Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 02:02 AM EST

PDB ID	:	1NYQ
Title	:	Structure of Staphylococcus aureus threonyl-tRNA synthetase complexed with an analogue of threonyl adenylate
Authors	:	Torres-Larios, A.; Sankaranarayanan, R.; Rees, B.; Dock-Bregeon, A.C.; Moras, D.
Deposited on	:	2003-02-13
Resolution	:	3.20 Å(reported)

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

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

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

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

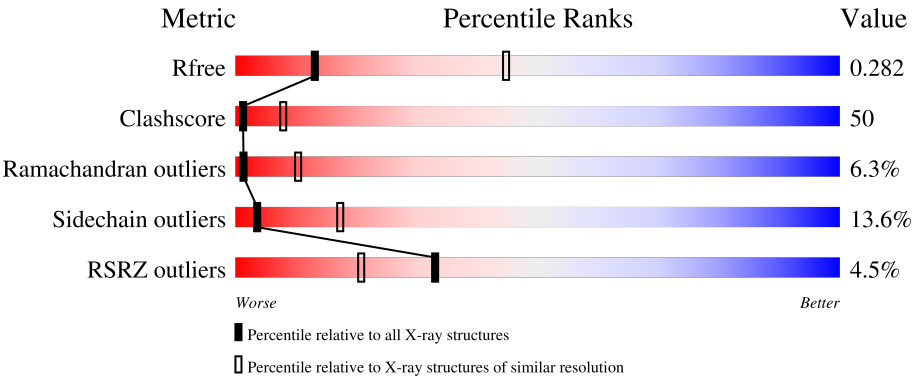
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	645	3% 35% 51% 13%
1	B	645	6% 34% 51% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10663 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.

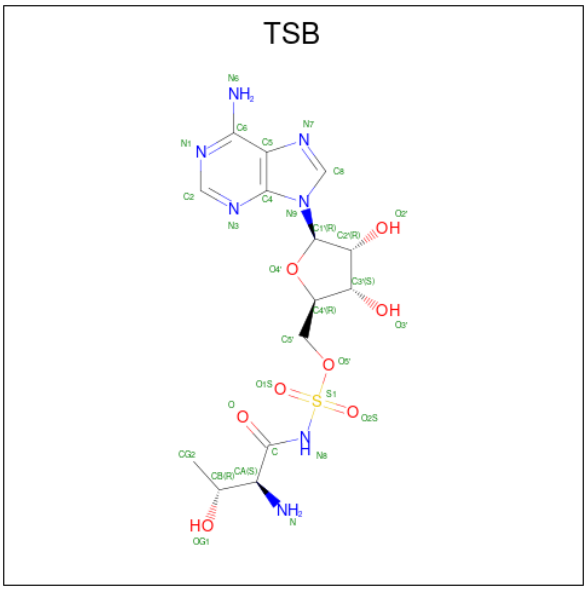
- Molecule 1 is a protein called threonyl-tRNA synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5216	3296	894	1003	23			
1	B	645	Total	C	N	O	S	0	0	0
			5242	3311	898	1009	24			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (three-letter code: TSB) (formula: $C_{14}H_{21}N_7O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	B	1	Total	C	N	O	S	0	0
			30	14	7	8	1		

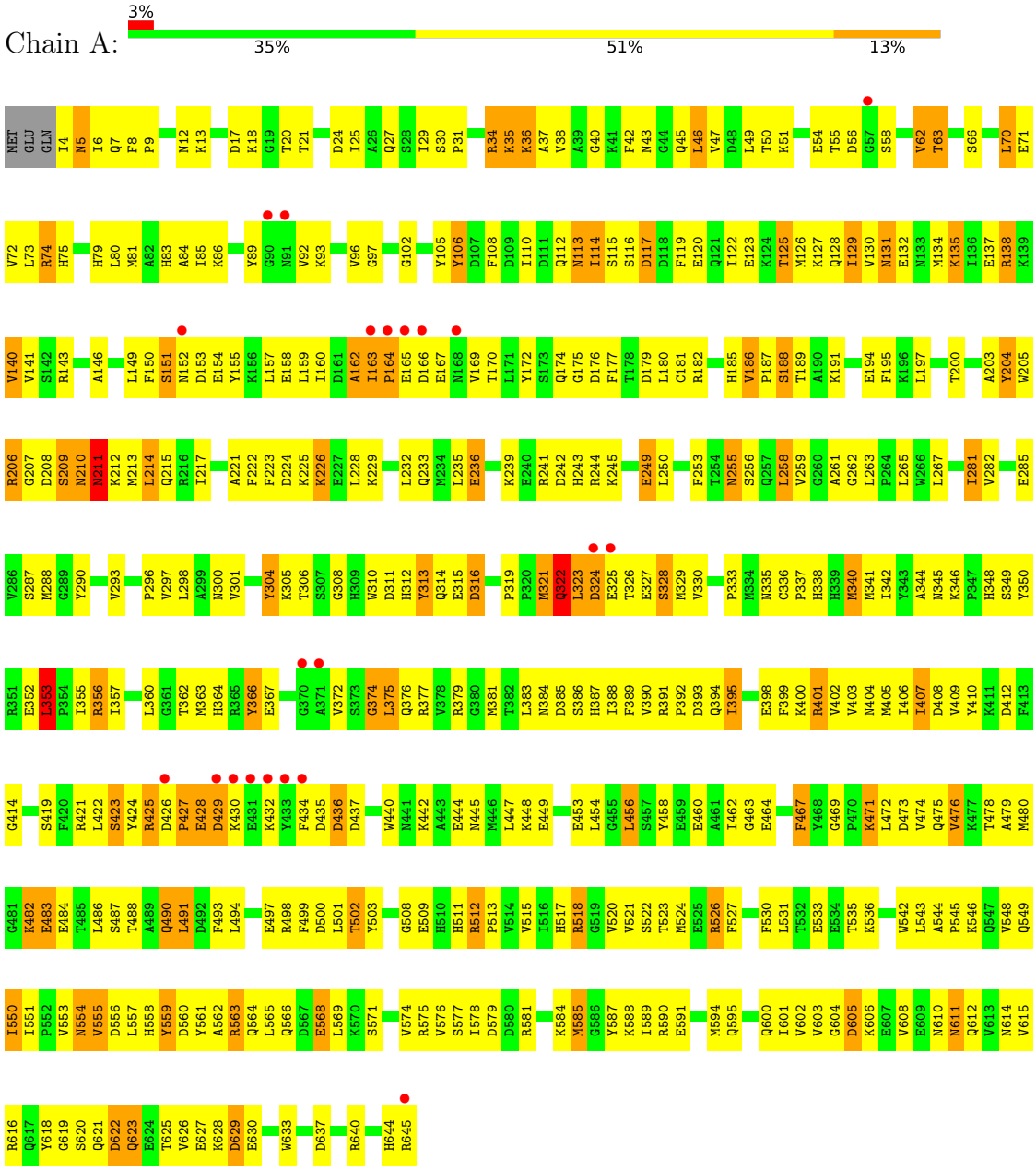
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	68	Total	O	0	0
			68	68		

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.

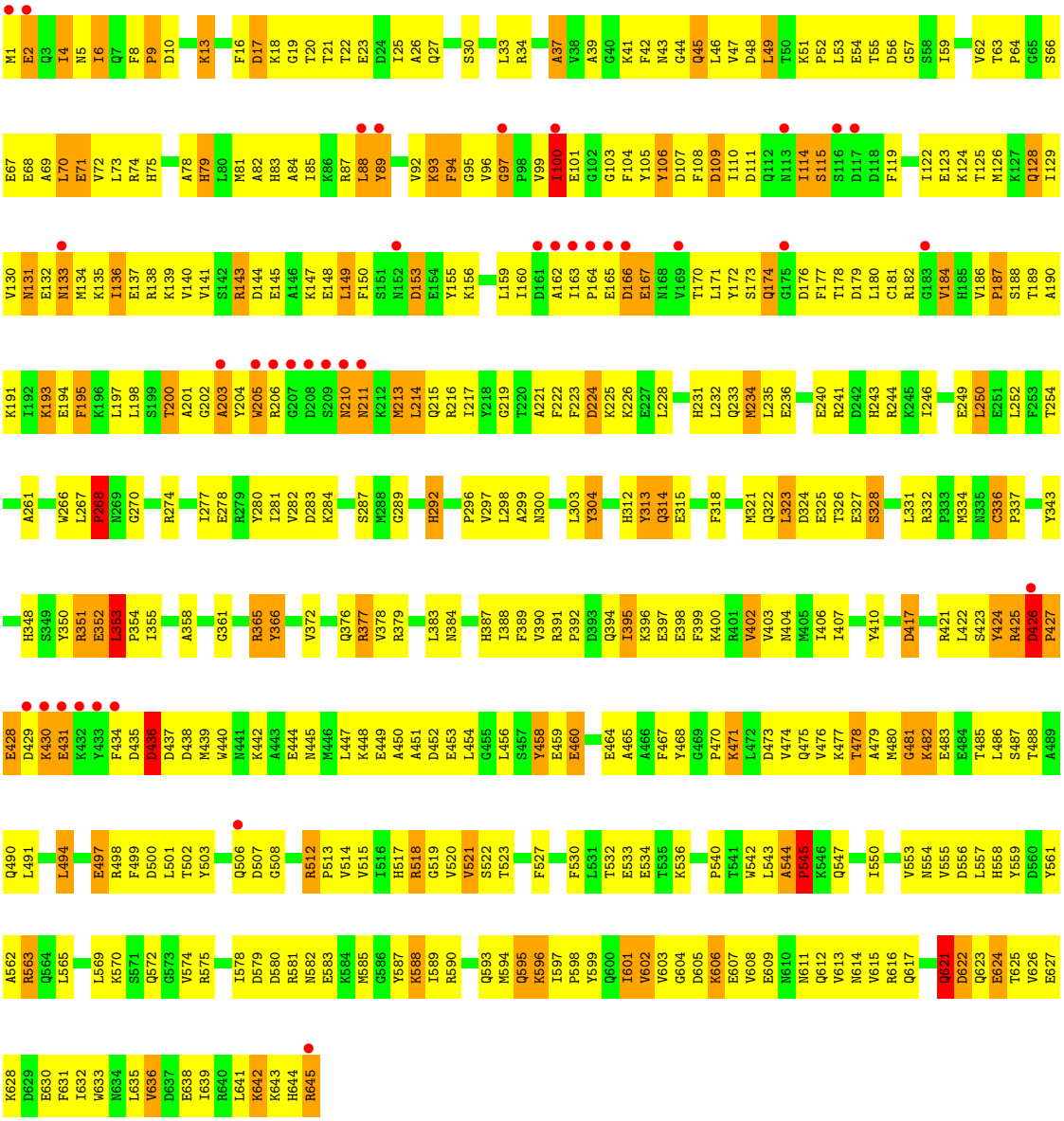
• Molecule 1: threonyl-tRNA synthetase 1



• Molecule 1: threonyl-tRNA synthetase 1

Chain B:


6%
34%
51%
14%


M1 E2 Q3 I4 N5 I6 Q7 F8 P9 D10 K13 F16 D17 K18 G19 T20 T21 T22 E23 D24 I25 A26 Q27 S30 L33 R34 A37 V38 A39 G40 K41 F42 N43 G44 Q45 L46 V47 D48 L49 T50 K51 P52 L53 E54 T55 D56 G57 S58 I59 V62 T63 P64 G65 S66
E67 E68 A69 L70 E71 V72 L73 R74 H75 A78 H79 L80 M81 A82 H83 A84 I85 K86 R87 L88 Y89 V92 K93 F94 G95 V96 G97 P98 V99 I100 E101 G102 G103 F104 Y105 Y106 D107 F108 D109 I110 D111 Q112 N113 I114 S115 S116 D117 D118 F119 I122 E123 K124 T125 M126 K127 Q128 I129
V130 N131 E132 N133 M134 K135 I136 E137 R138 K139 V140 V141 S142 R143 D144 E145 A146 K147 E148 L149 F150 S151 N152 D153 E154 Y155 K156 L159 I160 D161 A162 I163 P164 E165 D166 E167 N168 V169 T170 L171 Y172 S173 Q174 G175 D176 F177 T178 D179 L180 C181 R182 G183 V184 H185 V186 P187 S188 T189 A190
K191 I192 K193 E194 F195 K196 L197 L198 S199 T200 A201 G202 A203 Y204 W205 R206 G207 D208 S209 N210 N211 K212 M213 L214 Q215 R216 I217 Y218 G219 T220 A221 F222 F223 D224 K225 K226 E227 L228 H231 L232 Q233 M234 L235 E236 E240 R241 D242 H243 R244 K245 I246 E249 L250 E251 L252 F253 T254
A261 W266 L267 P268 N269 G270 R274 I277 E278 R279 Y280 I281 V282 D283 K284 S287 M288 G289 H292 P296 V297 L298 A299 N300 L303 Y304 H312 Y313 Q314 E315 F318 M321 Q322 L323 D324 E325 T326 E327 S328 L331 R332 P333 M334 N335 C336 P337 Y343
H348 S349 Y350 R351 E352 L353 P354 I355 A358 G361 R365 Y366 V372 Q376 R377 V378 R379 L383 N384 H387 I388 F389 V390 R391 P392 D393 Q394 I395 K396 E397 E398 F399 K400 R401 V402 V403 N404 M405 I406 I407 Y410 D417 R421 L422 S423 Y424 R425 D426 P427
E428 D429 K430 E431 K432 Y433 F434 D435 D436 D437 D438 M439 W440 N441 K442 A443 E444 N445 M446 L447 K448 E449 A450 A451 D452 E453 L454 G455 L456 S457 Y458 E459 E460 E464 A465 A466 F467 Y468 G469 P470 K471 L472 D473 V474 Q475 V476 K477 T478 A479 M480 G481 K482 E483 E484 T485 L486 S487 T488 A489
Q490 L491 L494 E497 R498 F499 D500 L501 T502 Y503 Q506 D507 G508 R512 P513 V514 V515 I516 H517 R518 G519 V520 V521 S522 T523 F527 F530 L531 T532 E533 E534 T535 K536 P540 T541 W542 L543 A544 P545 K546 Q547 I550 V553 N554 V555 D556 L557 H558 Y559 D560 Y561
A562 R563 Q564 L565 L569 K570 S571 Q572 G573 V574 R575 I578 D579 D580 R581 N582 E583 K584 M585 G586 Y587 K588 I589 R590 Q593 M594 Q595 K596 I597 P598 Y599 Q600 I601 V602 V603 G604 D605 K606 E607 V608 E609 M610 N611 Q612 V613 N614 V615 R616 Q617 Q621 D622 Q623 E624 T625 V626 E627
K628 D629 E630 F631 I632 W633 N634 L635 V636 D637 E638 I639 R640 L641 K642 K643 H644 R645

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.28Å 122.73Å 149.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 19.89 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-3.20) 95.1 (19.89-3.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 3.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.285 0.202 , 0.282	Depositor DCC
R_{free} test set	3182 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10663	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TSB, ZN

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	0.61	0/5325	0.83	4/7182 (0.1%)
1	B	0.56	0/5351	0.78	5/7216 (0.1%)
All	All	0.59	0/10676	0.81	9/14398 (0.1%)

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	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	GLY	N-CA-C	6.84	130.20	113.10
1	A	353	LEU	C-N-CA	-6.16	96.14	122.00
1	B	353	LEU	N-CA-C	5.77	126.59	111.00
1	B	519	GLY	N-CA-C	-5.61	99.07	113.10
1	A	353	LEU	N-CA-C	5.44	125.68	111.00
1	B	377	ARG	N-CA-C	-5.41	96.39	111.00
1	A	322	GLN	N-CA-C	5.37	125.51	111.00
1	B	424	TYR	N-CA-C	5.22	125.09	111.00
1	A	360	LEU	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	TYR	Sidechain
1	A	304	TYR	Sidechain
1	A	350	TYR	Sidechain
1	B	304	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	5216	0	5105	486	0
1	B	5242	0	5131	563	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	20	3	0
3	B	30	0	20	3	0
4	A	75	0	0	19	0
4	B	68	0	0	21	0
All	All	10663	0	10276	1035	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 50.

