Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:31 PM EST

PDB ID	:	3AL0
Title	:	Crystal structure of the glutamine transamidosome from Thermotoga maritima in the glutamylation state.
Authors	:	Ito, T.; Yokoyama, S.
Deposited on	:	2010-07-19
Resolution	:	3.37 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:

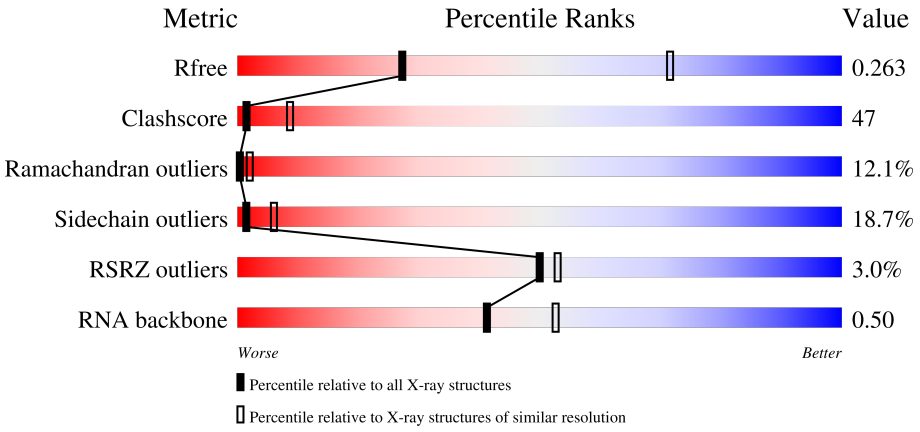
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.37 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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	475	4% 26% 54% 18% ··
2	B	482	5% 29% 47% 21% ·
3	C	592	% 29% 50% 14% · 5%
4	E	74	32% 54% 9% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GSU	C	1001	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13869 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3672	2342	625	690	15	0	0	0

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	482	3891	2462	662	744	23	0	0	0

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C,Linker,Glutamate--tRNA ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	564	4692	3007	794	874	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	expression tag	UNP Q9WY94
C	1	GLY	-	expression tag	UNP Q9WY94

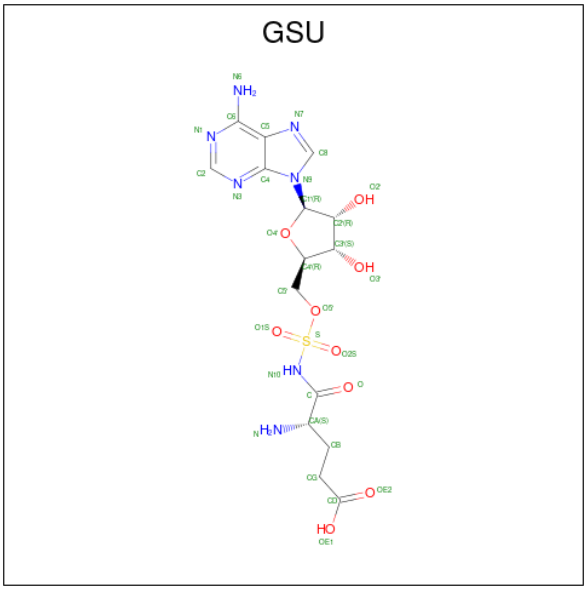
- Molecule 4 is a RNA chain called tRNAGln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	E	74	1581	703	281	523	74	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: $C_{15}H_{21}N_7O_9S$).

