LYS:O	1:A:307:PHE:N	2.51	0.44
1:B:103:PHE:HB2	1:B:129:GLU:HB3	2.00	0.44
1:A:445:GLY:O	1:A:457:ILE:HG21	2.17	0.44
1:A:178:ALA:O	1:A:180:LEU:N	2.51	0.44
1:A:577:THR:O	1:A:578:PRO:C	2.57	0.43
1:B:257:GLU:O	1:B:258:ASN:C	2.57	0.43
1:A:493:GLU:OE1	1:A:495:LYS:HD3	2.18	0.43
1:B:26:LYS:CD	1:B:69:GLU:HB2	2.49	0.43
1:A:11:ILE:HD11	1:A:37:MET:CE	2.48	0.43
1:A:63:GLU:HA	1:A:64:PRO:HD3	1.81	0.43
1:B:296:VAL:O	1:B:300:VAL:HG23	2.18	0.43
1:A:257:GLU:O	1:A:258:ASN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HA	1:A:570:LEU:O	2.18	0.43
1:A:59:ASN:O	1:A:60:ARG:C	2.57	0.43
1:B:212:ASP:O	1:B:213:ASP:HB2	2.18	0.43
1:A:436:TRP:O	1:A:437:ILE:C	2.56	0.43
1:A:335:TYR:CZ	1:B:301:THR:HG22	2.54	0.43
1:B:488:MET:O	1:B:492:VAL:HG23	2.19	0.43
1:A:44:MET:O	1:A:45:HIS:C	2.57	0.43
1:B:372:MET:HB2	1:B:372:MET:HE2	1.81	0.43
1:A:126:THR:HG22	1:A:127:LEU:N	2.34	0.43
1:B:305:LYS:C	1:B:307:PHE:N	2.72	0.43
1:B:304:LEU:HA	1:B:342:TYR:CE2	2.54	0.43
1:B:410:ILE:HD11	1:B:421:LEU:HD23	1.99	0.43
1:A:261:TYR:CE2	1:A:348:LEU:HD13	2.53	0.43
1:A:140:GLN:C	1:A:141:ILE:HD12	2.39	0.43
1:A:325:LEU:HD23	1:A:325:LEU:O	2.19	0.43
1:B:296:VAL:O	1:B:297:SER:C	2.55	0.43
1:B:3:LEU:HA	1:B:180:LEU:HD21	2.01	0.43
1:A:312:ARG:CB	1:A:312:ARG:HH11	2.32	0.42
1:B:305:LYS:O	1:B:308:ALA:N	2.52	0.42
1:B:561:THR:O	1:B:563:LYS:N	2.52	0.42
1:B:90:ASN:OD1	1:B:90:ASN:C	2.58	0.42
1:A:75:THR:OG1	1:A:77:THR:HG23	2.18	0.42
1:A:328:MET:C	1:A:330:LYS:N	2.72	0.42
1:A:410:ILE:HD11	1:A:421:LEU:HD23	2.01	0.42
1:A:343:SER:O	1:A:347:HIS:HB2	2.19	0.42
1:B:211:ALA:C	1:B:213:ASP:H	2.23	0.42
1:A:305:LYS:HB2	1:A:305:LYS:HE3	1.89	0.42
1:A:305:LYS:O	1:A:308:ALA:N	2.53	0.42
1:B:244:LEU:O	1:B:293:ILE:CD1	2.67	0.42
1:B:493:GLU:OE1	1:B:495:LYS:HD3	2.18	0.42
1:B:388:ILE:HG22	1:B:392:LEU:HD13	2.01	0.42
1:A:392:LEU:O	1:A:402:LYS:HE2	2.18	0.42
1:A:11:ILE:O	1:A:15:VAL:HB	2.19	0.42
1:B:75:THR:HA	1:B:76:PRO:HD3	1.86	0.42
1:A:141:ILE:HG12	1:A:552:MET:HG2	2.00	0.42
1:A:444:LEU:N	1:A:444:LEU:CD1	2.83	0.42
1:B:33:LEU:N	1:B:33:LEU:HD22	2.33	0.42
1:B:384:HIS:O	1:B:385:MET:SD	2.77	0.42
1:B:11:ILE:HD11	1:B:37:MET:CE	2.50	0.42
1:A:497:ASP:OD2	1:A:500:HIS:HB2	2.19	0.42
1:B:245:THR:HG21	1:B:553:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG11	1:A:65:LEU:HD12	2.00	0.42
1:B:383:ASP:O	1:B:384:HIS:CB	2.67	0.42
1:B:65:LEU:N	1:B:66:PRO:HD3	2.33	0.42
1:B:279:ASP:CG	1:B:281:LYS:HE2	2.40	0.42
1:B:44:MET:O	1:B:45:HIS:C	2.56	0.42
1:B:145:ASP:O	1:B:145:ASP:OD1	2.36	0.42
1:B:440:ASP:C	1:B:442:GLN:H	2.23	0.42
1:B:395:GLN:HA	1:B:395:GLN:OE1	2.20	0.42
1:A:89:GLN:CA	1:A:89:GLN:HE21	2.04	0.42
1:B:93:ASN:O	1:B:93:ASN:OD1	2.38	0.42
1:A:406:ILE:O	1:A:409:TYR:HB3	2.20	0.42
1:B:295:VAL:O	1:B:298:GLN:HB3	2.20	0.42