All (1035) 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:593:GLN:NE2	1:B:616:ARG:HH21	1.41	1.18
1:B:395:ILE:HD11	1:B:514:VAL:HG21	1.28	1.15
1:B:478:THR:HG22	1:B:479:ALA:H	1.08	1.13
1:A:426:ASP:HB3	1:A:427:PRO:HD2	1.31	1.10
1:B:74:ARG:HG2	1:B:221:ALA:HB3	1.28	1.08
1:B:135:LYS:HG2	1:B:136:ILE:H	1.19	1.08
1:B:322:GLN:HA	1:B:328:SER:HA	1.34	1.05
1:A:113:ASN:HA	1:A:215:GLN:HE22	1.25	1.01
1:B:593:GLN:HE21	1:B:616:ARG:NH2	1.58	1.00
1:B:27:GLN:NE2	1:B:34:ARG:HH11	1.59	1.00
1:A:20:THR:HG23	1:A:24:ASP:HB2	1.46	0.96
1:A:482:LYS:HZ2	1:A:483:GLU:H	1.08	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:HD22	1:A:521:VAL:H	0.97	0.95
1:B:580:ASP:HB3	4:B:2024:HOH:O	1.66	0.95
1:B:554:ASN:HB3	1:B:557:LEU:HB3	1.48	0.94
1:B:43:ASN:HD21	1:B:57:GLY:HA3	1.34	0.93
1:B:170:THR:HG23	1:B:182:ARG:NH1	1.85	0.92
1:B:303:LEU:HD21	1:B:337:PRO:HB2	1.50	0.92
1:A:554:ASN:ND2	1:A:556:ASP:H	1.69	0.91
1:B:27:GLN:HE22	1:B:34:ARG:HH11	1.16	0.91
1:A:18:LYS:HE2	1:A:54:GLU:HG3	1.50	0.90
1:B:601:ILE:HD11	1:B:615:VAL:HG12	1.54	0.90
1:B:170:THR:HG23	1:B:182:ARG:HH11	1.37	0.89
1:B:593:GLN:HE21	1:B:616:ARG:HH21	0.94	0.89
1:A:531:LEU:O	1:A:535:THR:HG22	1.69	0.89
1:B:4:ILE:HG23	1:B:5:ASN:N	1.88	0.89
1:A:74:ARG:NH2	1:A:102:GLY:HA2	1.87	0.88
1:A:384:ASN:ND2	1:A:521:VAL:H	1.71	0.88
1:B:4:ILE:HG12	1:B:5:ASN:H	1.35	0.88
1:A:478:THR:HG22	1:A:480:MET:H	1.37	0.88
1:A:482:LYS:HZ2	1:A:483:GLU:N	1.71	0.88
1:A:550:ILE:HD13	1:A:565:LEU:HD23	1.56	0.88
1:B:550:ILE:HG23	1:B:601:ILE:HG22	1.55	0.87
1:B:471:LYS:HG3	1:B:473:ASP:OD1	1.75	0.87
1:A:478:THR:HG21	1:A:480:MET:HG2	1.56	0.87
1:B:478:THR:HG22	1:B:479:ALA:N	1.90	0.86
1:A:256:SER:HB3	1:A:259:VAL:HG23	1.55	0.86
1:B:4:ILE:HD11	1:B:55:THR:O	1.74	0.86
1:A:554:ASN:C	1:A:554:ASN:HD22	1.78	0.85
1:B:497:GLU:HA	1:B:512:ARG:HE	1.39	0.85
1:B:163:ILE:N	1:B:164:PRO:HD3	1.92	0.85
1:A:312:HIS:NE2	1:A:429:ASP:HB2	1.93	0.83
1:B:6:ILE:O	1:B:13:LYS:HB2	1.79	0.83
1:A:406:ILE:HD13	1:A:487:SER:HB3	1.60	0.83
1:B:85:ILE:HG13	1:B:108:PHE:CZ	2.14	0.83
1:B:123:GLU:HB2	1:B:197:LEU:HD12	1.60	0.83
1:A:614:ASN:HD21	1:A:623:GLN:HG3	1.44	0.82
1:B:593:GLN:NE2	1:B:616:ARG:NH2	2.18	0.82
1:B:471:LYS:CB	1:B:490:GLN:HG2	2.09	0.82
1:B:43:ASN:ND2	1:B:57:GLY:HA3	1.94	0.82
1:B:494:LEU:HD11	4:B:2005:HOH:O	1.78	0.82
1:A:204:TYR:HE1	1:A:207:GLY:HA2	1.46	0.81
1:A:440:TRP:O	1:A:444:GLU:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HG2	1:B:180:LEU:HD12	1.62	0.81
1:B:430:LYS:HD2	1:B:436:ASP:OD2	1.80	0.81
1:A:566:GLN:HE21	1:A:577:SER:HA	1.46	0.81
1:B:521:VAL:HG22	1:B:527:PHE:CE1	2.15	0.81
1:A:616:ARG:HH21	1:A:623:GLN:HE22	1.28	0.81
1:A:553:VAL:HB	1:A:558:HIS:CE1	2.16	0.81
1:A:304:TYR:HE1	1:A:337:PRO:HG3	1.44	0.80
1:A:85:ILE:HG13	1:A:108:PHE:CE2	2.17	0.80
1:A:518:ARG:O	1:A:518:ARG:HD3	1.81	0.80
1:A:553:VAL:HB	1:A:558:HIS:ND1	1.97	0.80
1:A:482:LYS:NZ	1:A:483:GLU:H	1.79	0.80
1:A:544:ALA:O	1:A:575:ARG:NH1	2.15	0.80
1:B:563:ARG:O	1:B:563:ARG:HD3	1.81	0.79
1:B:353:LEU:HD13	1:B:390:VAL:HA	1.63	0.79
1:B:27:GLN:NE2	1:B:34:ARG:HD3	1.96	0.79
1:B:27:GLN:HE22	1:B:34:ARG:NH1	1.79	0.79
1:B:48:ASP:HB2	1:B:138:ARG:NH1	1.97	0.79
1:B:471:LYS:HB2	1:B:490:GLN:HG2	1.64	0.79
1:A:321:MET:O	1:A:322:GLN:HB2	1.79	0.79
1:B:421:ARG:HH21	1:B:464:GLU:HB3	1.45	0.79
1:A:445:ASN:O	1:A:449:GLU:HG3	1.83	0.79
1:B:160:ILE:HD11	1:B:180:LEU:CD1	2.13	0.79
1:A:426:ASP:HB3	1:A:427:PRO:CD	2.13	0.78
1:B:140:VAL:HA	1:B:170:THR:HG22	1.64	0.78
1:B:46:LEU:O	1:B:184:VAL:HG11	1.84	0.78
1:B:615:VAL:HG23	1:B:623:GLN:HB3	1.63	0.78
1:A:140:VAL:HG13	1:A:170:THR:HG22	1.63	0.78
1:B:92:VAL:HB	1:B:109:ASP:HB2	1.66	0.78
1:A:612:GLN:NE2	1:A:625:THR:HG21	1.98	0.77
1:B:399:PHE:O	1:B:403:VAL:HG23	1.84	0.77
1:A:400:LYS:HG2	1:A:454:LEU:HD13	1.66	0.77
1:A:204:TYR:CD2	1:A:209:SER:HA	2.20	0.77
1:B:395:ILE:CD1	1:B:514:VAL:HG21	2.13	0.77
1:B:421:ARG:NH2	1:B:464:GLU:HB3	1.99	0.77
1:B:395:ILE:CG2	1:B:491:LEU:HD11	2.14	0.76
1:B:627:GLU:HG3	1:B:630:GLU:H	1.50	0.76
1:A:163:ILE:N	1:A:164:PRO:HD3	1.99	0.76
1:A:113:ASN:HA	1:A:215:GLN:NE2	2.00	0.76
1:B:135:LYS:HG2	1:B:136:ILE:N	1.97	0.76
1:B:353:LEU:CD1	1:B:390:VAL:HA	2.15	0.76
1:B:454:LEU:HB3	1:B:456:LEU:HD13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:CE1	4:A:1003:HOH:O	2.38	0.76
1:A:604:GLY:O	1:A:608:VAL:HG23	1.86	0.76
1:B:490:GLN:HB2	1:B:517:HIS:HB2	1.68	0.76
1:A:618:TYR:O	1:A:620:SER:N	2.18	0.75
1:A:616:ARG:HH21	1:A:623:GLN:NE2	1.84	0.75
1:B:43:ASN:HD21	1:B:57:GLY:CA	1.98	0.75
1:B:323:LEU:HD12	1:B:324:ASP:H	1.52	0.75
1:B:521:VAL:HG22	1:B:527:PHE:CZ	2.21	0.75
1:A:554:ASN:HD22	1:A:556:ASP:H	1.33	0.75
1:B:478:THR:CG2	1:B:479:ALA:H	1.92	0.75
1:A:113:ASN:CA	1:A:215:GLN:HE22	1.99	0.74
1:B:223:PHE:O	1:B:224:ASP:HB3	1.88	0.74
1:B:18:LYS:HE3	1:B:54:GLU:OE1	1.87	0.73
1:B:143:ARG:HG2	1:B:167:GLU:OE2	1.85	0.73
1:B:353:LEU:HD13	1:B:353:LEU:O	1.88	0.73
1:B:477:LYS:HG3	1:B:483:GLU:HG2	1.70	0.73
1:A:20:THR:HG23	1:A:24:ASP:CB	2.19	0.73
1:B:4:ILE:HG22	1:B:16:PHE:H	1.54	0.73
1:B:384:ASN:HD22	1:B:521:VAL:H	1.36	0.73
1:A:589:ILE:HG23	1:A:600:GLN:HE22	1.54	0.72
1:B:312:HIS:CE1	1:B:429:ASP:HB2	2.23	0.72
1:A:262:GLY:O	1:A:263:LEU:HD23	1.90	0.72
1:A:128:GLN:HA	1:A:131:ASN:ND2	2.04	0.71
1:B:110:ILE:HB	1:B:215:GLN:HG2	1.70	0.71
1:A:256:SER:HB3	1:A:259:VAL:CG2	2.20	0.71
1:B:540:PRO:HG2	1:B:543:LEU:HD12	1.72	0.71
1:B:477:LYS:HE3	1:B:483:GLU:OE2	1.89	0.71
1:A:478:THR:CG2	1:A:480:MET:HG2	2.19	0.71
1:B:84:ALA:HB2	1:B:126:MET:HG2	1.72	0.71
1:A:591:GLU:O	1:A:595:GLN:HG3	1.91	0.71
1:A:5:ASN:O	1:A:56:ASP:HB2	1.90	0.70
1:B:85:ILE:HD11	1:B:122:ILE:HD13	1.73	0.70
1:B:428:GLU:HG2	1:B:440:TRP:HE1	1.56	0.70
1:B:174:GLN:HG3	1:B:189:THR:HG21	1.74	0.70
1:B:22:THR:HB	1:B:49:LEU:HD23	1.73	0.70
1:B:261:ALA:HB3	1:B:379:ARG:NH2	2.07	0.70
1:A:601:ILE:HD12	1:A:615:VAL:HG22	1.74	0.70
1:B:563:ARG:HA	1:B:578:ILE:HD11	1.74	0.70
1:A:89:TYR:HB2	1:A:92:VAL:CG2	2.22	0.70
1:A:114:ILE:HD11	1:A:215:GLN:CB	2.21	0.69
1:B:141:VAL:CG1	1:B:145:GLU:HB3	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:HIS:CD2	1:B:177:PHE:HB2	2.27	0.69
1:B:231:HIS:O	1:B:232:LEU:HD23	1.92	0.69
1:A:301:VAL:HG23	1:A:328:SER:O	1.91	0.69
1:B:431:GLU:O	1:B:431:GLU:HG2	1.92	0.69
1:A:424:TYR:OH	1:A:448:LYS:HE3	1.92	0.69
1:A:589:ILE:HG23	1:A:600:GLN:NE2	2.07	0.69
1:A:478:THR:HG22	1:A:479:ALA:N	2.05	0.69
1:A:114:ILE:HD11	1:A:215:GLN:HB2	1.74	0.69
1:A:384:ASN:HD22	1:A:521:VAL:N	1.82	0.69
1:A:18:LYS:CE	1:A:54:GLU:HG3	2.23	0.68
1:A:449:GLU:O	1:A:453:GLU:HG3	1.93	0.68
1:B:156:LYS:CG	1:B:180:LEU:HD12	2.22	0.68
1:A:298:LEU:HD23	1:B:331:LEU:HD11	1.75	0.68
1:B:4:ILE:CG2	1:B:16:PHE:H	2.05	0.68
1:B:490:GLN:N	1:B:517:HIS:O	2.22	0.68
1:A:488:THR:O	1:A:518:ARG:HA	1.94	0.68
1:B:110:ILE:HB	1:B:215:GLN:HE21	1.59	0.68
1:B:274:ARG:O	1:B:278:GLU:HG3	1.93	0.68
1:A:616:ARG:NH2	1:A:623:GLN:HE22	1.90	0.68
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.59	0.68
1:B:160:ILE:HD11	1:B:180:LEU:HD11	1.73	0.68
1:B:518:ARG:O	1:B:518:ARG:HD3	1.93	0.68
1:A:322:GLN:OE1	1:A:323:LEU:HD12	1.94	0.68
1:A:410:TYR:OH	1:A:486:LEU:HD23	1.94	0.68
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.58	0.67
1:B:353:LEU:HD12	1:B:391:ARG:N	2.09	0.67
1:A:185:HIS:NE2	4:A:1003:HOH:O	2.27	0.67
1:A:8:PHE:CD2	1:A:9:PRO:HD2	2.29	0.67
1:B:74:ARG:HD2	1:B:103:GLY:HA2	1.77	0.67
1:B:494:LEU:CD2	1:B:498:ARG:HD2	2.25	0.67
1:A:406:ILE:HD13	1:A:487:SER:CB	2.24	0.67
1:A:526:ARG:HH11	1:A:526:ARG:HB2	1.60	0.67
1:A:473:ASP:HB3	1:A:475:GLN:NE2	2.10	0.66
1:B:612:GLN:HG2	1:B:627:GLU:HA	1.78	0.66
1:A:174:GLN:HE22	1:A:189:THR:HG21	1.60	0.66
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.59	0.66
1:B:214:LEU:HD13	1:B:214:LEU:N	2.10	0.66
1:A:319:PRO:HG2	1:B:321:MET:HB2	1.77	0.66
1:A:8:PHE:CE2	1:A:29:ILE:HD11	2.30	0.66
1:A:113:ASN:O	1:A:114:ILE:HG23	1.96	0.66
1:B:488:THR:O	1:B:518:ARG:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:HG2	1:B:440:TRP:NE1	2.10	0.66
1:B:476:VAL:HG21	1:B:530:PHE:CZ	2.30	0.66
1:A:204:TYR:CE2	1:A:209:SER:HA	2.30	0.65
1:B:48:ASP:HB2	1:B:138:ARG:HH11	1.57	0.65
1:A:304:TYR:CE1	1:A:337:PRO:HG3	2.29	0.65
1:B:4:ILE:HG21	1:B:16:PHE:O	1.97	0.65
1:B:303:LEU:CD2	1:B:337:PRO:HB2	2.24	0.65
1:A:80:LEU:HG	1:A:126:MET:HB2	1.77	0.65
1:A:75:HIS:NE2	4:A:1003:HOH:O	2.30	0.65
1:A:323:LEU:HD13	1:A:323:LEU:O	1.95	0.65
1:B:75:HIS:CE1	1:B:181:CYS:SG	2.90	0.65
1:B:428:GLU:OE1	1:B:435:ASP:HA	1.97	0.65
1:B:497:GLU:HA	1:B:512:ARG:NE	2.10	0.65
1:A:36:LYS:HB2	1:A:36:LYS:NZ	2.12	0.65
1:A:323:LEU:HG	1:B:366:TYR:OH	1.96	0.65
1:A:454:LEU:HB3	1:A:456:LEU:CD1	2.27	0.65
1:B:579:ASP:OD2	1:B:581:ARG:NH2	2.29	0.65
1:A:146:ALA:O	1:A:149:LEU:HB3	1.96	0.65
1:A:281:ILE:CG2	1:A:282:VAL:N	2.60	0.65
1:B:160:ILE:HD11	1:B:180:LEU:HD13	1.78	0.65
1:A:8:PHE:CB	1:A:9:PRO:HD2	2.27	0.64
1:A:312:HIS:CE1	1:A:429:ASP:HB2	2.33	0.64
1:A:353:LEU:O	1:A:355:ILE:N	2.30	0.64
1:B:75:HIS:CE1	1:B:181:CYS:HG	2.15	0.64
1:A:403:VAL:HG12	1:A:407:ILE:CD1	2.28	0.64
1:A:403:VAL:HG12	1:A:407:ILE:HD12	1.80	0.64
1:A:554:ASN:ND2	1:A:554:ASN:C	2.51	0.64
1:B:89:TYR:OH	1:B:114:ILE:HG22	1.97	0.64
1:A:170:THR:OG1	1:A:182:ARG:HG2	1.97	0.64
1:A:305:LYS:HD3	1:A:310:TRP:CG	2.33	0.64
1:A:621:GLN:HG2	1:A:622:ASP:N	2.13	0.64
1:B:406:ILE:HD13	1:B:487:SER:HB2	1.78	0.64
1:A:323:LEU:HD11	1:A:326:THR:HG21	1.79	0.64
1:B:376:GLN:NE2	4:B:2055:HOH:O	2.31	0.64
1:B:156:LYS:CB	1:B:180:LEU:HD12	2.28	0.64
1:B:392:PRO:HA	1:B:395:ILE:HG13	1.79	0.63
1:B:287:SER:C	1:B:289:GLY:H	1.99	0.63
1:A:478:THR:CG2	1:A:479:ALA:N	2.62	0.63
1:B:429:ASP:N	4:B:2005:HOH:O	2.32	0.63
1:B:604:GLY:O	1:B:608:VAL:HG23	1.98	0.63
1:A:194:GLU:HG3	1:A:225:LYS:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:O	1:A:353:LEU:HD13	1.99	0.63
1:A:517:HIS:HB3	3:A:1002:TSB:OG1	1.99	0.63
1:B:126:MET:O	1:B:130:VAL:HG23	1.99	0.63
1:A:258:LEU:HD23	1:A:258:LEU:O	1.99	0.63
1:B:645:ARG:HD3	1:B:645:ARG:C	2.19	0.63
1:B:171:LEU:HD22	1:B:178:THR:CG2	2.28	0.63
1:B:25:ILE:HG21	1:B:59:ILE:CD1	2.29	0.62
1:B:323:LEU:HD12	1:B:324:ASP:N	2.14	0.62
1:B:601:ILE:HG22	1:B:601:ILE:O	1.97	0.62
1:A:467:PHE:CD1	1:A:467:PHE:C	2.72	0.62
1:A:391:ARG:NH1	1:A:393:ASP:OD1	2.32	0.62
1:A:522:SER:OG	1:A:523:THR:N	2.31	0.62
1:A:621:GLN:HG2	1:A:622:ASP:H	1.64	0.62
1:A:110:ILE:HG22	1:A:112:GLN:H	1.65	0.62
1:A:482:LYS:NZ	1:A:482:LYS:HA	2.14	0.62
1:B:606:LYS:H	1:B:606:LYS:HD2	1.64	0.62
1:A:323:LEU:HD13	1:A:326:THR:OG1	2.00	0.62
1:B:4:ILE:HG12	1:B:5:ASN:N	2.12	0.62
1:B:417:ASP:OD1	1:B:417:ASP:N	2.26	0.62
1:B:604:GLY:N	1:B:607:GLU:OE1	2.31	0.62
1:B:215:GLN:N	1:B:215:GLN:OE1	2.33	0.62
1:B:480:MET:C	1:B:482:LYS:H	2.03	0.62
1:A:143:ARG:HH11	1:A:163:ILE:HA	1.63	0.62
1:A:160:ILE:HD13	1:A:180:LEU:HD11	1.81	0.62
1:A:566:GLN:HB2	1:A:578:ILE:HD11	1.81	0.62
1:B:9:PRO:HD3	1:B:59:ILE:O	2.00	0.61
1:A:8:PHE:CG	1:A:9:PRO:HD2	2.34	0.61
1:A:129:ILE:HD12	1:A:129:ILE:O	2.01	0.61
1:B:471:LYS:HB3	1:B:490:GLN:HG2	1.82	0.61
1:B:130:VAL:O	1:B:132:GLU:N	2.34	0.61
1:B:518:ARG:HD3	1:B:518:ARG:C	2.21	0.61
1:A:584:LYS:O	1:A:587:TYR:N	2.34	0.61
1:B:587:TYR:C	1:B:589:ILE:H	2.04	0.61
1:B:488:THR:O	1:B:488:THR:HG23	2.01	0.61
1:A:143:ARG:NH1	1:A:163:ILE:HA	2.16	0.61
1:A:645:ARG:O	1:A:645:ARG:HG2	2.00	0.61
1:A:222:PHE:HD2	1:A:228:LEU:HD12	1.64	0.61
1:A:326:THR:HG22	1:A:327:GLU:HG3	1.82	0.61
1:A:42:PHE:O	1:A:43:ASN:HB2	2.01	0.60