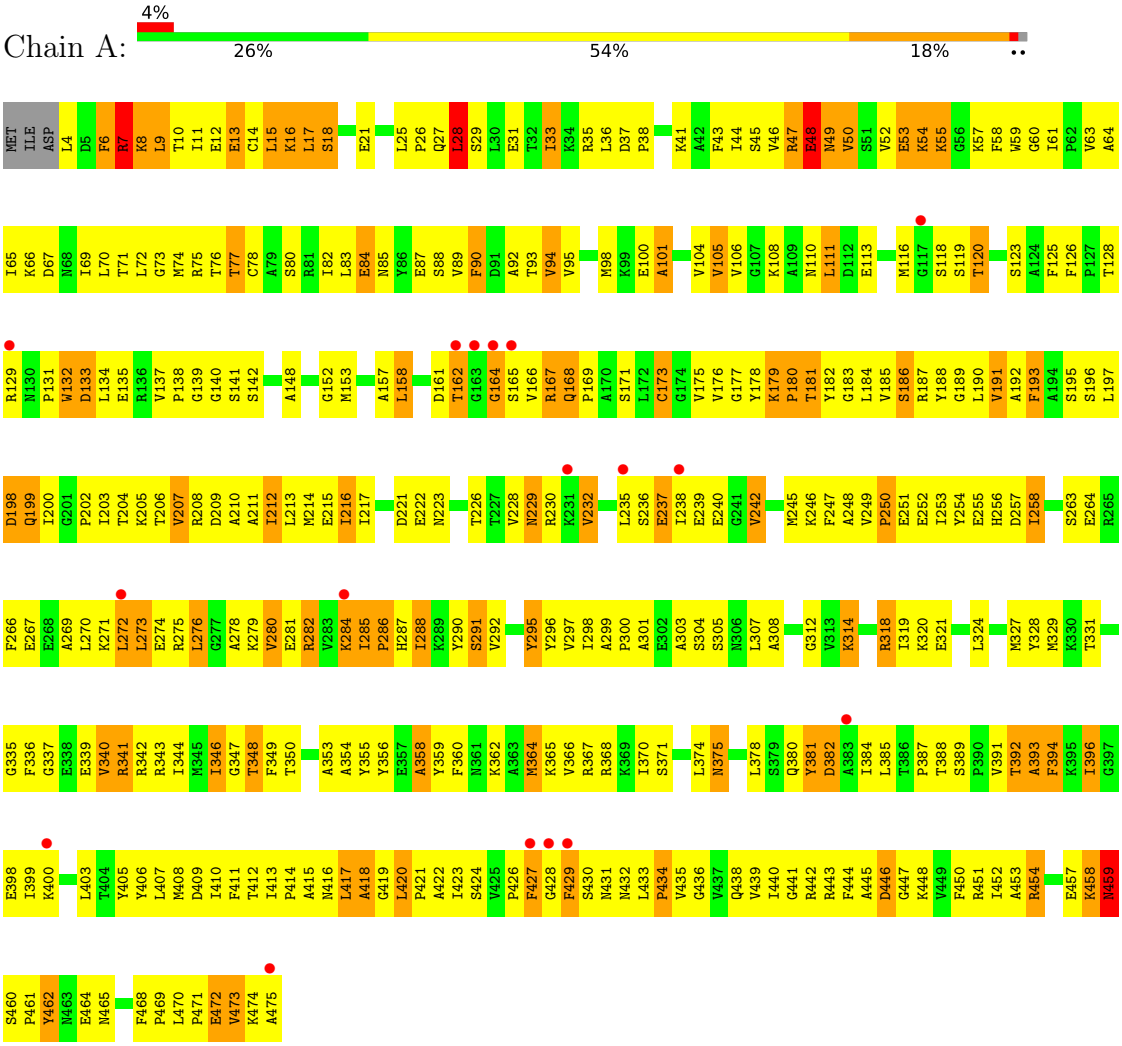


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 32	C 15	N 7	O 9	S 1	0	0

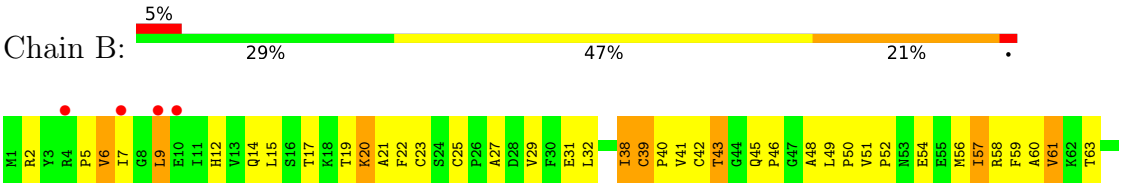
3 Residue-property plots (i)

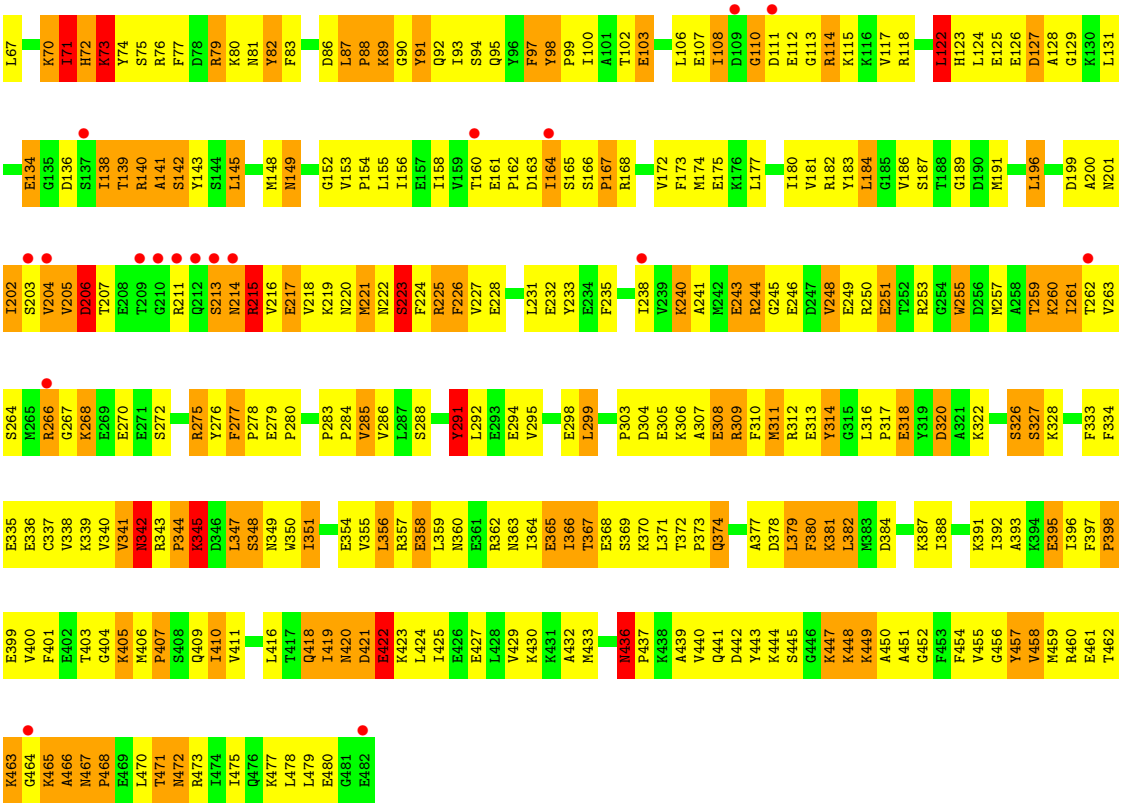
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