1:A:21:LYS:NZ	1:A:21:LYS:HB3	2.35	0.42
1:B:407:LEU:O	1:B:411:ILE:HG13	2.20	0.42
1:A:559:THR:O	1:A:563:LYS:HE3	2.20	0.41
1:B:94:PRO:HG3	1:B:123:PHE:HE2	1.84	0.41
1:B:386:ARG:O	1:B:387:ASN:C	2.58	0.41
1:B:386:ARG:C	1:B:388:ILE:N	2.73	0.41
1:A:6:ALA:HB1	1:A:179:THR:HG22	2.02	0.41
1:A:386:ARG:CG	1:A:387:ASN:N	2.83	0.41
1:A:65:LEU:N	1:A:66:PRO:HD3	2.35	0.41
1:B:312:ARG:HH11	1:B:312:ARG:CB	2.33	0.41
1:B:386:ARG:CG	1:B:387:ASN:N	2.82	0.41
1:A:370:LEU:HD13	1:A:409:TYR:HA	2.02	0.41
1:A:293:ILE:H	1:A:293:ILE:HD13	1.85	0.41
1:A:257:GLU:O	1:A:260:VAL:CG1	2.68	0.41
1:B:393:LEU:O	1:B:394:ASP:C	2.59	0.41
1:B:362:LYS:HZ1	1:B:396:LYS:HD2	1.86	0.41
1:B:561:THR:OG1	1:B:562:ALA:N	2.53	0.41
1:B:21:LYS:HB3	1:B:21:LYS:NZ	2.36	0.41
1:A:304:LEU:HA	1:A:342:TYR:CE2	2.56	0.41
1:A:436:TRP:HA	1:A:439:ASN:HD22	1.86	0.41
1:B:392:LEU:O	1:B:402:LYS:HE2	2.20	0.41
1:B:263:TYR:CZ	1:B:274:LYS:HG2	2.55	0.41
1:A:561:THR:OG1	1:A:562:ALA:N	2.53	0.41
1:B:327:GLN:N	1:B:327:GLN:CD	2.74	0.41
1:A:372:MET:HE2	1:A:372:MET:HB2	1.82	0.41
1:A:386:ARG:C	1:A:388:ILE:N	2.73	0.41
1:B:559:THR:O	1:B:563:LYS:HE3	2.21	0.41
1:B:360:VAL:O	1:B:361:ASP:C	2.58	0.41
1:A:211:ALA:C	1:A:213:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LYS:N	1:A:477:MET:HE3	2.36	0.41
1:B:163:ILE:N	1:B:164:PRO:CD	2.84	0.41
1:A:133:ALA:HB3	1:A:172:GLN:HA	2.02	0.41
1:B:274:LYS:HG3	1:B:275:GLU:N	2.36	0.41
1:B:244:LEU:CA	1:B:293:ILE:HD11	2.51	0.41
1:B:492:VAL:HG13	1:B:566:TRP:CG	2.56	0.41
1:A:4:LYS:NZ	1:A:280:GLU:HG3	2.36	0.41
1:B:126:THR:HG22	1:B:127:LEU:N	2.35	0.41
1:A:33:LEU:N	1:A:33:LEU:HD22	2.33	0.41
1:B:325:LEU:O	1:B:325:LEU:HD23	2.21	0.41
1:A:357:GLN:NE2	1:B:325:LEU:CD2	2.81	0.41
1:B:63:GLU:HA	1:B:64:PRO:HD3	1.80	0.41
1:A:296:VAL:O	1:A:297:SER:C	2.58	0.41
1:A:171:GLU:CA	1:A:205:LYS:HG2	2.51	0.41
1:A:58:ILE:HG13	1:A:83:CYS:HB3	2.03	0.41
1:B:436:TRP:O	1:B:437:ILE:C	2.59	0.41
1:B:134:PHE:HE2	1:B:136:PRO:HG3	1.85	0.41
1:B:328:MET:C	1:B:330:LYS:N	2.72	0.40
1:A:383:ASP:O	1:A:384:HIS:CB	2.68	0.40
1:B:242:HIS:CE1	1:B:404:ARG:NH1	2.89	0.40
1:A:327:GLN:N	1:A:327:GLN:CD	2.75	0.40
1:B:179:THR:O	1:B:179:THR:HG22	2.21	0.40
1:B:359:HIS:HB3	1:B:396:LYS:HD3	2.03	0.40
1:A:93:ASN:OD1	1:A:93:ASN:O	2.38	0.40
1:A:484:MET:SD	1:A:488:MET:HE2	2.61	0.40
1:B:436:TRP:HA	1:B:439:ASN:HD22	1.86	0.40
1:B:372:MET:C	1:B:374:THR:H	2.24	0.40
1:A:367:GLU:HG3	1:A:405:ILE:HD11	2.03	0.40
1:B:492:VAL:C	1:B:494:ASP:H	2.24	0.40
1:A:305:LYS:C	1:A:307:PHE:N	2.74	0.40
1:A:26:LYS:HG2	1:A:69:GLU:HB2	2.02	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	535/591 (90%)	424 (79%)	85 (16%)	26 (5%)	3 22
1	B	535/591 (90%)	423 (79%)	83 (16%)	29 (5%)	2 19
All	All	1070/1182 (90%)	847 (79%)	168 (16%)	55 (5%)	2 20