1:A:31:PRO:HA	1:A:34:ARG:HG2	1.83	0.60
1:A:224:ASP:HB2	4:A:1043:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:GLN:O	1:B:623:GLN:N	2.35	0.60
1:A:336:CYS:HB2	1:A:337:PRO:CD	2.31	0.60
1:A:478:THR:HG22	1:A:480:MET:N	2.13	0.60
1:B:95:GLY:HA2	1:B:155:TYR:HB2	1.83	0.60
1:B:110:ILE:HB	1:B:215:GLN:CG	2.31	0.60
1:B:404:ASN:HA	1:B:407:ILE:HD12	1.83	0.60
1:B:241:ARG:HG3	1:B:536:LYS:HG2	1.83	0.60
1:A:390:VAL:HB	1:A:394:GLN:HG3	1.83	0.60
1:B:554:ASN:HB3	1:B:557:LEU:CB	2.25	0.60
3:A:1002:TSB:H4'	4:A:1040:HOH:O	2.01	0.60
1:B:66:SER:HB3	1:B:69:ALA:HB3	1.82	0.60
1:B:304:TYR:HE1	1:B:337:PRO:HG3	1.66	0.60
1:B:545:PRO:O	1:B:575:ARG:HD2	2.01	0.60
1:A:105:TYR:HA	1:A:217:ILE:O	2.02	0.60
1:B:391:ARG:HB3	1:B:503:TYR:CZ	2.37	0.60
1:B:388:ILE:O	1:B:515:VAL:HA	2.01	0.60
1:B:186:VAL:CG1	1:B:191:LYS:HB3	2.31	0.59
1:B:326:THR:HB	4:B:2069:HOH:O	2.02	0.59
1:A:21:THR:HG22	1:A:50:THR:O	2.03	0.59
1:A:403:VAL:O	1:A:407:ILE:HD12	2.01	0.59
1:A:473:ASP:HB3	1:A:475:GLN:HE21	1.67	0.59
1:B:141:VAL:HG11	1:B:145:GLU:HB3	1.84	0.59
1:B:234:MET:SD	1:B:235:LEU:HD23	2.42	0.59
1:B:353:LEU:HD12	1:B:391:ARG:H	1.67	0.59
1:A:323:LEU:HD13	1:A:326:THR:CB	2.32	0.59
1:B:137:GLU:O	1:B:137:GLU:HG3	2.03	0.59
1:B:171:LEU:HD22	1:B:178:THR:HG22	1.83	0.59
1:A:73:LEU:HD22	1:A:223:PHE:CE1	2.37	0.59
1:B:41:LYS:HA	1:B:45:GLN:O	2.03	0.59
1:A:20:THR:HG21	1:A:25:ILE:HG13	1.83	0.59
1:B:322:GLN:HB3	1:B:328:SER:HB3	1.83	0.59
1:A:321:MET:HE3	1:B:321:MET:SD	2.43	0.59
1:B:612:GLN:HA	1:B:628:LYS:H	1.68	0.59
1:A:181:CYS:HB3	4:A:1003:HOH:O	2.02	0.59
1:A:285:GLU:OE2	1:A:518:ARG:NH2	2.36	0.58
1:B:27:GLN:HA	1:B:27:GLN:HE21	1.68	0.58
1:A:235:LEU:O	1:A:239:LYS:HG3	2.03	0.58
1:B:81:MET:HA	1:B:126:MET:SD	2.43	0.58
1:B:83:HIS:NE2	1:B:177:PHE:HB2	2.19	0.58
1:A:316:ASP:N	1:A:316:ASP:OD1	2.36	0.58
1:A:398:GLU:O	1:A:402:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ILE:HG23	1:A:588:LYS:HD3	1.85	0.58
1:B:582:ASN:O	1:B:583:GLU:HG2	2.04	0.58
1:A:388:ILE:N	1:A:388:ILE:HD12	2.17	0.58
1:B:4:ILE:CG2	1:B:16:PHE:O	2.52	0.58
1:B:579:ASP:OD1	1:B:581:ARG:NE	2.36	0.58
1:A:306:THR:O	1:A:498:ARG:HB3	2.04	0.58
1:A:308:GLY:O	1:A:312:HIS:HD2	1.87	0.58
1:B:422:LEU:HG	1:B:447:LEU:HD11	1.86	0.58
1:B:550:ILE:HG23	1:B:601:ILE:CG2	2.30	0.58
1:A:322:GLN:HG2	1:A:329:MET:HG2	1.84	0.57
1:B:565:LEU:CD2	1:B:601:ILE:HG21	2.34	0.57
1:A:601:ILE:CD1	1:A:615:VAL:HG22	2.33	0.57
1:B:336:CYS:N	1:B:337:PRO:HD2	2.19	0.57
1:B:383:LEU:HD22	3:B:2002:TSB:H5'1	1.85	0.57
1:A:612:GLN:HE22	1:A:625:THR:HG21	1.67	0.57
1:B:422:LEU:HG	1:B:447:LEU:CD1	2.35	0.57
1:B:428:GLU:CG	1:B:440:TRP:HE1	2.16	0.57
1:B:471:LYS:NZ	1:B:473:ASP:OD2	2.37	0.57
1:A:242:ASP:OD1	1:A:244:ARG:HB2	2.04	0.57
1:B:110:ILE:HB	1:B:215:GLN:NE2	2.19	0.57
1:B:198:LEU:HG	1:B:219:GLY:HA2	1.86	0.57
1:A:186:VAL:HG13	1:A:188:SER:H	1.69	0.57
1:B:194:GLU:HG3	1:B:225:LYS:N	2.19	0.57
1:A:8:PHE:HE2	1:A:29:ILE:HD11	1.69	0.57
1:A:342:ILE:HD13	1:B:267:LEU:HD23	1.87	0.57
1:A:366:TYR:CE2	1:B:323:LEU:HB2	2.40	0.57
1:A:410:TYR:CZ	1:A:486:LEU:HD23	2.39	0.57
1:A:559:TYR:O	1:A:562:ALA:N	2.37	0.57
1:A:563:ARG:HG3	1:A:563:ARG:HH11	1.69	0.57
1:B:125:THR:O	1:B:129:ILE:HG13	2.04	0.57
1:B:553:VAL:HG23	1:B:603:VAL:O	2.04	0.57
1:B:134:MET:HB2	1:B:174:GLN:OE1	2.04	0.57
1:B:521:VAL:HG13	1:B:521:VAL:O	2.05	0.57
1:B:585:MET:HA	1:B:588:LYS:HB2	1.85	0.57
1:A:4:ILE:HD13	1:A:18:LYS:HA	1.86	0.57
1:A:163:ILE:HG22	1:A:163:ILE:O	2.04	0.57
1:A:423:SER:HB2	1:A:464:GLU:C	2.25	0.57
1:B:82:ALA:HB2	1:B:106:TYR:CD2	2.39	0.57
1:B:139:LYS:HE3	1:B:141:VAL:HG21	1.86	0.57
1:A:157:LEU:O	1:A:160:ILE:HG22	2.05	0.57
1:A:554:ASN:HD22	1:A:555:VAL:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:HB2	1:A:92:VAL:HG21	1.86	0.57
1:A:424:TYR:O	1:A:462:ILE:HD12	2.05	0.57
1:B:5:ASN:HB3	1:B:56:ASP:OD1	2.03	0.57
1:B:569:LEU:CD2	1:B:632:ILE:HG13	2.35	0.57
1:A:324:ASP:O	1:A:326:THR:N	2.37	0.56
1:A:554:ASN:ND2	1:A:557:LEU:H	2.03	0.56
1:B:66:SER:HB3	1:B:69:ALA:CB	2.34	0.56
1:A:288:MET:SD	1:A:405:MET:CE	2.93	0.56
1:A:454:LEU:HB3	1:A:456:LEU:HD13	1.85	0.56
1:A:115:SER:C	1:A:117:ASP:H	2.09	0.56
1:A:313:TYR:CE1	1:A:316:ASP:HB2	2.41	0.56
1:B:139:LYS:HE3	1:B:141:VAL:CG2	2.36	0.56
1:A:259:VAL:O	1:B:299:ALA:HA	2.05	0.56
1:A:456:LEU:CD1	1:A:456:LEU:N	2.69	0.56
1:A:621:GLN:HG2	1:A:622:ASP:CG	2.25	0.56
1:A:323:LEU:CD1	1:A:326:THR:CB	2.83	0.56
1:B:148:GLU:O	1:B:150:PHE:N	2.38	0.56
1:B:162:ALA:HB1	1:B:164:PRO:HD3	1.87	0.56
1:A:353:LEU:O	1:A:389:PHE:O	2.23	0.56
1:B:49:LEU:HD12	1:B:187:PRO:HG3	1.86	0.56
1:B:234:MET:SD	1:B:234:MET:C	2.85	0.56
1:B:322:GLN:CA	1:B:328:SER:HA	2.23	0.56
1:A:336:CYS:N	1:A:337:PRO:HD2	2.21	0.55
1:A:637:ASP:OD2	1:A:640:ARG:NH2	2.37	0.55
1:B:114:ILE:HD11	1:B:200:THR:HG21	1.88	0.55
1:B:327:GLU:OE1	1:B:327:GLU:HA	2.05	0.55
1:B:390:VAL:HB	1:B:394:GLN:OE1	2.05	0.55
1:B:473:ASP:HB3	1:B:485:THR:HG23	1.87	0.55
1:A:130:VAL:HG13	1:A:189:THR:O	2.07	0.55
1:B:351:ARG:HG3	1:B:351:ARG:NH1	2.21	0.55
1:A:34:ARG:HG3	1:A:35:LYS:N	2.21	0.55
1:A:204:TYR:CE1	1:A:207:GLY:HA2	2.35	0.55
1:A:409:VAL:O	1:A:412:ASP:HB2	2.06	0.55
1:B:73:LEU:HD21	1:B:222:PHE:O	2.06	0.55
1:B:136:ILE:HG13	1:B:136:ILE:O	2.05	0.55
1:B:522:SER:OG	1:B:523:THR:N	2.39	0.55
1:A:119:PHE:O	1:A:123:GLU:HB2	2.07	0.55
1:B:193:LYS:N	1:B:193:LYS:HD2	2.22	0.55
1:A:579:ASP:OD1	1:A:588:LYS:HE2	2.07	0.55
1:A:384:ASN:ND2	1:A:521:VAL:HG12	2.22	0.55
1:A:428:GLU:CB	1:A:440:TRP:HE1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG13	1:B:292:HIS:CE1	2.41	0.55
1:A:4:ILE:O	1:A:6:ILE:HG13	2.07	0.55
1:A:162:ALA:HB3	1:A:167:GLU:OE2	2.06	0.55
1:A:376:GLN:NE2	1:A:484:GLU:OE1	2.40	0.55
1:B:6:ILE:HD13	1:B:25:ILE:HD13	1.88	0.55
1:A:340:MET:HG3	1:A:501:LEU:HD11	1.88	0.55
1:A:584:LYS:O	1:A:585:MET:C	2.46	0.54
1:A:115:SER:C	1:A:117:ASP:N	2.61	0.54
1:A:480:MET:HE3	1:A:482:LYS:HG3	1.89	0.54
1:A:45:GLN:NE2	4:A:1062:HOH:O	2.40	0.54
1:A:163:ILE:N	1:A:164:PRO:CD	2.69	0.54
1:A:288:MET:SD	1:A:405:MET:HE3	2.48	0.54
1:A:561:TYR:O	1:A:564:GLN:HB3	2.07	0.54
1:B:430:LYS:CG	1:B:431:GLU:H	2.20	0.54
1:B:556:ASP:HB2	4:B:2033:HOH:O	2.07	0.54
1:A:425:ARG:NH2	1:A:437:ASP:HA	2.23	0.54
1:A:324:ASP:C	1:A:326:THR:H	2.10	0.54
1:B:83:HIS:CE1	1:B:177:PHE:HB2	2.42	0.54
1:B:143:ARG:O	1:B:147:LYS:HB2	2.07	0.54
1:A:29:ILE:O	1:A:30:SER:HB3	2.08	0.54
1:A:323:LEU:CD1	1:A:326:THR:HB	2.37	0.54
1:B:149:LEU:HG	1:B:150:PHE:CD1	2.42	0.54
1:B:214:LEU:HD13	1:B:214:LEU:H	1.71	0.54
1:B:423:SER:HB3	1:B:465:ALA:N	2.22	0.54
1:B:448:LYS:O	1:B:451:ALA:HB3	2.08	0.54
1:A:181:CYS:SG	4:A:1003:HOH:O	2.59	0.54
1:B:8:PHE:CE1	1:B:59:ILE:HD11	2.43	0.54
1:B:449:GLU:O	1:B:453:GLU:HG3	2.08	0.54
1:A:155:TYR:CD1	1:A:205:TRP:CZ3	2.96	0.54
1:A:429:ASP:O	1:A:494:LEU:HD11	2.08	0.54
1:B:428:GLU:CB	1:B:440:TRP:HE1	2.21	0.54
1:B:644:HIS:N	1:B:644:HIS:CD2	2.74	0.54
1:A:344:ALA:O	1:A:346:LYS:N	2.41	0.53
1:B:147:LYS:HA	1:B:160:ILE:HG21	1.90	0.53
1:B:250:LEU:HD11	1:B:595:GLN:HA	1.89	0.53
1:B:445:ASN:O	1:B:449:GLU:HG3	2.08	0.53
1:A:174:GLN:O	1:A:176:ASP:N	2.38	0.53
1:A:490:GLN:CG	1:A:517:HIS:HB2	2.38	0.53
1:B:163:ILE:N	1:B:164:PRO:CD	2.68	0.53
1:B:231:HIS:O	1:B:231:HIS:ND1	2.41	0.53
1:B:244:ARG:HB3	4:B:2015:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:CD1	1:B:267:LEU:HD23	2.38	0.53
1:A:467:PHE:HD1	1:A:467:PHE:O	1.92	0.53
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.74	0.53
1:B:547:GLN:HG3	1:B:575:ARG:HB2	1.90	0.53
1:A:85:ILE:HG13	1:A:108:PHE:CZ	2.43	0.53
1:B:87:ARG:HD2	1:B:125:THR:HG23	1.90	0.53
1:B:132:GLU:OE1	1:B:134:MET:HE1	2.08	0.53
1:A:20:THR:CG2	1:A:21:THR:N	2.70	0.53
1:A:566:GLN:NE2	1:A:578:ILE:HD12	2.24	0.53
1:A:21:THR:CG2	1:A:50:THR:O	2.57	0.53
1:A:212:LYS:HG3	1:A:213:MET:N	2.24	0.53
1:A:367:GLU:OE1	1:A:377:ARG:HD2	2.09	0.53
1:A:554:ASN:CG	1:A:557:LEU:HB2	2.28	0.53
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.23	0.53
1:B:494:LEU:HD22	1:B:498:ARG:HD2	1.91	0.53
1:A:391:ARG:HD3	1:A:503:TYR:CE1	2.43	0.53
1:B:475:GLN:NE2	1:B:485:THR:HG23	2.23	0.53
1:B:590:ARG:O	1:B:594:MET:HG3	2.08	0.53
1:A:37:ALA:HB3	1:A:49:LEU:HD11	1.89	0.53
1:B:136:ILE:C	1:B:136:ILE:HD12	2.29	0.53
1:B:354:PRO:HA	1:B:390:VAL:HG12	1.91	0.53
1:B:105:TYR:HA	1:B:217:ILE:O	2.09	0.52
1:B:402:VAL:O	1:B:406:ILE:HG13	2.09	0.52
1:A:253:PHE:CE2	1:A:375:LEU:HG	2.45	0.52
1:A:526:ARG:HH11	1:A:526:ARG:CB	2.20	0.52
1:B:21:THR:HG22	1:B:52:PRO:HA	1.91	0.52
1:B:570:LYS:C	1:B:572:GLN:N	2.61	0.52
1:A:115:SER:O	1:A:117:ASP:N	2.42	0.52
1:A:618:TYR:C	1:A:620:SER:H	2.12	0.52
1:B:479:ALA:O	1:B:480:MET:HG3	2.09	0.52
1:A:70:LEU:HD23	1:A:74:ARG:CZ	2.40	0.52
1:B:298:LEU:CD2	1:B:331:LEU:HD23	2.39	0.52
1:B:631:PHE:HD2	1:B:632:ILE:HD12	1.74	0.52
1:A:245:LYS:O	1:A:249:GLU:HB2	2.10	0.52
1:A:132:GLU:OE1	1:A:134:MET:HE2	2.09	0.52
1:A:135:LYS:HE2	1:A:137:GLU:HG2	1.92	0.52
1:B:21:THR:O	1:B:25:ILE:HG13	2.09	0.52
1:B:22:THR:HB	1:B:49:LEU:CD2	2.38	0.52
1:A:20:THR:CG2	1:A:25:ILE:HG13	2.40	0.52
1:A:337:PRO:O	1:A:340:MET:HB2	2.10	0.52
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:O	1:B:224:ASP:CB	2.57	0.52
1:B:561:TYR:CD2	1:B:608:VAL:HG22	2.45	0.52
1:B:570:LYS:C	1:B:572:GLN:H	2.13	0.52
1:A:186:VAL:HG13	1:A:188:SER:O	2.09	0.52
1:A:281:ILE:HG23	1:A:282:VAL:N	2.24	0.52
1:A:388:ILE:N	1:A:388:ILE:CD1	2.72	0.52
1:A:518:ARG:HD3	1:A:518:ARG:C	2.27	0.52
1:A:612:GLN:NE2	1:A:625:THR:CG2	2.69	0.52
1:B:542:TRP:CZ2	1:B:543:LEU:HD21	2.45	0.52
1:B:598:PRO:HB2	1:B:599:TYR:HD1	1.75	0.52
1:A:79:HIS:CD2	1:A:185:HIS:NE2	2.78	0.52
1:A:243:HIS:HB3	1:A:533:GLU:HG3	1.92	0.52
1:A:322:GLN:CB	1:A:327:GLU:O	2.58	0.52
1:B:174:GLN:CG	1:B:189:THR:HG21	2.40	0.52
1:B:246:ILE:HG21	1:B:532:THR:CG2	2.40	0.52
1:B:429:ASP:O	1:B:430:LYS:HB2	2.09	0.52
1:B:434:PHE:HE2	1:B:438:ASP:OD1	1.92	0.52
1:B:224:ASP:OD2	1:B:226:LYS:HB3	2.10	0.51
1:A:4:ILE:HG23	1:A:18:LYS:HB2	1.91	0.51
1:A:392:PRO:HG3	4:A:1075:HOH:O	2.09	0.51
1:A:426:ASP:OD1	1:A:463:GLY:HA2	2.09	0.51
1:A:515:VAL:HG12	1:A:517:HIS:CD2	2.45	0.51
1:B:563:ARG:HG3	1:B:563:ARG:HH11	1.75	0.51
1:B:95:GLY:O	1:B:155:TYR:HB2	2.11	0.51
1:B:481:GLY:O	1:B:483:GLU:N	2.43	0.51
1:A:157:LEU:HA	1:A:160:ILE:HG22	1.92	0.51
1:A:384:ASN:HD21	1:A:520:VAL:HB	1.75	0.51
1:B:565:LEU:HD21	1:B:601:ILE:HG21	1.93	0.51
1:A:258:LEU:HD21	1:B:303:LEU:HA	1.93	0.51
1:B:392:PRO:HA	1:B:395:ILE:CD1	2.40	0.51
1:A:114:ILE:HD11	1:A:215:GLN:HB3	1.91	0.51
1:A:321:MET:O	1:A:328:SER:HA	2.11	0.51
1:B:261:ALA:HB3	1:B:379:ARG:HH21	1.73	0.51
1:B:458:TYR:CD1	1:B:458:TYR:N	2.79	0.51
1:B:477:LYS:CE	1:B:483:GLU:OE2	2.59	0.51
1:B:615:VAL:HG23	1:B:623:GLN:CB	2.37	0.51
1:A:554:ASN:OD1	1:A:557:LEU:HB2	2.11	0.51
1:A:591:GLU:HG2	1:A:595:GLN:NE2	2.26	0.51
1:B:83:HIS:CE1	1:B:174:GLN:HE21	2.29	0.51
1:B:186:VAL:O	1:B:188:SER:N	2.44	0.51
1:B:188:SER:C	1:B:190:ALA:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD22	1:A:223:PHE:CD1	2.46	0.51
1:A:419:SER:O	1:A:475:GLN:N	2.40	0.51
1:A:336:CYS:HA	1:A:387:HIS:CE1	2.46	0.51
1:B:42:PHE:H	1:B:47:VAL:CG1	2.24	0.51
1:B:84:ALA:HA	1:B:129:ILE:CD1	2.41	0.51
1:B:543:LEU:O	1:B:544:ALA:C	2.48	0.51
1:A:422:LEU:HD22	1:A:447:LEU:HD21	1.93	0.50
1:A:426:ASP:O	1:A:428:GLU:N	2.44	0.50
1:A:482:LYS:HA	1:A:482:LYS:HZ3	1.75	0.50
1:B:131:ASN:H	1:B:131:ASN:ND2	2.10	0.50
1:B:459:GLU:O	1:B:460:GLU:C	2.49	0.50
1:A:132:GLU:OE1	1:A:134:MET:CE	2.59	0.50