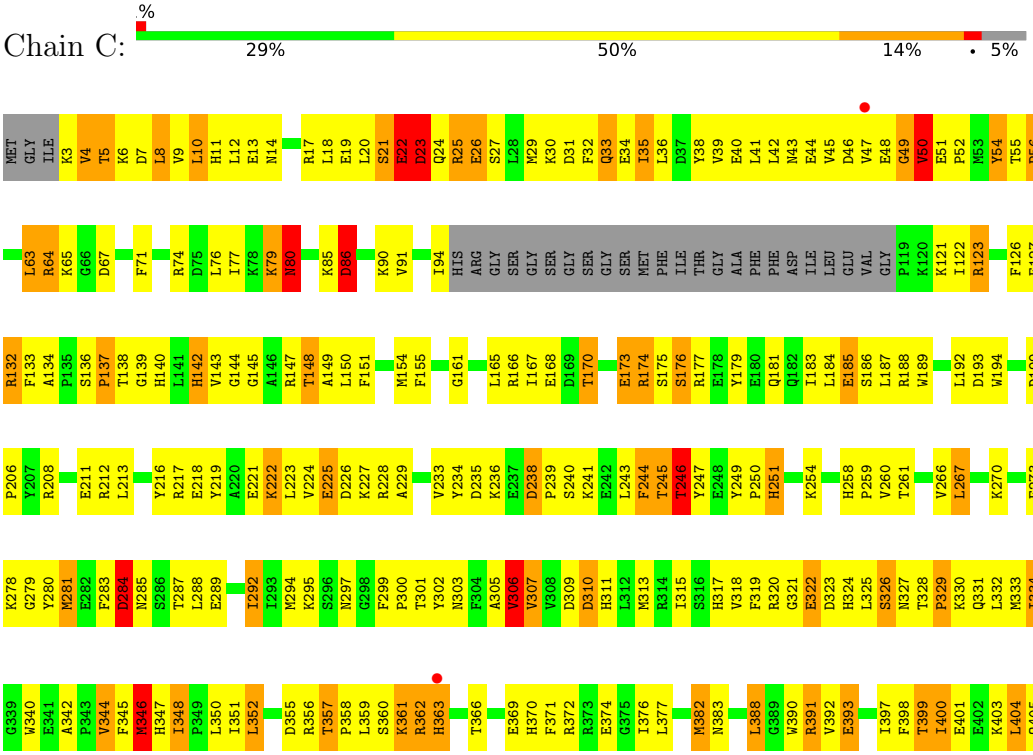
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

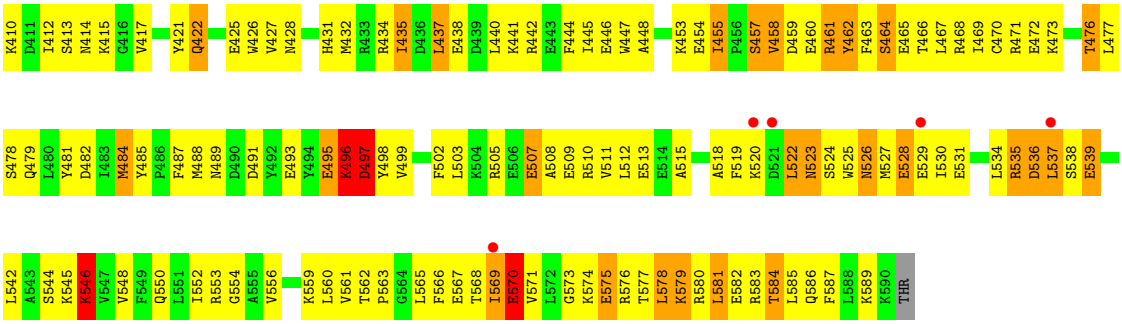




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C,Linker,Glutamate--tRNA ligase 2

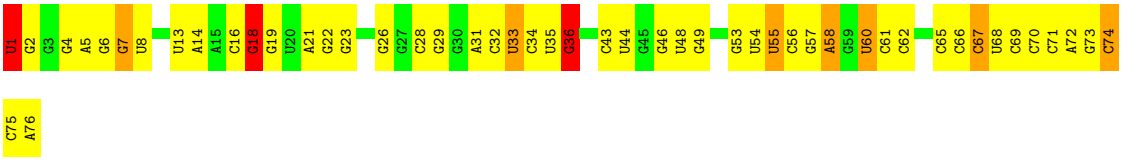
Chain C:





• Molecule 4: tRNAGln

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	76.95Å 125.66Å 313.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 3.37 48.67 – 3.37	Depositor EDS
% Data completeness (in resolution range)	92.7 (48.67-3.37) 92.7 (48.67-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	5.11 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.195 , 0.269 0.181 , 0.263	Depositor DCC
R_{free} test set	2068 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 99.9	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	0.94	EDS
Total number of atoms	13869	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: GSU, 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	0.31	0/3740	0.54	0/5047
2	B	0.40	0/3964	0.63	0/5336
3	C	0.43	0/4798	0.65	2/6453 (0.0%)
4	E	0.84	1/1765 (0.1%)	0.93	5/2749 (0.2%)
All	All	0.47	1/14267 (0.0%)	0.66	7/19585 (0.0%)

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
4	E	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	U	OP3-P	-7.12	1.52	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	23	G	OP2-P-O3'	6.15	118.74	105.20
3	C	223	LEU	CA-CB-CG	5.33	127.55	115.30
3	C	306	VAL	CB-CA-C	-5.23	101.47	111.40
4	E	36	G	O4'-C1'-N9	-5.21	104.03	108.20
4	E	55	U	C5'-C4'-C3'	-5.13	107.80	116.00
4	E	1	U	OP1-P-OP2	-5.10	111.95	119.60
4	E	36	G	C4-N9-C1'	5.08	133.10	126.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	1	U	Sidechain
4	E	18	G	Sidechain
4	E	67	C	Sidechain
4	E	7	G	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	3672	0	3734	377	0
2	B	3891	0	3905	444	0
3	C	4692	0	4654	429	0
4	E	1581	0	800	68	0
5	B	1	0	0	0	0
6	C	32	0	20	11	0
All	All	13869	0	13113	1258	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 47.