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ALA
1	A	93	ASN
1	A	220	PRO
1	A	223	ASP
1	A	376	ALA
1	A	379	GLU
1	A	381	ILE
1	A	385	MET
1	A	387	ASN
1	A	450	GLN
1	B	23	ALA
1	B	93	ASN
1	B	220	PRO
1	B	223	ASP
1	B	376	ALA
1	B	379	GLU
1	B	381	ILE
1	B	385	MET
1	B	387	ASN
1	B	450	GLN
1	A	22	ASN
1	A	222	LYS
1	A	296	VAL
1	A	359	HIS
1	A	384	HIS
1	A	452	GLY
1	B	22	ASN
1	B	222	LYS
1	B	296	VAL
1	B	359	HIS
1	B	384	HIS
1	B	452	GLY
1	A	96	TYR

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Mol	Chain	Res	Type
1	A	219	GLY
1	B	219	GLY
1	B	386	ARG
1	A	179	THR
1	A	212	ASP
1	A	386	ARG
1	B	96	TYR
1	B	179	THR
1	B	212	ASP
1	B	562	ALA
1	A	394	ASP
1	A	562	ALA
1	B	32	GLN
1	B	298	GLN
1	B	306	GLN
1	A	388	ILE
1	B	394	ASP
1	B	388	ILE
1	A	213	ASP
1	A	91	PRO
1	B	91	PRO
1	B	213	ASP

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	485/523 (93%)	445 (92%)	40 (8%)	14	50
1	B	485/523 (93%)	443 (91%)	42 (9%)	13	45
All	All	970/1046 (93%)	888 (92%)	82 (8%)	13	47

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR

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Mol	Chain	Res	Type
1	A	25	TRP
1	A	42	CYS
1	A	60	ARG
1	A	62	ARG
1	A	84	LEU
1	A	89	GLN
1	A	111	LEU
1	A	115	LEU
1	A	129	GLU
1	A	140	GLN
1	A	153	TYR
1	A	193	ASP
1	A	206	LEU
1	A	220	PRO
1	A	228	LEU
1	A	232	ARG
1	A	241	LEU
1	A	246	PHE
1	A	289	ARG
1	A	293	ILE
1	A	330	LYS
1	A	332	MET
1	A	340	SER
1	A	345	HIS
1	A	354	LYS
1	A	358	GLN
1	A	359	HIS
1	A	375	ASP
1	A	380	LYS
1	A	382	ARG
1	A	384	HIS
1	A	395	GLN
1	A	436	TRP
1	A	497	ASP
1	A	504	LEU
1	A	544	VAL
1	A	577	THR
1	A	582	LEU
1	A	588	ILE
1	B	5	THR
1	B	25	TRP
1	B	42	CYS