1:B:97:GLY:HA3	1:B:106:TYR:CD1	2.45	0.50
1:B:449:GLU:O	1:B:453:GLU:CG	2.60	0.50
1:A:21:THR:H	1:A:24:ASP:HB2	1.76	0.50
1:A:154:GLU:O	1:A:158:GLU:HG2	2.11	0.50
1:B:13:LYS:HD3	1:B:13:LYS:O	2.12	0.50
1:B:114:ILE:O	1:B:115:SER:HB3	2.11	0.50
1:A:428:GLU:HB3	1:A:440:TRP:HE1	1.75	0.50
1:B:1:MET:O	1:B:1:MET:HG2	2.11	0.50
1:A:322:GLN:OE1	1:A:323:LEU:CD1	2.59	0.50
1:B:139:LYS:HG2	1:B:141:VAL:HG23	1.93	0.50
1:B:383:LEU:HD12	1:B:384:ASN:H	1.77	0.50
1:B:392:PRO:HA	1:B:395:ILE:CG1	2.42	0.50
1:A:261:ALA:O	1:A:379:ARG:HD2	2.11	0.50
1:B:249:GLU:O	1:B:595:GLN:NE2	2.45	0.50
1:B:376:GLN:HG2	4:B:2059:HOH:O	2.10	0.50
1:B:439:MET:O	1:B:442:LYS:HB3	2.12	0.50
1:A:181:CYS:CB	4:A:1003:HOH:O	2.60	0.50
1:A:630:GLU:O	1:A:633:TRP:HB3	2.10	0.50
1:A:313:TYR:CD1	1:A:316:ASP:HB2	2.47	0.50
1:A:555:VAL:CG2	1:A:555:VAL:O	2.59	0.50
1:B:303:LEU:HD23	1:B:304:TYR:CZ	2.46	0.50
1:A:8:PHE:HB3	1:A:9:PRO:HD2	1.92	0.50
1:A:84:ALA:HB2	1:A:126:MET:HB3	1.94	0.49
1:B:5:ASN:HB3	1:B:56:ASP:CG	2.32	0.49
1:B:129:ILE:O	1:B:129:ILE:HG22	2.12	0.49
1:B:428:GLU:OE1	1:B:435:ASP:CA	2.60	0.49
1:A:242:ASP:OD1	1:A:244:ARG:N	2.35	0.49
1:B:83:HIS:HE1	1:B:174:GLN:HE21	1.58	0.49
1:B:132:GLU:HB2	1:B:134:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:CG	1:B:136:ILE:H	2.04	0.49
1:B:287:SER:C	1:B:289:GLY:N	2.66	0.49
1:B:422:LEU:N	1:B:422:LEU:CD1	2.75	0.49
1:B:444:GLU:HG2	1:B:470:PRO:HB3	1.94	0.49
1:A:288:MET:SD	1:A:405:MET:HE1	2.53	0.49
1:B:139:LYS:HG2	1:B:141:VAL:CG2	2.42	0.49
1:B:470:PRO:HD2	1:B:491:LEU:O	2.11	0.49
1:B:500:ASP:HA	1:B:512:ARG:NH2	2.26	0.49
1:A:4:ILE:C	1:A:56:ASP:HB3	2.32	0.49
1:A:110:ILE:HB	1:A:112:GLN:O	2.13	0.49
1:A:383:LEU:HD23	1:A:385:ASP:HB2	1.94	0.49
1:B:163:ILE:H	1:B:164:PRO:HD3	1.71	0.49
1:B:569:LEU:HD21	1:B:632:ILE:HG13	1.93	0.49
1:A:490:GLN:HG2	1:A:517:HIS:HB2	1.94	0.49
1:A:7:GLN:HG2	1:A:13:LYS:HG2	1.95	0.49
1:A:155:TYR:HB3	1:A:205:TRP:CZ3	2.48	0.49
1:A:174:GLN:NE2	1:A:189:THR:HG21	2.28	0.49
1:A:424:TYR:HH	1:A:448:LYS:HE3	1.77	0.49
1:A:621:GLN:CG	1:A:622:ASP:H	2.21	0.49
1:B:132:GLU:HB2	1:B:134:MET:CE	2.42	0.49
1:A:5:ASN:HB3	1:A:56:ASP:OD2	2.13	0.49
1:A:322:GLN:HB3	1:A:327:GLU:O	2.13	0.49
1:A:500:ASP:HA	1:A:512:ARG:NH1	2.27	0.49
1:A:568:GLU:O	1:A:571:SER:OG	2.25	0.49
1:B:27:GLN:HE21	1:B:34:ARG:HD3	1.76	0.49
1:B:137:GLU:HG2	4:B:2021:HOH:O	2.12	0.49
1:B:187:PRO:HA	4:B:2045:HOH:O	2.12	0.49
1:B:422:LEU:N	1:B:422:LEU:HD12	2.27	0.49
1:B:195:PHE:CD1	1:B:195:PHE:N	2.81	0.49
1:B:210:ASN:O	1:B:211:ASN:CG	2.51	0.49
1:B:318:PHE:HE1	1:B:365:ARG:O	1.96	0.49
1:B:323:LEU:HD13	1:B:324:ASP:OD2	2.12	0.49
1:B:480:MET:O	1:B:482:LYS:N	2.40	0.49
1:B:583:GLU:O	1:B:588:LYS:HE2	2.11	0.49
1:A:428:GLU:CG	1:A:440:TRP:HE1	2.26	0.49
1:A:569:LEU:HB3	1:A:574:VAL:HB	1.94	0.49
1:B:325:GLU:O	1:B:327:GLU:HG2	2.12	0.49
1:A:313:TYR:O	1:A:315:GLU:N	2.45	0.48
1:A:432:LYS:O	1:A:434:PHE:CD2	2.66	0.48
1:B:2:GLU:HA	1:B:17:ASP:HB3	1.95	0.48
1:B:148:GLU:O	1:B:149:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PRO:O	1:A:188:SER:HB2	2.13	0.48
1:A:554:ASN:HD21	1:A:556:ASP:HB2	1.79	0.48
1:A:602:VAL:O	1:A:614:ASN:HB3	2.12	0.48
1:B:395:ILE:HD11	1:B:514:VAL:CG2	2.20	0.48
1:B:397:GLU:OE1	1:B:398:GLU:N	2.46	0.48
1:A:399:PHE:HE2	1:A:472:LEU:HD12	1.79	0.48
1:B:355:ILE:N	4:B:2048:HOH:O	2.45	0.48
1:B:593:GLN:O	1:B:596:LYS:N	2.46	0.48
1:B:601:ILE:CD1	1:B:615:VAL:HG12	2.36	0.48
1:A:122:ILE:O	1:A:126:MET:HG2	2.13	0.48
1:B:312:HIS:HE1	1:B:429:ASP:HB2	1.75	0.48
1:A:486:LEU:O	1:A:522:SER:HB2	2.13	0.48
1:A:531:LEU:O	1:A:535:THR:CG2	2.54	0.48
1:B:140:VAL:HG22	1:B:170:THR:CG2	2.44	0.48
1:B:203:ALA:O	1:B:214:LEU:HD22	2.13	0.48
1:B:210:ASN:O	1:B:211:ASN:ND2	2.46	0.48
1:B:410:TYR:H	1:B:410:TYR:HD1	1.61	0.48
1:B:473:ASP:HB3	1:B:475:GLN:HE21	1.77	0.48
1:B:558:HIS:NE2	1:B:604:GLY:C	2.67	0.48
1:A:169:VAL:HG23	1:A:169:VAL:O	2.13	0.48
1:A:194:GLU:HG3	1:A:225:LYS:CA	2.44	0.48
1:A:458:TYR:N	1:A:458:TYR:CD1	2.81	0.48
1:A:555:VAL:O	1:A:555:VAL:HG23	2.13	0.48
1:B:277:ILE:O	1:B:280:TYR:HB3	2.14	0.48
1:A:281:ILE:HG22	1:A:282:VAL:H	1.77	0.48
1:A:356:ARG:NH1	1:A:398:GLU:OE2	2.46	0.48
1:A:395:ILE:HG21	1:A:491:LEU:HD21	1.95	0.48
1:B:281:ILE:HG23	1:B:282:VAL:N	2.29	0.48
1:B:593:GLN:O	1:B:594:MET:C	2.51	0.48
1:A:210:ASN:O	1:A:211:ASN:O	2.32	0.48
1:B:96:VAL:HG23	1:B:107:ASP:OD2	2.14	0.48
1:B:313:TYR:O	1:B:314:GLN:C	2.52	0.48
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.73	0.48
1:B:392:PRO:O	1:B:395:ILE:HG13	2.14	0.48
1:A:176:ASP:C	1:A:176:ASP:OD1	2.52	0.48
1:B:587:TYR:C	1:B:589:ILE:N	2.67	0.48
1:B:587:TYR:HA	1:B:590:ARG:HG2	1.96	0.48
1:A:428:GLU:OE2	1:A:435:ASP:C	2.53	0.47
1:B:46:LEU:O	1:B:184:VAL:CG1	2.58	0.47
1:B:389:PHE:HE2	1:B:501:LEU:HD13	1.78	0.47
1:A:74:ARG:HH22	1:A:102:GLY:HA2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:C	1:B:132:GLU:N	2.67	0.47
1:B:394:GLN:O	1:B:396:LYS:N	2.48	0.47
1:B:502:THR:HA	1:B:513:PRO:HD3	1.96	0.47
1:B:579:ASP:CG	1:B:581:ARG:HH21	2.17	0.47
1:B:595:GLN:O	1:B:597:ILE:HG13	2.15	0.47
1:B:55:THR:HB	1:B:56:ASP:H	1.58	0.47
1:B:87:ARG:O	1:B:88:LEU:HB2	2.15	0.47
1:B:110:ILE:CB	1:B:215:GLN:HE21	2.26	0.47
1:B:85:ILE:CD1	1:B:122:ILE:HD13	2.44	0.47
1:B:172:TYR:CD1	1:B:173:SER:N	2.82	0.47
1:B:473:ASP:HB3	1:B:475:GLN:NE2	2.29	0.47
1:B:574:VAL:HG12	1:B:575:ARG:N	2.30	0.47
1:B:606:LYS:HD3	1:B:607:GLU:CD	2.35	0.47
1:A:253:PHE:HA	1:A:267:LEU:HG	1.95	0.47
1:A:349:SER:O	1:A:352:GLU:HG2	2.13	0.47
1:B:561:TYR:HE2	1:B:603:VAL:HG11	1.78	0.47
1:A:262:GLY:C	1:A:263:LEU:HD23	2.35	0.47
1:A:399:PHE:CE2	1:A:472:LEU:HD12	2.49	0.47
1:A:425:ARG:HA	1:A:440:TRP:CZ3	2.50	0.47
1:A:471:LYS:HA	1:A:490:GLN:HA	1.97	0.47
1:A:500:ASP:HA	1:A:512:ARG:HH12	1.79	0.47
1:A:549:GLN:HA	1:A:549:GLN:OE1	2.14	0.47
1:A:602:VAL:HG23	4:A:1019:HOH:O	2.13	0.47
1:B:93:LYS:HB2	1:B:93:LYS:NZ	2.29	0.47
1:B:297:VAL:HG22	4:B:2004:HOH:O	2.14	0.47
1:B:410:TYR:N	1:B:410:TYR:CD1	2.81	0.47
1:A:423:SER:HB3	1:A:464:GLU:CB	2.44	0.47
1:A:610:ASN:HB3	4:A:1004:HOH:O	2.15	0.47
1:B:46:LEU:HG	1:B:184:VAL:HG11	1.97	0.47
1:B:130:VAL:HG13	1:B:190:ALA:HA	1.97	0.47
1:B:155:TYR:CZ	1:B:159:LEU:HD22	2.50	0.47
1:B:174:GLN:O	1:B:174:GLN:NE2	2.47	0.47
1:A:71:GLU:HB3	4:A:1068:HOH:O	2.15	0.47
1:A:125:THR:C	1:A:127:LYS:N	2.66	0.47
1:A:298:LEU:C	1:A:298:LEU:HD12	2.35	0.47
1:A:391:ARG:H	1:A:394:GLN:CG	2.28	0.47
1:A:581:ARG:O	1:A:588:LYS:NZ	2.45	0.47
1:A:625:THR:CG2	1:A:626:VAL:N	2.78	0.47
1:A:611:ASN:HD22	1:A:611:ASN:HA	1.56	0.47
1:B:123:GLU:HB2	1:B:197:LEU:CD1	2.37	0.47
1:A:46:LEU:HG	4:A:1021:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG23	1:A:362:THR:O	2.14	0.46
1:A:386:SER:HB3	1:A:518:ARG:HD2	1.97	0.46
1:A:399:PHE:O	1:A:403:VAL:HG23	2.15	0.46
1:A:205:TRP:O	1:A:207:GLY:N	2.47	0.46
1:A:323:LEU:O	1:A:324:ASP:O	2.33	0.46
1:A:502:THR:HA	1:A:513:PRO:HD3	1.96	0.46
1:B:395:ILE:HG23	1:B:491:LEU:HD11	1.96	0.46
1:B:643:LYS:C	1:B:644:HIS:HD2	2.18	0.46
1:B:202:GLY:O	1:B:203:ALA:HB2	2.15	0.46
1:A:8:PHE:CZ	1:A:29:ILE:HD11	2.51	0.46
1:A:191:LYS:HE3	4:A:1007:HOH:O	2.14	0.46
1:A:454:LEU:HB3	1:A:456:LEU:HD11	1.97	0.46
1:B:8:PHE:C	1:B:10:ASP:H	2.19	0.46
1:B:222:PHE:CD2	1:B:228:LEU:HD13	2.51	0.46
1:B:459:GLU:O	1:B:460:GLU:O	2.33	0.46
1:A:34:ARG:O	1:A:36:LYS:N	2.47	0.46
1:B:93:LYS:HB2	1:B:93:LYS:HZ2	1.81	0.46
1:B:140:VAL:HG22	1:B:170:THR:HG22	1.98	0.46
1:B:388:ILE:HG21	1:B:398:GLU:HG2	1.97	0.46
1:B:467:PHE:CD1	1:B:468:TYR:N	2.84	0.46
1:A:406:ILE:HG21	1:A:474:VAL:HG21	1.97	0.46
1:A:471:LYS:NZ	1:A:473:ASP:OD2	2.48	0.46
1:A:476:VAL:HG13	1:A:530:PHE:CE1	2.50	0.46
1:A:157:LEU:O	1:A:160:ILE:CG2	2.64	0.46
1:A:469:GLY:HA3	1:A:491:LEU:O	2.16	0.46
1:A:113:ASN:C	1:A:215:GLN:HE22	2.18	0.46
1:A:150:PHE:O	1:A:157:LEU:HD21	2.15	0.46
1:A:177:PHE:CZ	1:A:179:ASP:HB2	2.51	0.46
1:B:396:LYS:HG3	1:B:397:GLU:N	2.31	0.46
1:A:38:VAL:O	1:A:187:PRO:HD3	2.16	0.46
1:B:39:ALA:O	1:B:62:VAL:HB	2.16	0.46
1:B:236:GLU:O	1:B:240:GLU:HG2	2.16	0.46
1:B:467:PHE:CD1	1:B:467:PHE:C	2.88	0.46
1:B:478:THR:CG2	1:B:479:ALA:N	2.62	0.46
1:B:550:ILE:HG21	1:B:562:ALA:HB1	1.97	0.46
1:B:27:GLN:NE2	1:B:27:GLN:HA	2.29	0.46
1:B:156:LYS:HB3	1:B:180:LEU:HD12	1.96	0.46
1:A:125:THR:O	1:A:129:ILE:HG23	2.17	0.45
1:A:323:LEU:CG	1:B:366:TYR:OH	2.63	0.45
1:A:471:LYS:HG2	1:A:490:GLN:HB3	1.96	0.45
1:A:478:THR:CG2	1:A:479:ALA:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASP:O	1:B:609:GLU:HB2	2.16	0.45
1:A:73:LEU:HB2	1:A:223:PHE:CZ	2.50	0.45
1:A:335:ASN:HB2	1:A:385:ASP:OD2	2.16	0.45
1:B:70:LEU:HD22	1:B:74:ARG:CZ	2.46	0.45
1:B:383:LEU:HA	1:B:523:THR:HA	1.98	0.45
1:A:186:VAL:HG22	1:A:187:PRO:HD2	1.98	0.45
1:A:298:LEU:CD2	1:B:331:LEU:HD11	2.44	0.45
1:B:547:GLN:OE1	1:B:574:VAL:HG13	2.16	0.45
1:B:17:ASP:OD1	1:B:17:ASP:N	2.50	0.45
1:B:73:LEU:HD22	1:B:223:PHE:CD1	2.51	0.45
1:B:124:LYS:O	1:B:128:GLN:HB2	2.17	0.45
1:B:636:VAL:HA	1:B:639:ILE:HD12	1.98	0.45
1:A:195:PHE:HA	1:A:221:ALA:HA	1.98	0.45
1:A:203:ALA:O	1:A:214:LEU:HB2	2.16	0.45
1:A:503:TYR:CE2	1:A:511:HIS:HB3	2.51	0.45
1:B:234:MET:SD	1:B:235:LEU:N	2.90	0.45
1:A:40:GLY:HA2	1:A:62:VAL:HG23	1.98	0.45
1:A:93:LYS:HB3	1:A:153:ASP:OD1	2.16	0.45
1:A:97:GLY:HA3	1:A:106:TYR:CE2	2.52	0.45
1:A:204:TYR:HE2	1:A:209:SER:HG	1.63	0.45
1:B:303:LEU:HD23	1:B:304:TYR:CE1	2.51	0.45
1:B:501:LEU:O	1:B:513:PRO:HD2	2.16	0.45
1:A:521:VAL:HG22	1:A:527:PHE:CE1	2.52	0.45
1:B:83:HIS:CE1	1:B:174:GLN:NE2	2.84	0.45
1:B:99:VAL:HG12	1:B:104:PHE:HB3	1.97	0.45
1:B:130:VAL:C	1:B:132:GLU:H	2.20	0.45
1:B:614:ASN:HB2	1:B:625:THR:HG22	1.98	0.45
1:A:428:GLU:HG2	1:A:429:ASP:N	2.32	0.45
1:B:425:ARG:NH1	4:B:2003:HOH:O	2.49	0.45
1:B:430:LYS:CG	1:B:431:GLU:N	2.79	0.45
1:B:487:SER:HB3	1:B:520:VAL:O	2.16	0.45
1:B:512:ARG:HG3	1:B:512:ARG:NH1	2.27	0.45
1:B:602:VAL:O	1:B:614:ASN:HB3	2.17	0.45
1:B:614:ASN:HA	1:B:625:THR:HA	1.99	0.45
1:A:388:ILE:HG21	1:A:398:GLU:HG2	1.98	0.45
1:A:589:ILE:O	1:A:589:ILE:HG22	2.16	0.45
1:B:62:VAL:HG13	1:B:69:ALA:HB2	1.98	0.45
1:B:66:SER:O	1:B:67:GLU:C	2.54	0.45
1:B:143:ARG:HH11	1:B:143:ARG:CG	2.27	0.45
1:B:75:HIS:O	1:B:78:ALA:HB3	2.17	0.45
1:B:298:LEU:HD23	1:B:331:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LEU:HD13	1:B:458:TYR:HB3	1.99	0.45
1:A:353:LEU:CD1	1:A:390:VAL:HA	2.47	0.44
1:A:404:ASN:O	1:A:408:ASP:N	2.42	0.44
1:A:521:VAL:HG22	1:A:527:PHE:CD1	2.52	0.44
1:B:27:GLN:HE21	1:B:27:GLN:CA	2.26	0.44
1:B:222:PHE:HD2	1:B:228:LEU:HD13	1.82	0.44
1:B:452:ASP:C	1:B:454:LEU:N	2.70	0.44
1:B:473:ASP:HB3	1:B:485:THR:CG2	2.47	0.44
1:B:641:LEU:O	1:B:642:LYS:C	2.52	0.44
1:A:114:ILE:HG12	1:A:215:GLN:NE2	2.32	0.44
1:A:123:GLU:HA	1:A:126:MET:HG2	1.98	0.44
1:A:249:GLU:HB3	1:A:250:LEU:HD13	2.00	0.44
1:A:255:ASN:N	1:A:255:ASN:ND2	2.64	0.44
1:A:398:GLU:HA	1:A:401:ARG:HH21	1.81	0.44
1:A:566:GLN:CD	1:A:578:ILE:HD12	2.37	0.44
1:B:43:ASN:ND2	1:B:57:GLY:CA	2.69	0.44
1:B:167:GLU:CG	1:B:167:GLU:O	2.65	0.44
1:A:180:LEU:HD23	1:A:180:LEU:O	2.18	0.44
1:B:313:TYR:O	1:B:315:GLU:N	2.50	0.44
1:B:315:GLU:H	1:B:315:GLU:HG2	1.48	0.44
1:B:388:ILE:HG22	1:B:390:VAL:HG13	1.98	0.44
1:B:612:GLN:HB3	1:B:626:VAL:O	2.17	0.44
1:A:157:LEU:HA	1:A:160:ILE:CG2	2.47	0.44
1:A:181:CYS:SG	1:A:182:ARG:N	2.90	0.44
1:A:205:TRP:NE1	1:A:206:ARG:HG3	2.33	0.44
1:A:296:PRO:HG3	4:B:2009:HOH:O	2.16	0.44
1:A:326:THR:O	1:A:327:GLU:CG	2.65	0.44
1:A:340:MET:HE1	1:A:389:PHE:CZ	2.51	0.44