All (1258) 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)
3:C:546:LYS:NZ	4:E:35:U:H5'	1.59	1.16
1:A:8:LYS:HB3	1:A:470:LEU:HD12	1.38	1.05
1:A:52:VAL:HG22	1:A:104:VAL:HG11	1.32	1.05
4:E:6:G:H2'	4:E:7:G:H5'	1.36	1.04
1:A:378:LEU:HG	1:A:442:ARG:HA	1.40	1.01
3:C:143:VAL:HG23	3:C:351:ILE:HD11	1.40	0.99
2:B:181:VAL:HG13	2:B:186:VAL:HG23	1.45	0.98
3:C:148:THR:HG21	6:C:1001:GSU:N3	1.77	0.98
1:A:250:PRO:HB2	1:A:253:ILE:HB	1.45	0.97
3:C:546:LYS:HZ3	4:E:35:U:H5'	0.83	0.96
3:C:473:LYS:HD2	4:E:36:G:H21	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:SER:HB2	2:B:291:TYR:HB3	1.47	0.95
1:A:267:GLU:HA	1:A:270:LEU:HD13	1.49	0.94
1:A:132:TRP:CZ2	1:A:434:PRO:HG2	2.01	0.94
1:A:17:LEU:O	1:A:21:GLU:HB2	1.67	0.93
1:A:202:PRO:HB3	1:A:213:LEU:HD12	1.49	0.92
3:C:132:ARG:HH12	6:C:1001:GSU:CD	1.82	0.92
2:B:200:ALA:O	2:B:217:GLU:HA	1.69	0.92
3:C:422:GLN:HE21	3:C:422:GLN:H	1.14	0.91
1:A:442:ARG:HB3	1:A:445:ALA:HB3	1.53	0.90
1:A:120:THR:HG21	1:A:128:THR:HB	1.53	0.90
1:A:207:VAL:HG11	1:A:453:ALA:HB1	1.53	0.90
2:B:75:SER:HB3	2:B:285:VAL:HG12	1.52	0.89
3:C:546:LYS:HZ3	4:E:35:U:C5'	1.79	0.89
2:B:45:GLN:HG3	2:B:46:PRO:HD2	1.55	0.88
2:B:351:ILE:HA	2:B:355:VAL:HB	1.56	0.88
1:A:367:ARG:O	1:A:371:SER:HB2	1.73	0.88
1:A:349:PHE:HB2	3:C:12:LEU:HD21	1.56	0.88
2:B:76:ARG:HG3	2:B:76:ARG:HH11	1.39	0.88
1:A:65:ILE:HD11	1:A:69:ILE:HG21	1.56	0.87
3:C:400:ILE:HD13	3:C:400:ILE:H	1.38	0.87
2:B:111:ASP:HB3	2:B:168:ARG:HD2	1.55	0.86
1:A:246:LYS:HG2	1:A:279:LYS:HD2	1.57	0.86
3:C:576:ARG:HD3	3:C:580:ARG:HH21	1.39	0.86
1:A:188:TYR:CD1	1:A:223:ASN:HB3	2.11	0.86
1:A:141:SER:HB2	1:A:165:SER:HB3	1.58	0.85
1:A:285:ILE:HD13	1:A:288:ILE:HG21	1.58	0.85
1:A:181:THR:HG21	1:A:444:PHE:H	1.40	0.85
2:B:457:TYR:HE2	2:B:461:GLU:HG3	1.40	0.85
2:B:464:GLY:O	2:B:465:LYS:HB2	1.74	0.85
1:A:285:ILE:HD12	1:A:285:ILE:H	1.42	0.84
2:B:86:ASP:O	2:B:128:ALA:HB1	1.78	0.83
1:A:166:VAL:HB	1:A:203:ILE:HD11	1.58	0.83
1:A:111:LEU:O	1:A:123:SER:HB2	1.79	0.83
2:B:457:TYR:CE2	2:B:461:GLU:HG3	2.13	0.83
1:A:161:ASP:HA	1:A:165:SER:HB2	1.58	0.83
1:A:169:PRO:O	1:A:173:CYS:HB2	1.78	0.83
1:A:392:THR:HG22	1:A:433:LEU:HB2	1.60	0.83
2:B:432:ALA:HA	2:B:457:TYR:CE1	2.13	0.82
1:A:374:LEU:HD11	1:A:414:PRO:HB2	1.62	0.81
3:C:36:LEU:O	3:C:39:VAL:HG12	1.81	0.81
3:C:139:GLY:HA2	3:C:179:TYR:CD1	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ARG:HD3	2:B:278:PRO:HB3	1.64	0.80
3:C:362:ARG:H	3:C:362:ARG:HD3	1.47	0.80
2:B:19:THR:HG21	3:C:64:ARG:HD2	1.64	0.80
3:C:527:MET:O	3:C:530:ILE:HG22	1.83	0.79
3:C:132:ARG:NH1	6:C:1001:GSU:OE1	2.15	0.79
1:A:365:LYS:HD3	3:C:50:VAL:HG23	1.65	0.79
3:C:128:LEU:HD23	3:C:128:LEU:H	1.46	0.78
3:C:138:THR:HA	3:C:174:ARG:O	1.83	0.78
1:A:217:ILE:HG13	1:A:217:ILE:O	1.83	0.78
2:B:392:ILE:O	2:B:396:ILE:HG12	1.84	0.78
2:B:95:GLN:HB2	2:B:123:HIS:HB2	1.64	0.78
3:C:332:LEU:O	3:C:336:GLU:HG2	1.82	0.78
1:A:93:THR:HG21	1:A:221:ASP:OD2	1.84	0.77
2:B:420:ASN:HD22	2:B:420:ASN:C	1.88	0.77
3:C:437:LEU:H	3:C:437:LEU:CD1	1.98	0.77
3:C:509:GLU:O	3:C:513:GLU:HB2	1.84	0.77
2:B:126:GLU:HG2	2:B:152:GLY:HA2	1.67	0.77
3:C:139:GLY:HA2	3:C:179:TYR:HD1	1.48	0.77
2:B:205:VAL:HG12	2:B:206:ASP:N	2.00	0.77
4:E:6:G:C2'	4:E:7:G:H5'	2.15	0.77