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Mol	Chain	Res	Type
1	B	60	ARG
1	B	62	ARG
1	B	84	LEU
1	B	89	GLN
1	B	111	LEU
1	B	115	LEU
1	B	129	GLU
1	B	131	ASN
1	B	135	LEU
1	B	140	GLN
1	B	153	TYR
1	B	193	ASP
1	B	206	LEU
1	B	220	PRO
1	B	228	LEU
1	B	232	ARG
1	B	241	LEU
1	B	246	PHE
1	B	289	ARG
1	B	293	ILE
1	B	309	ASP
1	B	330	LYS
1	B	332	MET
1	B	345	HIS
1	B	354	LYS
1	B	358	GLN
1	B	359	HIS
1	B	375	ASP
1	B	380	LYS
1	B	382	ARG
1	B	384	HIS
1	B	395	GLN
1	B	436	TRP
1	B	497	ASP
1	B	504	LEU
1	B	544	VAL
1	B	577	THR
1	B	582	LEU
1	B	588	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	93	ASN
1	A	95	GLN
1	A	140	GLN
1	A	165	ASN
1	A	258	ASN
1	A	299	ASN
1	A	347	HIS
1	A	357	GLN
1	A	359	HIS
1	A	368	GLN
1	A	387	ASN
1	A	439	ASN
1	A	459	GLN
1	A	462	HIS
1	A	464	HIS
1	A	465	ASN
1	A	560	GLN
1	A	565	ASN
1	A	574	HIS
1	B	89	GLN
1	B	93	ASN
1	B	95	GLN
1	B	165	ASN
1	B	258	ASN
1	B	299	ASN
1	B	336	GLN
1	B	347	HIS
1	B	357	GLN
1	B	359	HIS
1	B	368	GLN
1	B	387	ASN
1	B	439	ASN
1	B	462	HIS
1	B	464	HIS
1	B	465	ASN
1	B	560	GLN
1	B	574	HIS

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	543/591 (91%)	-0.10	22 (4%)	41	27	30, 63, 104, 131	1 (0%)
1	B	543/591 (91%)	-0.11	29 (5%)	30	17	28, 65, 105, 131	1 (0%)
All	All	1086/1182 (91%)	-0.11	51 (4%)	35	22	28, 64, 105, 131	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	GLY	7.4
1	B	327	GLN	5.8
1	A	507	GLY	5.4
1	A	506	GLY	4.9
1	B	472	ASP	4.3
1	A	452	GLY	4.2
1	A	117	LYS	3.8
1	A	453	GLY	3.7
1	B	312	ARG	3.7
1	A	312	ARG	3.4
1	A	377	ASP	3.3
1	A	89	GLN	3.3
1	B	220	PRO	3.2
1	B	273	GLU	3.1
1	A	79	GLU	3.1
1	A	454	ARG	3.1
1	A	472	ASP	2.9
1	B	89	GLN	2.9
1	A	451	ASP	2.9
1	A	22	ASN	2.8
1	B	45	HIS	2.7
1	B	507	GLY	2.7
1	B	109	GLU	2.7
1	A	508	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	118	SER	2.6
1	B	464	HIS	2.6
1	A	109	GLU	2.6
1	B	564	ASN	2.5
1	B	223	ASP	2.5
1	B	456	LYS	2.5
1	A	160	GLN	2.5
1	B	375	ASP	2.5
1	B	264	VAL	2.4
1	B	454	ARG	2.4
1	A	384	HIS	2.4
1	B	377	ASP	2.3
1	A	455	ARG	2.3
1	B	451	ASP	2.3
1	B	110	GLU	2.2
1	A	45	HIS	2.2
1	B	384	HIS	2.2
1	B	217	GLY	2.2
1	B	160	GLN	2.2
1	B	471	ALA	2.1
1	B	455	ARG	2.1
1	B	25	TRP	2.0
1	B	452	GLY	2.0
1	A	273	GLU	2.0
1	B	396	LYS	2.0
1	B	565	ASN	2.0
1	A	591	PRO	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.