1:A:589:ILE:O	1:A:589:ILE:CG2	2.66	0.44
1:B:147:LYS:CA	1:B:160:ILE:HG21	2.47	0.44
1:A:548:VAL:O	1:A:576:VAL:HA	2.17	0.44
1:B:16:PHE:O	1:B:17:ASP:C	2.55	0.44
1:B:79:HIS:CD2	1:B:172:TYR:OH	2.71	0.44
1:B:84:ALA:HB2	1:B:126:MET:CG	2.44	0.44
1:B:126:MET:HE1	1:B:197:LEU:HD21	2.00	0.44
1:B:202:GLY:HA2	1:B:214:LEU:O	2.17	0.44
1:B:283:ASP:HB2	4:B:2026:HOH:O	2.18	0.44
1:B:350:TYR:CE2	1:B:506:GLN:HA	2.53	0.44
1:B:378:VAL:HG23	1:B:379:ARG:N	2.33	0.44
1:B:379:ARG:NH2	4:B:2038:HOH:O	2.31	0.44
1:B:534:GLU:OE1	1:B:534:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ALA:HB1	1:A:125:THR:HG22	1.97	0.44
1:A:561:TYR:CD2	1:A:608:VAL:HG22	2.53	0.44
1:B:410:TYR:HD1	1:B:410:TYR:N	2.16	0.44
1:B:434:PHE:O	1:B:435:ASP:HB2	2.17	0.44
1:B:554:ASN:O	1:B:557:LEU:N	2.47	0.44
1:B:561:TYR:CE2	1:B:603:VAL:HG11	2.53	0.44
1:B:597:ILE:HA	1:B:598:PRO:HD2	1.74	0.44
1:B:602:VAL:HG23	1:B:614:ASN:OD1	2.18	0.44
1:A:323:LEU:O	1:A:323:LEU:CD1	2.66	0.44
1:A:589:ILE:HG21	1:A:616:ARG:HH12	1.83	0.44
1:A:612:GLN:HB2	1:A:626:VAL:O	2.18	0.44
1:B:8:PHE:O	1:B:10:ASP:N	2.51	0.44
1:B:42:PHE:HD1	1:B:59:ILE:HG23	1.83	0.44
1:B:261:ALA:N	4:B:2038:HOH:O	2.48	0.44
1:B:434:PHE:O	1:B:434:PHE:CD1	2.71	0.44
1:B:479:ALA:C	1:B:480:MET:HG3	2.38	0.44
1:B:540:PRO:CG	1:B:543:LEU:HD12	2.45	0.44
1:A:323:LEU:HD13	1:A:326:THR:HB	1.99	0.44
1:A:558:HIS:NE2	1:A:605:ASP:OD1	2.43	0.44
1:B:131:ASN:ND2	1:B:131:ASN:N	2.64	0.44
1:B:297:VAL:O	1:B:332:ARG:HG2	2.18	0.44
1:B:331:LEU:HB3	4:B:2032:HOH:O	2.18	0.44
1:B:377:ARG:HA	3:B:2002:TSB:N1	2.32	0.44
1:B:422:LEU:HD13	1:B:458:TYR:CB	2.48	0.44
1:B:638:GLU:O	1:B:638:GLU:HG2	2.18	0.44
1:B:172:TYR:O	1:B:178:THR:HG23	2.17	0.44
1:B:186:VAL:HG11	1:B:191:LYS:HB3	2.00	0.44
1:A:34:ARG:HG3	1:A:35:LYS:H	1.83	0.43
1:A:186:VAL:CG1	1:A:188:SER:O	2.66	0.43
1:B:163:ILE:HG22	1:B:163:ILE:O	2.18	0.43
1:B:322:GLN:OE1	1:B:322:GLN:N	2.51	0.43
1:B:598:PRO:O	1:B:617:GLN:HA	2.18	0.43
1:A:80:LEU:CG	1:A:126:MET:HB2	2.48	0.43
1:A:259:VAL:O	1:B:300:ASN:N	2.46	0.43
1:A:338:HIS:O	1:A:341:MET:HB2	2.19	0.43
1:A:353:LEU:CD1	1:A:390:VAL:C	2.87	0.43
1:B:353:LEU:C	1:B:355:ILE:H	2.21	0.43
1:B:458:TYR:HD2	1:B:460:GLU:HG3	1.83	0.43
1:A:499:PHE:HB2	1:A:501:LEU:HG	2.00	0.43
1:A:524:MET:CE	1:A:524:MET:HA	2.49	0.43
1:B:42:PHE:H	1:B:47:VAL:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD13	1:B:250:LEU:HA	1.66	0.43
1:B:569:LEU:HD23	1:B:632:ILE:HG13	1.99	0.43
1:B:598:PRO:C	1:B:599:TYR:CD1	2.91	0.43
1:B:606:LYS:HD3	1:B:607:GLU:OE2	2.17	0.43
1:A:224:ASP:OD1	1:A:226:LYS:HB2	2.19	0.43
1:A:250:LEU:CD1	1:A:250:LEU:N	2.81	0.43
1:A:410:TYR:OH	1:A:486:LEU:HB3	2.18	0.43
1:A:442:LYS:HE3	1:A:493:PHE:CE1	2.53	0.43
1:A:494:LEU:O	1:A:497:GLU:HB2	2.19	0.43
1:B:422:LEU:HD21	1:B:451:ALA:CB	2.48	0.43
1:B:450:ALA:HA	1:B:453:GLU:HG3	2.00	0.43
1:B:559:TYR:CE2	1:B:563:ARG:HG3	2.53	0.43
1:A:337:PRO:O	1:A:338:HIS:C	2.57	0.43
1:A:374:GLY:O	1:A:376:GLN:N	2.47	0.43
1:A:423:SER:HB3	1:A:464:GLU:HB2	2.01	0.43
1:B:42:PHE:CD1	1:B:53:LEU:HD13	2.53	0.43
1:B:343:TYR:O	1:B:348:HIS:NE2	2.48	0.43
1:B:613:VAL:HG13	1:B:628:LYS:HA	2.00	0.43
1:A:47:VAL:HB	1:A:51:LYS:HG2	2.01	0.43
1:A:138:ARG:HD2	1:A:138:ARG:C	2.39	0.43
1:A:229:LYS:O	1:A:233:GLN:HG3	2.18	0.43
1:B:132:GLU:O	1:B:133:ASN:C	2.56	0.43
1:B:204:TYR:HA	1:B:213:MET:HA	1.99	0.43
1:B:243:HIS:HB3	1:B:533:GLU:HG3	1.99	0.43
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.82	0.43
1:A:80:LEU:CD1	1:A:129:ILE:HG12	2.49	0.43
1:A:110:ILE:HG22	1:A:112:GLN:N	2.32	0.43
1:A:526:ARG:CG	1:A:526:ARG:NH1	2.81	0.43
1:A:106:TYR:CD1	1:A:108:PHE:CE1	3.06	0.43
1:A:311:ASP:HB2	1:A:312:HIS:CD2	2.54	0.43
1:B:292:HIS:HA	1:B:358:ALA:O	2.19	0.43
1:A:36:LYS:HB2	1:A:36:LYS:HZ2	1.82	0.43
1:A:79:HIS:O	1:A:80:LEU:C	2.56	0.43
1:A:155:TYR:O	1:A:159:LEU:HD13	2.18	0.43
1:A:236:GLU:OE2	1:A:239:LYS:HD2	2.19	0.43
1:B:45:GLN:HB3	1:B:47:VAL:HG12	1.99	0.43
1:B:72:VAL:HG22	1:B:184:VAL:HG22	2.00	0.43
1:B:119:PHE:O	1:B:123:GLU:N	2.48	0.43
1:B:298:LEU:HD21	1:B:331:LEU:HD23	2.01	0.43
1:A:376:GLN:O	1:A:526:ARG:NH1	2.52	0.43
1:B:48:ASP:OD1	1:B:49:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLU:O	1:B:167:GLU:HG2	2.19	0.43
1:B:281:ILE:CG2	1:B:282:VAL:N	2.82	0.43
1:A:128:GLN:HA	1:A:131:ASN:HD22	1.81	0.42
1:A:151:SER:O	1:A:153:ASP:N	2.52	0.42
1:A:353:LEU:HD22	1:A:353:LEU:HA	1.78	0.42
1:A:374:GLY:C	1:A:376:GLN:H	2.23	0.42
1:A:385:ASP:OD1	1:A:386:SER:N	2.52	0.42
1:A:554:ASN:ND2	1:A:556:ASP:N	2.51	0.42
1:B:165:GLU:O	1:B:166:ASP:HB3	2.19	0.42
1:B:458:TYR:CD2	1:B:460:GLU:HG3	2.54	0.42
1:B:478:THR:HG21	1:B:480:MET:HE2	2.01	0.42
1:B:631:PHE:CD2	1:B:632:ILE:HD12	2.54	0.42
1:A:157:LEU:CA	1:A:160:ILE:HG22	2.49	0.42
1:A:326:THR:O	1:A:327:GLU:HG2	2.20	0.42
1:B:42:PHE:CB	1:B:47:VAL:HG11	2.49	0.42
1:B:87:ARG:HH12	1:B:128:GLN:HG3	1.83	0.42
1:B:231:HIS:O	1:B:231:HIS:CG	2.71	0.42
1:B:384:ASN:ND2	1:B:521:VAL:H	2.12	0.42
1:B:428:GLU:OE2	1:B:435:ASP:HB3	2.18	0.42
1:A:6:ILE:HD13	1:A:25:ILE:HD11	2.02	0.42
1:A:162:ALA:O	1:A:167:GLU:OE1	2.38	0.42
1:A:265:LEU:HD23	1:B:296:PRO:CD	2.49	0.42
1:A:300:ASN:HD22	1:A:327:GLU:HB3	1.84	0.42
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.86	0.42
1:B:186:VAL:HA	1:B:187:PRO:HD2	1.76	0.42
1:B:494:LEU:HD21	1:B:498:ARG:HD2	1.99	0.42
1:A:20:THR:HG22	1:A:21:THR:N	2.33	0.42
1:A:605:ASP:O	1:A:606:LYS:C	2.55	0.42
1:B:336:CYS:HA	1:B:387:HIS:CE1	2.55	0.42
1:B:391:ARG:HB3	1:B:503:TYR:OH	2.19	0.42
1:A:108:PHE:O	1:A:214:LEU:HG	2.19	0.42
1:A:155:TYR:HB3	1:A:205:TRP:HZ3	1.84	0.42
1:A:281:ILE:HD12	1:A:281:ILE:HA	1.74	0.42
1:A:625:THR:HG22	1:A:626:VAL:N	2.35	0.42
1:B:51:LYS:HA	1:B:52:PRO:HD3	1.87	0.42
1:B:74:ARG:CG	1:B:221:ALA:HB3	2.20	0.42
1:B:81:MET:O	1:B:85:ILE:HG12	2.20	0.42
1:B:471:LYS:HB2	1:B:490:GLN:CG	2.41	0.42
1:A:79:HIS:NE2	4:A:1003:HOH:O	2.11	0.42
1:A:563:ARG:HH11	1:A:563:ARG:CG	2.31	0.42
1:B:19:GLY:O	1:B:20:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLU:O	1:B:75:HIS:N	2.43	0.42
1:B:205:TRP:HB2	1:B:211:ASN:ND2	2.35	0.42
1:A:258:LEU:O	1:A:258:LEU:CD2	2.67	0.42
1:A:353:LEU:HD12	1:A:391:ARG:N	2.34	0.42
1:A:566:GLN:NE2	1:A:577:SER:HA	2.23	0.42
1:B:153:ASP:HB2	1:B:156:LYS:HD2	2.01	0.42
1:A:265:LEU:HD23	1:B:296:PRO:HD3	2.02	0.42
1:A:363:MET:O	1:A:381:MET:HG2	2.20	0.42
1:A:627:GLU:O	1:A:628:LYS:C	2.54	0.42
1:B:352:GLU:O	1:B:355:ILE:HG13	2.19	0.42
1:B:553:VAL:HG21	1:B:604:GLY:HA3	2.02	0.42
1:A:460:GLU:OE1	1:A:460:GLU:HA	2.20	0.42
1:A:546:LYS:HE2	1:A:577:SER:OG	2.20	0.42
1:B:85:ILE:HG13	1:B:108:PHE:CE2	2.54	0.42
1:B:92:VAL:HB	1:B:109:ASP:CB	2.44	0.42
1:B:135:LYS:O	1:B:174:GLN:HG2	2.19	0.42
1:B:633:TRP:CD1	1:B:633:TRP:C	2.93	0.42
1:A:34:ARG:NH2	4:A:1045:HOH:O	2.48	0.41
1:A:72:VAL:O	1:A:73:LEU:C	2.58	0.41
1:A:447:LEU:HD11	1:A:471:LYS:C	2.40	0.41
1:A:589:ILE:CG2	1:A:616:ARG:NH1	2.83	0.41
1:B:8:PHE:HB3	1:B:10:ASP:OD1	2.20	0.41
1:B:194:GLU:CD	1:B:225:LYS:HG2	2.40	0.41
1:B:423:SER:HB3	1:B:464:GLU:C	2.40	0.41
1:A:400:LYS:CG	1:A:454:LEU:HD13	2.43	0.41
1:A:644:HIS:ND1	1:A:645:ARG:N	2.68	0.41
1:B:334:MET:SD	3:B:2002:TSB:N	2.83	0.41
1:B:448:LYS:HD3	1:B:460:GLU:OE2	2.19	0.41
1:B:545:PRO:HB2	4:B:2012:HOH:O	2.19	0.41
1:A:364:HIS:HA	1:A:379:ARG:O	2.20	0.41
1:B:33:LEU:O	1:B:37:ALA:N	2.42	0.41
1:B:107:ASP:OD1	1:B:216:ARG:HB2	2.20	0.41
1:A:70:LEU:CD2	1:A:74:ARG:CZ	2.99	0.41
1:A:645:ARG:O	1:A:645:ARG:CG	2.62	0.41
1:B:94:PHE:CE2	1:B:108:PHE:HE1	2.39	0.41
1:B:430:LYS:HG2	1:B:431:GLU:H	1.85	0.41
1:A:490:GLN:HG2	1:A:490:GLN:H	1.55	0.41
1:B:82:ALA:HB1	1:B:94:PHE:CD2	2.55	0.41
1:B:114:ILE:HG13	1:B:115:SER:N	2.35	0.41
1:B:402:VAL:HG22	1:B:403:VAL:N	2.34	0.41
1:A:8:PHE:CB	1:A:9:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:OE1	1:A:27:GLN:HA	2.21	0.41
1:A:83:HIS:ND1	1:A:177:PHE:HB3	2.36	0.41
1:A:410:TYR:HH	1:A:487:SER:HG	1.57	0.41
1:B:23:GLU:O	1:B:26:ALA:HB3	2.21	0.41
1:B:203:ALA:O	1:B:214:LEU:CD2	2.69	0.41
1:B:636:VAL:O	1:B:639:ILE:HB	2.20	0.41
1:A:36:LYS:HE3	1:A:63:THR:OG1	2.21	0.41
1:A:204:TYR:HE1	1:A:207:GLY:CA	2.25	0.41
1:A:340:MET:CE	1:A:389:PHE:CE2	3.04	0.41
1:A:340:MET:CE	1:A:389:PHE:CZ	3.04	0.41
1:A:414:GLY:HA3	1:A:644:HIS:CE1	2.55	0.41
1:B:72:VAL:HG22	1:B:184:VAL:CG2	2.50	0.41
1:B:252:LEU:HD22	1:B:270:GLY:HA2	2.03	0.41
1:B:422:LEU:HD21	1:B:451:ALA:HB2	2.03	0.41
1:A:7:GLN:O	1:A:58:SER:HA	2.20	0.41
1:A:45:GLN:O	1:A:47:VAL:HG13	2.21	0.41
1:A:584:LYS:O	1:A:587:TYR:HB3	2.21	0.41
1:B:47:VAL:O	1:B:47:VAL:CG2	2.69	0.41
1:B:105:TYR:CD1	1:B:105:TYR:C	2.93	0.41
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.31	0.41
1:B:143:ARG:NH2	1:B:160:ILE:O	2.54	0.41
1:B:174:GLN:HE21	1:B:174:GLN:HB3	1.64	0.41
1:B:267:LEU:HB3	4:B:2014:HOH:O	2.20	0.41
1:B:304:TYR:OH	1:B:332:ARG:HB3	2.21	0.41
1:B:521:VAL:CG2	1:B:527:PHE:CE1	2.97	0.41
1:A:120:GLU:O	1:A:120:GLU:HG2	2.20	0.41
1:A:348:HIS:HA	1:A:352:GLU:OE2	2.21	0.41
1:A:353:LEU:HD13	1:A:390:VAL:HA	2.03	0.41
1:A:499:PHE:O	1:A:500:ASP:C	2.59	0.41
1:A:521:VAL:CG2	1:A:527:PHE:CE1	3.03	0.41
1:B:94:PHE:HE2	1:B:108:PHE:HE1	1.69	0.41
1:B:100:ILE:HB	1:B:101:GLU:H	1.49	0.41
1:B:426:ASP:O	1:B:427:PRO:C	2.59	0.41
1:B:480:MET:C	1:B:482:LYS:N	2.72	0.41
1:B:581:ARG:HE	1:B:581:ARG:HB2	1.75	0.41
1:B:585:MET:CE	1:B:602:VAL:HG11	2.51	0.41
1:B:623:GLN:O	1:B:624:GLU:C	2.59	0.41
1:B:628:LYS:O	1:B:632:ILE:HD13	2.21	0.41
1:A:467:PHE:CD1	1:A:467:PHE:O	2.72	0.41
1:A:482:LYS:HZ2	1:A:482:LYS:CA	2.34	0.41
1:A:542:TRP:CE2	1:A:543:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:TYR:O	1:B:465:ALA:HB3	2.20	0.41
1:A:81:MET:SD	1:A:197:LEU:HD21	2.61	0.40
1:A:293:VAL:HB	1:B:266:TRP:O	2.20	0.40
1:A:435:ASP:O	1:A:436:ASP:C	2.60	0.40
1:A:603:VAL:HG12	1:A:603:VAL:O	2.21	0.40
1:B:83:HIS:CG	1:B:177:PHE:HB2	2.55	0.40
1:B:131:ASN:N	1:B:131:ASN:HD22	2.18	0.40
1:B:155:TYR:OH	1:B:159:LEU:HD22	2.21	0.40
1:B:268:PRO:N	4:B:2014:HOH:O	2.53	0.40
1:B:336:CYS:HB2	1:B:337:PRO:CD	2.50	0.40
1:B:454:LEU:HB3	1:B:456:LEU:CD1	2.44	0.40
1:B:544:ALA:O	1:B:545:PRO:C	2.59	0.40
1:B:85:ILE:HG22	1:B:85:ILE:O	2.21	0.40
1:B:122:ILE:O	1:B:126:MET:HE3	2.21	0.40
1:B:622:ASP:O	1:B:623:GLN:C	2.60	0.40
1:A:30:SER:HA	1:A:31:PRO:HD3	1.88	0.40
1:A:324:ASP:C	1:A:326:THR:N	2.75	0.40
1:A:405:MET:SD	1:A:520:VAL:HG21	2.61	0.40
1:A:498:ARG:H	1:A:498:ARG:HG2	1.69	0.40
1:A:612:GLN:HB3	4:A:1004:HOH:O	2.22	0.40
1:B:143:ARG:CG	1:B:143:ARG:NH1	2.83	0.40
1:B:499:PHE:HB2	1:B:501:LEU:HG	2.03	0.40
1:A:191:LYS:CE	4:A:1007:HOH:O	2.70	0.40
1:A:357:ILE:N	1:A:357:ILE:HD13	2.37	0.40
1:A:526:ARG:NH1	3:A:1002:TSB:N3	2.69	0.40
1:B:4:ILE:HG22	1:B:16:PHE:N	2.29	0.40
1:B:68:GLU:H	1:B:68:GLU:HG2	1.74	0.40
1:B:93:LYS:H	1:B:109:ASP:HB2	1.86	0.40
1:B:343:TYR:CG	1:B:389:PHE:CD2	3.10	0.40
1:B:474:VAL:HB	1:B:487:SER:OG	2.21	0.40
1:A:386:SER:HB3	1:A:518:ARG:NH1	2.37	0.40
1:A:430:LYS:HB3	1:A:434:PHE:O	2.21	0.40
1:A:627:GLU:HG3	1:A:629:ASP:HB2	2.03	0.40
1:B:83:HIS:HE1	1:B:174:GLN:NE2	2.19	0.40
1:B:126:MET:C	1:B:128:GLN:H	2.24	0.40
1:B:326:THR:HG22	1:B:326:THR:O	2.21	0.40
1:B:392:PRO:HA	1:B:395:ILE:HD11	2.03	0.40
1:B:396:LYS:HD3	1:B:400:LYS:NZ	2.36	0.40
1:B:477:LYS:HB3	1:B:481:GLY:HA2	2.04	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	640/645 (99%)	525 (82%)	81 (13%)	34 (5%)	2 15
1	B	643/645 (100%)	471 (73%)	125 (19%)	47 (7%)	1 7
All	All	1283/1290 (100%)	996 (78%)	206 (16%)	81 (6%)	1 10