1:A:209:ASP:HA	1:A:212:ILE:HG22	1.65	0.77
2:B:183:TYR:CE2	2:B:303:PRO:HD3	2.19	0.77
1:A:365:LYS:HE2	3:C:52:PRO:HD3	1.67	0.76
2:B:255:TRP:HB2	2:B:262:THR:HG22	1.67	0.76
3:C:143:VAL:HG23	3:C:351:ILE:CD1	2.14	0.76
2:B:354:GLU:HB3	2:B:397:PHE:CE2	2.19	0.76
1:A:178:TYR:HD2	1:A:423:ILE:HG12	1.50	0.76
2:B:314:TYR:OH	2:B:338:VAL:HG11	1.84	0.76
1:A:178:TYR:CD2	1:A:423:ILE:HG12	2.21	0.76
3:C:525:TRP:CD1	3:C:525:TRP:O	2.39	0.75
3:C:132:ARG:HG2	3:C:315:ILE:HD13	1.69	0.75
3:C:422:GLN:HE21	3:C:422:GLN:N	1.85	0.75
2:B:341:VAL:HG12	2:B:343:ARG:HG2	1.68	0.75
2:B:455:VAL:HG11	4:E:19:G:C2	2.22	0.75
3:C:5:THR:HG21	3:C:8:LEU:HD13	1.68	0.75
1:A:384:ILE:HG22	1:A:385:LEU:H	1.51	0.75
3:C:9:VAL:HG21	3:C:25:ARG:HH22	1.52	0.75
1:A:140:GLY:H	1:A:168:GLN:NE2	1.84	0.74
1:A:252:GLU:HA	1:A:255:GLU:HG3	1.68	0.74
1:A:304:SER:HB2	1:A:348:THR:HG23	1.69	0.74
2:B:97:PHE:O	2:B:98:TYR:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:ILE:HD11	2:B:411:VAL:HG21	1.69	0.74
1:A:65:ILE:HD12	1:A:158:LEU:HD23	1.70	0.74
1:A:161:ASP:HB2	1:A:166:VAL:HG13	1.69	0.73
2:B:20:LYS:HA	2:B:27:ALA:HB2	1.69	0.73
1:A:328:TYR:HE1	2:B:83:PHE:HB3	1.53	0.73
2:B:261:ILE:HG22	2:B:262:THR:H	1.53	0.73
2:B:318:GLU:H	2:B:318:GLU:CD	1.91	0.73
2:B:38:ILE:HD13	2:B:38:ILE:H	1.52	0.73
2:B:432:ALA:HA	2:B:457:TYR:HE1	1.52	0.73
1:A:52:VAL:CG2	1:A:104:VAL:HG11	2.14	0.73
2:B:7:ILE:HD13	2:B:231:LEU:HD13	1.71	0.73
3:C:10:LEU:O	3:C:14:ASN:HB2	1.88	0.72
3:C:307:VAL:HG11	3:C:334:ILE:HG22	1.72	0.72
2:B:181:VAL:C	2:B:183:TYR:H	1.93	0.72
3:C:147:ARG:NH2	3:C:412:ILE:HD11	2.03	0.72
1:A:418:ALA:HB3	1:A:420:LEU:HG	1.69	0.72
2:B:51:VAL:HG23	2:B:51:VAL:O	1.89	0.72
3:C:129:VAL:O	3:C:130:ARG:HG2	1.90	0.72
2:B:337:CYS:HB3	2:B:347:LEU:HD11	1.71	0.71
2:B:379:LEU:O	2:B:382:LEU:HB3	1.89	0.71
3:C:317:HIS:HB3	3:C:319:PHE:CE1	2.25	0.71
2:B:29:VAL:HG22	2:B:29:VAL:O	1.90	0.71
2:B:140:ARG:NH2	2:B:141:ALA:HA	2.04	0.71
2:B:263:VAL:HG12	2:B:264:SER:N	2.05	0.71
2:B:177:LEU:O	2:B:181:VAL:HG23	1.90	0.71
1:A:248:ALA:HB2	1:A:381:TYR:CE1	2.25	0.71
2:B:134:GLU:HB3	2:B:141:ALA:HB3	1.70	0.71
3:C:224:VAL:HG13	3:C:229:ALA:O	1.89	0.71
3:C:400:ILE:HD13	3:C:400:ILE:N	2.05	0.71
3:C:515:ALA:HA	3:C:537:LEU:HD11	1.71	0.71
2:B:166:SER:HB2	2:B:168:ARG:HG2	1.72	0.71
2:B:320:ASP:OD2	2:B:348:SER:OG	2.06	0.71
3:C:582:GLU:HA	3:C:585:LEU:HD12	1.73	0.71
1:A:406:TYR:CD2	3:C:35:ILE:HD11	2.25	0.71
2:B:29:VAL:HG23	2:B:32:LEU:CD2	2.20	0.71
2:B:86:ASP:HB2	2:B:129:GLY:O	1.90	0.71
3:C:574:LYS:HG2	3:C:578:LEU:HD23	1.73	0.71
1:A:11:ILE:HG23	1:A:61:ILE:HD13	1.72	0.70
1:A:12:GLU:HA	1:A:15:LEU:HG	1.74	0.70
2:B:181:VAL:HG11	2:B:187:SER:HB3	1.74	0.70
2:B:424:LEU:HA	2:B:427:GLU:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:HB2	3:C:346:MET:HG2	1.74	0.70
2:B:19:THR:HG23	2:B:23:CYS:O	1.91	0.69
3:C:573:GLY:O	3:C:577:THR:HG23	1.91	0.69
2:B:25:CYS:SG	2:B:39:CYS:HB3	2.31	0.69
3:C:472:GLU:O	3:C:473:LYS:HD3	1.92	0.69
2:B:181:VAL:CG1	2:B:186:VAL:HG23	2.22	0.69
2:B:127:ASP:HB2	2:B:155:LEU:HG	1.75	0.69
3:C:458:VAL:HG23	3:C:459:ASP:N	2.08	0.69
1:A:458:LYS:HG3	1:A:459:ASN:HD22	1.58	0.69
3:C:32:PHE:O	3:C:35:ILE:HG22	1.91	0.69
3:C:132:ARG:NH2	6:C:1001:GSU:OE2	2.21	0.69
3:C:142:HIS:CD2	3:C:145:GLY:H	2.11	0.69