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	113	ASN
1	A	114	ILE
1	A	206	ARG
1	A	211	ASN
1	A	322	GLN
1	A	324	ASP
1	A	325	GLU
1	A	345	ASN
1	A	425	ARG
1	A	436	ASP
1	A	619	GLY
1	B	4	ILE
1	B	88	LEU
1	B	131	ASN
1	B	149	LEU
1	B	210	ASN
1	B	224	ASP
1	B	430	LYS
1	B	460	GLU
1	B	478	THR
1	B	482	LYS
1	B	555	VAL
1	B	596	LYS
1	B	622	ASP

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Mol	Chain	Res	Type
1	A	35	LYS
1	A	151	SER
1	A	152	ASN
1	A	162	ALA
1	A	164	PRO
1	A	175	GLY
1	A	188	SER
1	A	314	GLN
1	A	374	GLY
1	A	375	LEU
1	A	395	ILE
1	A	536	LYS
1	B	187	PRO
1	B	205	TRP
1	B	206	ARG
1	B	211	ASN
1	B	314	GLN
1	B	621	GLN
1	B	635	LEU
1	A	116	SER
1	A	427	PRO
1	A	508	GLY
1	A	559	TYR
1	B	100	ILE
1	B	352	GLU
1	B	436	ASP
1	B	544	ALA
1	B	642	LYS
1	A	62	VAL
1	A	209	SER
1	A	560	ASP
1	A	585	MET
1	B	9	PRO
1	B	115	SER
1	B	166	ASP
1	B	203	ALA
1	B	426	ASP
1	B	624	GLU
1	B	37	ALA
1	B	97	GLY
1	B	114	ILE
1	B	201	ALA