3:C:317:HIS:CD2	3:C:344:VAL:HG21	2.27	0.69
2:B:12:HIS:HD2	2:B:155:LEU:HD13	1.56	0.69
2:B:183:TYR:OH	2:B:328:LYS:HG3	1.92	0.69
2:B:180:ILE:HG23	2:B:184:LEU:HD21	1.74	0.68
3:C:138:THR:HG21	3:C:174:ARG:NH1	2.08	0.68
3:C:437:LEU:N	3:C:437:LEU:HD12	2.08	0.68
2:B:180:ILE:O	2:B:183:TYR:HB3	1.93	0.68
2:B:362:ARG:HD2	2:B:364:ILE:HD11	1.74	0.68
1:A:423:ILE:HD12	1:A:453:ALA:HB2	1.75	0.68
2:B:284:PRO:HG2	3:C:59:ASP:HB2	1.76	0.68
1:A:398:GLU:HG2	1:A:405:TYR:OH	1.93	0.68
2:B:110:GLY:C	2:B:112:GLU:H	1.97	0.68
1:A:238:ILE:HG23	1:A:239:GLU:H	1.59	0.68
3:C:266:VAL:HG22	3:C:333:MET:SD	2.33	0.68
3:C:79:LYS:O	3:C:79:LYS:HG3	1.94	0.68
3:C:577:THR:O	3:C:581:LEU:HB2	1.94	0.68
1:A:69:ILE:O	1:A:71:THR:HG23	1.93	0.68
1:A:89:VAL:HG12	3:C:76:LEU:HB3	1.75	0.68
1:A:164:GLY:HA3	1:A:412:THR:HB	1.76	0.68
2:B:317:PRO:HG2	2:B:320:ASP:HB2	1.75	0.68
3:C:355:ASP:O	3:C:357:THR:HG22	1.93	0.67
2:B:118:ARG:HB2	2:B:161:GLU:HG3	1.76	0.67
3:C:388:LEU:HD13	3:C:417:VAL:HG21	1.75	0.67
3:C:165:LEU:HD21	3:C:184:LEU:CD2	2.23	0.67
2:B:295:VAL:HG12	2:B:295:VAL:O	1.95	0.67
3:C:228:ARG:CZ	3:C:267:LEU:HD23	2.25	0.67
1:A:119:SER:HA	1:A:139:GLY:HA2	1.76	0.67
2:B:443:TYR:CD2	2:B:479:LEU:HD22	2.30	0.67
3:C:56:PRO:O	3:C:57:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:HH21	1:A:457:GLU:HG2	1.59	0.66
2:B:181:VAL:CG1	2:B:187:SER:HB3	2.24	0.66
3:C:170:THR:HG21	3:C:300:PRO:HG2	1.76	0.66
1:A:181:THR:H	1:A:184:LEU:HD12	1.61	0.66
2:B:335:GLU:HA	2:B:338:VAL:HG12	1.77	0.66
2:B:337:CYS:HB3	2:B:347:LEU:CD1	2.25	0.66
1:A:44:ILE:HD11	1:A:110:ASN:HD22	1.60	0.66
1:A:94:VAL:HG21	1:A:200:ILE:CD1	2.26	0.66
3:C:235:ASP:OD2	3:C:241:LYS:HE3	1.95	0.66
3:C:421:TYR:CE2	3:C:425:GLU:HB2	2.30	0.66
3:C:213:LEU:HD12	3:C:213:LEU:H	1.60	0.66
2:B:205:VAL:HG12	2:B:206:ASP:H	1.59	0.66
3:C:9:VAL:O	3:C:13:GLU:HG2	1.95	0.66
3:C:320:ARG:NH2	3:C:345:PHE:HE1	1.94	0.66
1:A:94:VAL:HG21	1:A:200:ILE:HD12	1.78	0.66
1:A:242:VAL:HG11	1:A:452:ILE:HG12	1.77	0.66
1:A:71:THR:HG22	1:A:95:VAL:HG21	1.78	0.66
2:B:294:GLU:O	2:B:298:GLU:HG2	1.95	0.66
2:B:424:LEU:HA	2:B:427:GLU:HG2	1.76	0.66
3:C:523:ASN:ND2	3:C:524:SER:H	1.94	0.66
2:B:344:PRO:HD2	2:B:345:LYS:HG2	1.77	0.66
2:B:455:VAL:HG22	2:B:472:ASN:HD21	1.59	0.66
2:B:473:ARG:HH21	2:B:473:ARG:HG2	1.59	0.66
3:C:325:LEU:C	3:C:327:ASN:H	2.00	0.66
3:C:576:ARG:HB3	3:C:580:ARG:HE	1.60	0.66
3:C:177:ARG:HH22	3:C:208:ARG:CZ	2.10	0.65
1:A:185:VAL:H	1:A:199:GLN:HE22	1.43	0.65
1:A:211:ALA:HB2	1:A:450:PHE:CD1	2.32	0.65
2:B:235:PHE:HA	2:B:238:ILE:HG22	1.78	0.65
1:A:252:GLU:HG3	1:A:255:GLU:HB2	1.78	0.65
4:E:6:G:H2'	4:E:7:G:C5'	2.22	0.65
3:C:128:LEU:H	3:C:128:LEU:CD2	2.09	0.65
1:A:8:LYS:HB3	1:A:470:LEU:CD1	2.23	0.65
2:B:112:GLU:HB2	2:B:168:ARG:HH21	1.61	0.65
3:C:498:TYR:CE1	3:C:554:GLY:HA3	2.32	0.65
2:B:278:PRO:O	2:B:280:PRO:HD3	1.97	0.65
2:B:305:GLU:HA	2:B:308:GLU:HB2	1.78	0.65
2:B:433:MET:CE	2:B:440:VAL:HG11	2.27	0.65
1:A:196:SER:HB2	1:A:367:ARG:HH12	1.62	0.65
3:C:338:PHE:HB3	3:C:340:TRP:CE2	2.32	0.64
2:B:263:VAL:HG12	2:B:264:SER:H	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ARG:NH2	3:C:362:ARG:HH12	1.95	0.64
1:A:140:GLY:HA3	1:A:169:PRO:HD3	1.79	0.64
2:B:437:PRO:HA	2:B:440:VAL:HG12	1.79	0.64