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Mol	Chain	Res	Type
1	B	588	LYS
1	B	64	PRO
1	B	133	ASN
1	B	268	PRO
1	B	481	GLY
1	B	545	PRO
1	A	372	VAL
1	B	395	ILE
1	B	427	PRO
1	B	44	GLY
1	B	508	GLY
1	A	163	ILE
1	B	30	SER
1	B	636	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	567/570 (100%)	485 (86%)	82 (14%)	3	15
1	B	570/570 (100%)	497 (87%)	73 (13%)	4	20
All	All	1137/1140 (100%)	982 (86%)	155 (14%)	3	17

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	17	ASP
1	A	34	ARG
1	A	36	LYS
1	A	46	LEU
1	A	55	THR
1	A	63	THR
1	A	66	SER
1	A	70	LEU

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Mol	Chain	Res	Type
1	A	74	ARG
1	A	86	LYS
1	A	96	VAL
1	A	106	TYR
1	A	117	ASP
1	A	125	THR
1	A	129	ILE
1	A	131	ASN
1	A	135	LYS
1	A	138	ARG
1	A	140	VAL
1	A	141	VAL
1	A	165	GLU
1	A	166	ASP
1	A	172	TYR
1	A	186	VAL
1	A	200	THR
1	A	204	TYR
1	A	208	ASP
1	A	210	ASN
1	A	211	ASN
1	A	214	LEU
1	A	226	LYS
1	A	232	LEU
1	A	236	GLU
1	A	241	ARG
1	A	249	GLU
1	A	255	ASN
1	A	258	LEU
1	A	281	ILE
1	A	287	SER
1	A	313	TYR
1	A	316	ASP
1	A	321	MET
1	A	323	LEU
1	A	328	SER
1	A	330	VAL
1	A	333	PRO
1	A	340	MET
1	A	353	LEU
1	A	356	ARG
1	A	366	TYR

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Mol	Chain	Res	Type
1	A	401	ARG
1	A	407	ILE
1	A	421	ARG
1	A	423	SER
1	A	428	GLU
1	A	429	ASP
1	A	456	LEU
1	A	467	PHE
1	A	471	LYS
1	A	476	VAL
1	A	482	LYS
1	A	483	GLU
1	A	490	GLN
1	A	491	LEU
1	A	502	THR
1	A	509	GLU
1	A	512	ARG
1	A	518	ARG
1	A	526	ARG
1	A	545	PRO
1	A	550	ILE
1	A	554	ASN
1	A	555	VAL
1	A	563	ARG
1	A	568	GLU
1	A	594	MET
1	A	605	ASP
1	A	611	ASN
1	A	622	ASP
1	A	623	GLN
1	A	629	ASP
1	B	2	GLU
1	B	6	ILE
1	B	13	LYS
1	B	17	ASP
1	B	45	GLN
1	B	49	LEU
1	B	63	THR
1	B	70	LEU
1	B	71	GLU
1	B	79	HIS
1	B	89	TYR

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Mol	Chain	Res	Type
1	B	93	LYS
1	B	94	PHE
1	B	100	ILE
1	B	106	TYR
1	B	109	ASP
1	B	111	ASP
1	B	128	GLN
1	B	136	ILE
1	B	143	ARG
1	B	144	ASP
1	B	153	ASP
1	B	167	GLU
1	B	174	GLN
1	B	176	ASP
1	B	179	ASP
1	B	184	VAL
1	B	193	LYS
1	B	195	PHE
1	B	200	THR
1	B	213	MET
1	B	214	LEU
1	B	233	GLN
1	B	234	MET
1	B	250	LEU
1	B	254	THR
1	B	268	PRO
1	B	284	LYS
1	B	292	HIS
1	B	313	TYR
1	B	323	LEU
1	B	328	SER
1	B	336	CYS
1	B	351	ARG
1	B	353	LEU
1	B	365	ARG
1	B	366	TYR
1	B	372	VAL
1	B	402	VAL
1	B	417	ASP
1	B	425	ARG
1	B	426	ASP
1	B	428	GLU