1:A:242:VAL:HG12	1:A:245:MET:SD	2.37	0.64
1:A:409:ASP:O	1:A:411:PHE:N	2.31	0.64
2:B:110:GLY:C	2:B:112:GLU:N	2.46	0.64
2:B:226:PHE:CE2	2:B:257:MET:HB2	2.33	0.64
2:B:433:MET:HE2	2:B:440:VAL:HG11	1.80	0.64
3:C:569:ILE:HG23	3:C:577:THR:HG21	1.80	0.64
1:A:110:ASN:ND2	1:A:111:LEU:H	1.95	0.64
1:A:307:LEU:HD22	1:A:344:ILE:HD11	1.78	0.64
2:B:139:THR:OG1	2:B:140:ARG:HG3	1.97	0.64
3:C:138:THR:HG21	3:C:174:ARG:HH11	1.63	0.64
3:C:303:ASN:O	3:C:306:VAL:HG23	1.97	0.64
2:B:136:ASP:OD2	2:B:139:THR:HG23	1.97	0.63
3:C:473:LYS:HD2	4:E:36:G:N2	2.08	0.63
2:B:57:ILE:O	2:B:61:VAL:HG13	1.98	0.63
2:B:51:VAL:HG21	3:C:64:ARG:NH2	2.13	0.63
3:C:42:LEU:O	3:C:45:VAL:HG13	1.98	0.63
1:A:16:LYS:O	1:A:17:LEU:HD23	1.97	0.63
1:A:350:THR:HG22	1:A:360:PHE:HB2	1.79	0.63
1:A:367:ARG:HG3	1:A:417:LEU:HB3	1.80	0.63
1:A:13:GLU:O	1:A:17:LEU:HD21	1.99	0.63
2:B:75:SER:HB3	2:B:285:VAL:CG1	2.26	0.63
3:C:388:LEU:HD13	3:C:417:VAL:CG2	2.29	0.63
1:A:116:MET:CE	1:A:340:VAL:HA	2.29	0.63
2:B:295:VAL:HA	2:B:298:GLU:HG2	1.80	0.63
1:A:77:THR:HB	1:A:84:GLU:HA	1.80	0.63
1:A:93:THR:OG1	1:A:186:SER:HB3	1.98	0.63
2:B:191:MET:HG2	2:B:196:LEU:HB3	1.79	0.63
2:B:364:ILE:HG22	2:B:365:GLU:N	2.13	0.62
3:C:321:GLY:O	3:C:323:ASP:N	2.32	0.62
2:B:143:TYR:CD1	3:C:90:LYS:HE3	2.34	0.62
3:C:463:PHE:HD1	3:C:488:MET:CE	2.12	0.62
1:A:43:PHE:HE1	1:A:148:ALA:HB1	1.64	0.62
2:B:249:GLU:HG2	2:B:250:ARG:N	2.14	0.62
3:C:561:VAL:HG12	4:E:35:U:O2'	1.99	0.62
2:B:93:ILE:HD12	2:B:93:ILE:N	2.15	0.62
2:B:455:VAL:HG22	2:B:472:ASN:ND2	2.14	0.62
3:C:49:GLY:O	3:C:50:VAL:HG13	2.00	0.62
3:C:217:ARG:N	3:C:294:MET:HE1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:THR:O	2:B:260:LYS:HB2	2.00	0.62
3:C:283:PHE:CD2	3:C:329:PRO:HG3	2.34	0.62
3:C:428:ASN:ND2	3:C:476:THR:HA	2.14	0.62
2:B:429:VAL:O	2:B:432:ALA:HB3	1.98	0.62
1:A:216:ILE:HG22	1:A:217:ILE:HG23	1.81	0.62
1:A:403:LEU:HD21	3:C:34:GLU:HB3	1.80	0.62
3:C:277:LEU:HD12	3:C:278:LYS:NZ	2.14	0.62
3:C:325:LEU:O	3:C:327:ASN:N	2.32	0.62
1:A:137:VAL:HG21	1:A:394:PHE:CE1	2.34	0.62
1:A:137:VAL:HG21	1:A:394:PHE:CZ	2.35	0.61
1:A:161:ASP:CG	1:A:165:SER:H	2.03	0.61
2:B:463:LYS:O	2:B:464:GLY:C	2.38	0.61
1:A:407:LEU:C	1:A:409:ASP:H	2.04	0.61
2:B:447:LYS:HB2	2:B:447:LYS:NZ	2.14	0.61
2:B:226:PHE:HE2	2:B:257:MET:HA	1.65	0.61
3:C:463:PHE:HD1	3:C:488:MET:HE1	1.66	0.61
1:A:427:PHE:CE2	1:A:460:SER:HB2	2.35	0.61
2:B:477:LYS:HG2	2:B:478:LEU:HD23	1.81	0.61
3:C:40:GLU:C	3:C:42:LEU:H	2.04	0.61
3:C:472:GLU:C	3:C:473:LYS:HD3	2.20	0.61
2:B:241:ALA:C	2:B:243:GLU:H	2.03	0.61
3:C:531:GLU:HG3	3:C:566:PHE:CZ	2.35	0.61
1:A:375:ASN:HD21	1:A:443:ARG:HB2	1.65	0.61
2:B:388:ILE:CG2	2:B:393:ALA:HB2	2.30	0.61
2:B:420:ASN:HB3	2:B:467:ASN:HB2	1.82	0.61
1:A:196:SER:CB	1:A:367:ARG:HH12	2.13	0.61
2:B:7:ILE:CG1	2:B:202:ILE:HG22	2.30	0.61
3:C:129:VAL:C	3:C:130:ARG:HG2	2.20	0.61
2:B:17:THR:HG21	2:B:154:PRO:HG2	1.83	0.61
1:A:177:GLY:HA2	1:A:203:ILE:HD13	1.82	0.60
1:A:206:THR:HG22	1:A:208:ARG:H	1.64	0.60
3:C:281:MET:HE1	4:E:4:G:O3'	2.01	0.60
1:A:67:ASP:OD2	1:A:77:THR:HG23	2.01	0.60
2:B:76:ARG:HG3	2:B:76:ARG:NH1	2.14	0.60
2:B:122:LEU:HD23	2:B:158:ILE:HG23	1.83	0.60
3:C:22:GLU:HA	3:C:25:ARG:HG3	1.82	0.60
3:C:139:GLY:CA	3:C:179:TYR:HD1	2.14	0.60