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Mol	Chain	Res	Type
1	B	431	GLU
1	B	436	ASP
1	B	437	ASP
1	B	458	TYR
1	B	471	LYS
1	B	494	LEU
1	B	497	GLU
1	B	507	ASP
1	B	512	ARG
1	B	518	ARG
1	B	521	VAL
1	B	545	PRO
1	B	563	ARG
1	B	595	GLN
1	B	601	ILE
1	B	602	VAL
1	B	606	LYS
1	B	611	ASN
1	B	621	GLN
1	B	645	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	128	GLN
1	A	131	ASN
1	A	168	ASN
1	A	174	GLN
1	A	210	ASN
1	A	215	GLN
1	A	255	ASN
1	A	312	HIS
1	A	384	ASN
1	A	441	ASN
1	A	475	GLN
1	A	554	ASN
1	A	564	GLN
1	A	566	GLN
1	A	582	ASN
1	A	595	GLN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	611	ASN
1	A	612	GLN
1	A	623	GLN
1	B	7	GLN
1	B	27	GLN
1	B	43	ASN
1	B	83	HIS
1	B	131	ASN
1	B	211	ASN
1	B	233	GLN
1	B	269	ASN
1	B	376	GLN
1	B	384	ASN
1	B	445	ASN
1	B	475	GLN
1	B	582	ASN
1	B	593	GLN
1	B	595	GLN
1	B	600	GLN
1	B	611	ASN
1	B	612	GLN
1	B	617	GLN
1	B	634	ASN
1	B	644	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TSB	B	2002	2	29,32,32	2.11	3 (10%)	33,48,48	1.15	3 (9%)
3	TSB	A	1002	2	29,32,32	2.23	3 (10%)	33,48,48	1.17	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TSB	B	2002	2	-	1/18/39/39	0/3/3/3
3	TSB	A	1002	2	-	0/18/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	TSB	O2S-S1	8.79	1.49	1.42
3	B	2002	TSB	O2S-S1	8.20	1.49	1.42
3	A	1002	TSB	O1S-S1	6.77	1.48	1.42
3	B	2002	TSB	O1S-S1	6.49	1.48	1.42
3	A	1002	TSB	C-N8	-2.94	1.32	1.37
3	B	2002	TSB	C-N8	-2.77	1.32	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	TSB	C-CA-N	3.53	115.67	110.28
3	A	1002	TSB	C-CA-N	3.07	114.97	110.28
3	B	2002	TSB	C-N8-S1	-2.77	120.12	124.61
3	A	1002	TSB	C5'-O5'-S1	2.41	122.35	117.37
3	A	1002	TSB	C5-C6-N6	2.40	124.00	120.35
3	B	2002	TSB	C5-C6-N6	2.24	123.75	120.35
3	A	1002	TSB	C-N8-S1	-2.16	121.11	124.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	TSB	C4'-C5'-O5'-S1

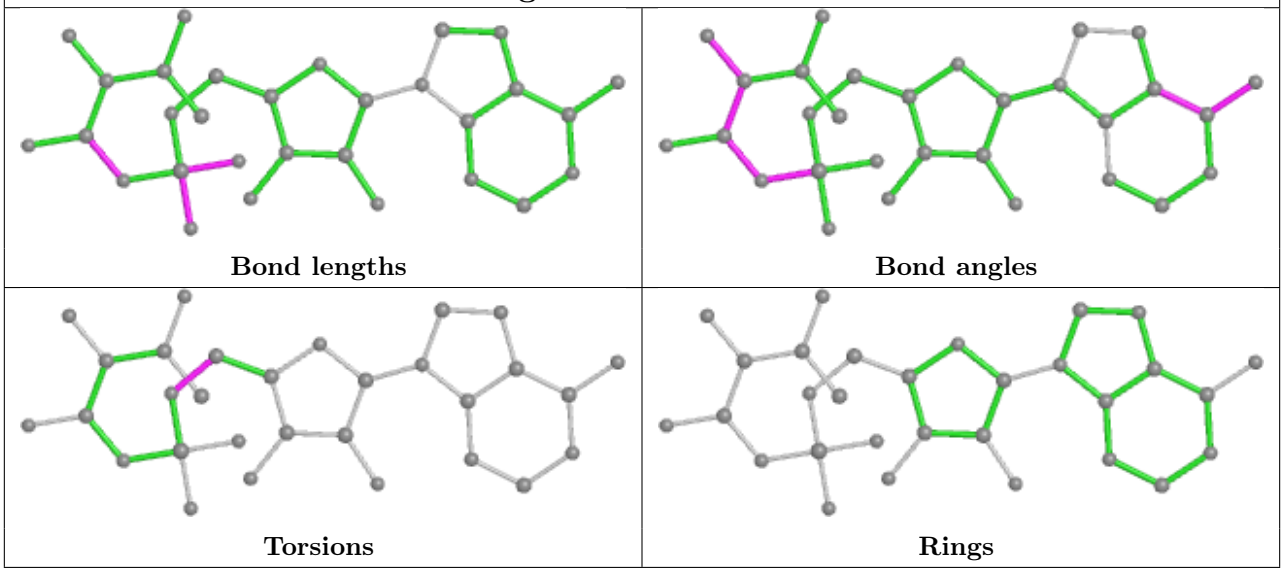
There are no ring outliers.

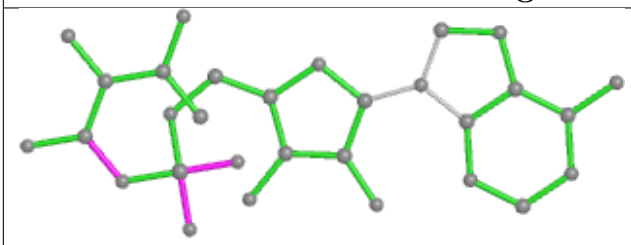
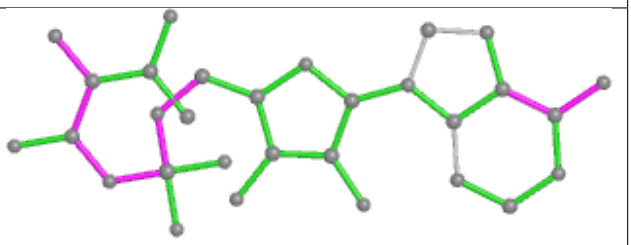
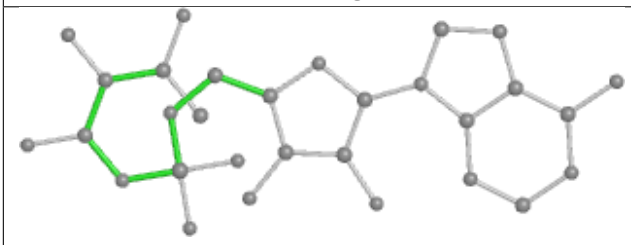
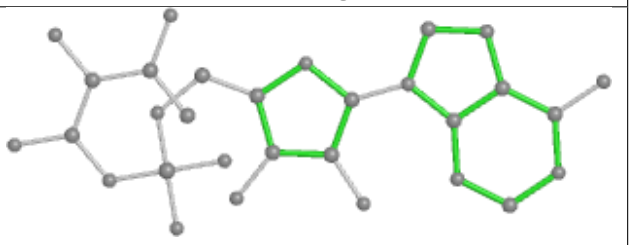
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2002	TSB	3	0
3	A	1002	TSB	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TSB B 2002



Ligand TSB A 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

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	642/645 (99%)	-0.34	21 (3%)	46	30	19, 54, 113, 144	0
1	B	645/645 (100%)	-0.05	37 (5%)	23	13	24, 71, 156, 182	0
All	All	1287/1290 (99%)	-0.20	58 (4%)	33	21	19, 61, 144, 182	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	9.3
1	B	211	ASN	5.8
1	B	152	ASN	5.6
1	B	2	GLU	5.0
1	A	433	TYR	4.8
1	B	162	ALA	4.8
1	A	430	LYS	4.7
1	A	164	PRO	4.5
1	B	431	GLU	4.4
1	B	208	ASP	4.3
1	B	164	PRO	4.1
1	A	426	ASP	4.0
1	B	163	ILE	4.0
1	B	433	TYR	4.0
1	B	183	GLY	3.7
1	B	117	ASP	3.7
1	B	175	GLY	3.6
1	B	1	MET	3.6
1	A	429	ASP	3.6
1	B	645	ARG	3.5
1	A	371	ALA	3.5
1	A	434	PHE	3.5
1	A	166	ASP	3.4
1	B	113	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	SER	3.3
1	A	432	LYS	3.2
1	B	210	ASN	3.2
1	B	165	GLU	3.1
1	A	325	GLU	3.1
1	B	434	PHE	3.1
1	B	100	ILE	3.1
1	A	370	GLY	3.1
1	A	165	GLU	2.9
1	B	133	ASN	2.9
1	A	324	ASP	2.9
1	B	166	ASP	2.9
1	A	431	GLU	2.9
1	B	88	LEU	2.8
1	A	163	ILE	2.7
1	B	207	GLY	2.7
1	A	168	ASN	2.7
1	B	97	GLY	2.7
1	B	116	SER	2.7
1	B	169	VAL	2.7
1	B	89	TYR	2.6
1	B	430	LYS	2.5
1	A	91	ASN	2.5
1	A	152	ASN	2.5
1	B	206	ARG	2.4
1	B	203	ALA	2.3
1	A	90	GLY	2.2
1	B	506	GLN	2.2
1	B	432	LYS	2.2
1	B	429	ASP	2.2
1	A	645	ARG	2.1
1	B	205	TRP	2.1
1	B	426	ASP	2.1
1	A	57	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

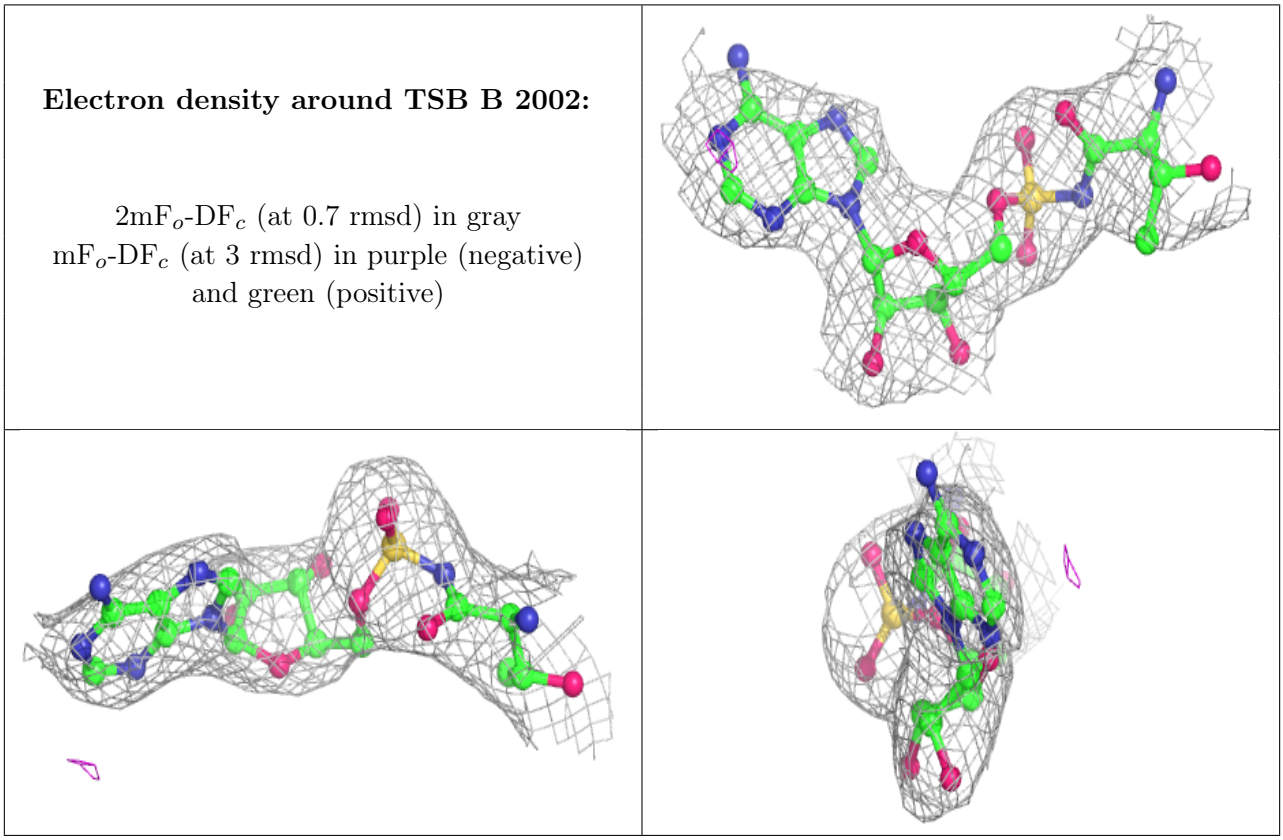
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TSB	B	2002	30/30	0.95	0.18	41,48,50,51	0
3	TSB	A	1002	30/30	0.97	0.16	33,37,41,41	0
2	ZN	B	2001	1/1	0.99	0.15	52,52,52,52	0
2	ZN	A	1001	1/1	1.00	0.15	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

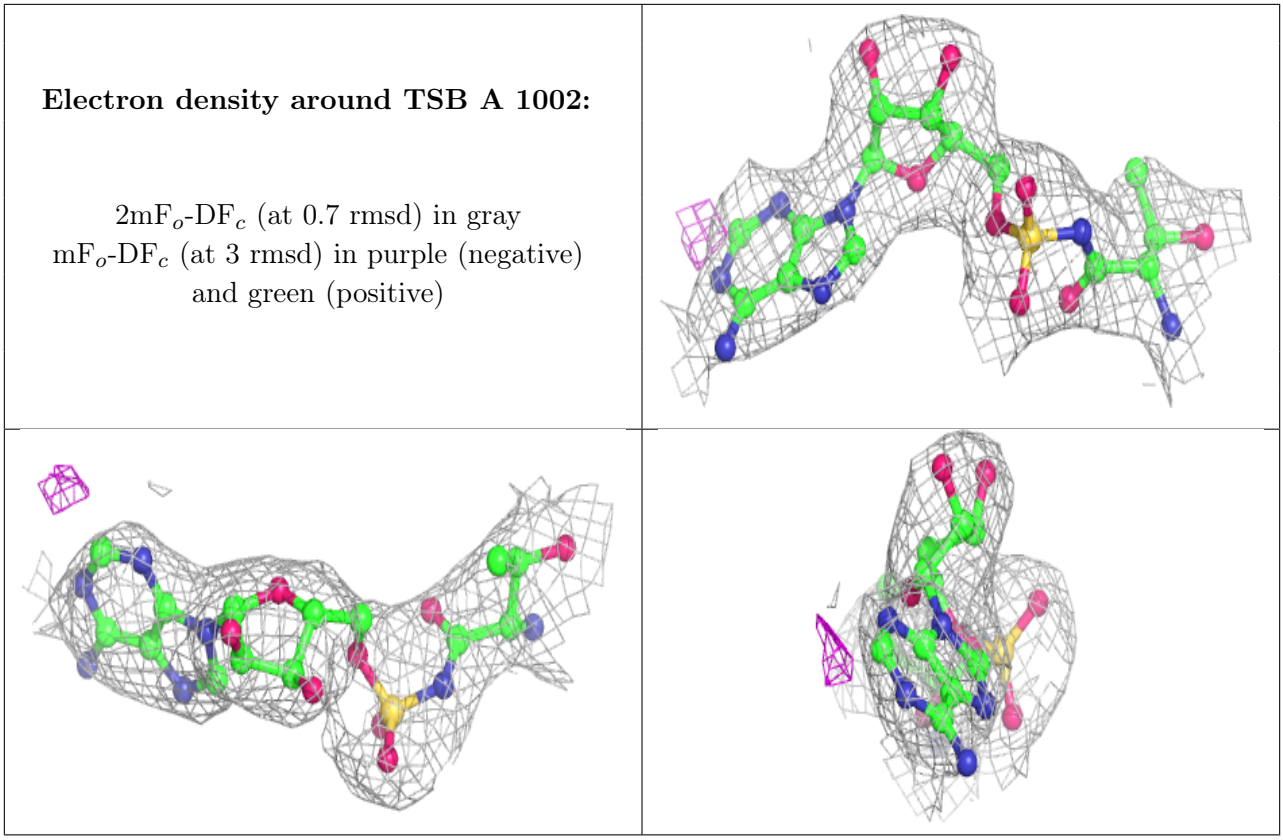
Electron density around TSB B 2002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around TSB A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.