1:A:45:SER:HB2	1:A:108:LYS:H	1.66	0.60
2:B:350:TRP:HH2	2:B:393:ALA:O	1.83	0.60
2:B:341:VAL:HG21	2:B:377:ALA:HA	1.83	0.60
3:C:221:GLU:HA	3:C:224:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:512:LEU:HB3	3:C:585:LEU:HD21	1.83	0.60
2:B:358:GLU:HB3	2:B:362:ARG:HH11	1.67	0.60
3:C:31:ASP:O	3:C:35:ILE:HB	2.01	0.60
4:E:61:C:H2'	4:E:61:C:O2	2.01	0.60
2:B:166:SER:CB	2:B:168:ARG:HG2	2.31	0.60
3:C:498:TYR:CE2	3:C:503:LEU:HD13	2.37	0.60
1:A:208:ARG:HE	1:A:238:ILE:HD13	1.67	0.60
2:B:7:ILE:CD1	2:B:231:LEU:HD13	2.32	0.60
1:A:215:GLU:O	1:A:215:GLU:HG3	2.00	0.60
1:A:407:LEU:O	1:A:409:ASP:N	2.33	0.60
2:B:143:TYR:CE1	2:B:145:LEU:HD11	2.36	0.60
3:C:487:PHE:CZ	3:C:568:THR:HG23	2.37	0.60
1:A:119:SER:HB3	1:A:394:PHE:HZ	1.66	0.60
2:B:391:LYS:CD	2:B:459:MET:HE2	2.32	0.60
3:C:321:GLY:HA3	6:C:1001:GSU:O2'	2.02	0.60
1:A:384:ILE:HB	1:A:440:ILE:HB	1.84	0.59
2:B:448:LYS:O	2:B:450:ALA:N	2.35	0.59
3:C:350:LEU:HD13	3:C:358:PRO:HB3	1.84	0.59
2:B:224:PHE:O	2:B:227:VAL:HG12	2.02	0.59
2:B:425:ILE:N	2:B:425:ILE:HD12	2.17	0.59
2:B:29:VAL:HG23	2:B:32:LEU:HD23	1.84	0.59
2:B:310:PHE:HA	2:B:314:TYR:HB2	1.84	0.59
3:C:5:THR:HG23	3:C:8:LEU:H	1.68	0.59
1:A:179:LYS:HD2	1:A:179:LYS:O	2.02	0.59
3:C:273:PHE:HE2	3:C:283:PHE:HE2	1.49	0.59
1:A:94:VAL:HG12	1:A:217:ILE:HB	1.84	0.59
1:A:314:LYS:H	1:A:314:LYS:HD3	1.67	0.59
1:A:342:ARG:O	1:A:346:ILE:HG23	2.02	0.59
2:B:7:ILE:HG12	2:B:202:ILE:HG22	1.83	0.59
3:C:132:ARG:CG	3:C:315:ILE:HD13	2.32	0.59
3:C:437:LEU:CD1	3:C:437:LEU:N	2.59	0.59
1:A:403:LEU:H	1:A:403:LEU:HD12	1.67	0.59
2:B:266:ARG:HG2	2:B:267:GLY:N	2.18	0.59
2:B:381:LYS:O	2:B:382:LEU:HB2	2.03	0.59
3:C:241:LYS:NZ	3:C:243:LEU:HD11	2.18	0.59
1:A:258:ILE:HD12	1:A:263:SER:HB2	1.85	0.59
2:B:134:GLU:OE1	2:B:142:SER:HB3	2.03	0.59
3:C:13:GLU:OE2	3:C:20:LEU:HD12	2.03	0.59
3:C:33:GLN:HE21	3:C:33:GLN:HA	1.67	0.59
2:B:451:ALA:HB1	2:B:475:ILE:HG21	1.85	0.59
3:C:138:THR:OG1	3:C:361:LYS:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLN:HA	3:C:27:SER:OG	2.03	0.58
3:C:148:THR:CG2	6:C:1001:GSU:N3	2.60	0.58
3:C:151:PHE:CD2	3:C:348:ILE:HD11	2.38	0.58
3:C:151:PHE:CG	3:C:348:ILE:HD11	2.38	0.58
3:C:526:ASN:ND2	3:C:528:GLU:H	2.01	0.58
4:E:67:C:H2'	4:E:68:U:H6	1.68	0.58
2:B:112:GLU:HB2	2:B:168:ARG:NH2	2.18	0.58
3:C:400:ILE:H	3:C:400:ILE:CD1	2.07	0.58
1:A:47:ARG:HB2	1:A:106:VAL:O	2.02	0.58
3:C:276:LEU:HD12	3:C:276:LEU:H	1.68	0.58
3:C:519:PHE:HZ	3:C:534:LEU:HD11	1.67	0.58
3:C:586:GLN:O	3:C:589:LYS:HE2	2.03	0.58
1:A:116:MET:HE2	1:A:340:VAL:HG22	1.85	0.58
2:B:213:SER:O	2:B:248:VAL:HG22	2.03	0.58
2:B:250:ARG:O	2:B:251:GLU:HB3	2.04	0.58
3:C:147:ARG:HH21	3:C:412:ILE:HD11	1.66	0.58
3:C:311:HIS:CD2	3:C:340:TRP:CD2	2.91	0.58
3:C:470:CYS:SG	3:C:484:MET:HA	2.42	0.58
1:A:6:PHE:CD2	1:A:6:PHE:C	2.77	0.58
1:A:171:SER:O	1:A:435:VAL:HA	2.03	0.58
3:C:470:CYS:SG	3:C:484:MET:HG2	2.43	0.58
1:A:415:ALA:HA	1:A:420:LEU:HD12	1.86	0.58
2:B:20:LYS:HG2	2:B:27:ALA:HB2	1.85	0.58
2:B:338:VAL:HG13	2:B:339:LYS:N	2.19	0.58
1:A:43:PHE:HE1	1:A:148:ALA:CB	2.16	0.58
1:A:65:ILE:HG22	1:A:105:VAL:CG1	2.34	0.58
1:A:237:GLU:O	1:A:451:ARG:HG3	2.03	0.58
3:C:128:LEU:CD2	3:C:128:LEU:N	2.66	0.58
3:C:71:PHE:HB3	3:C:74:ARG:HG3	1.86	0.58
1:A:337:GLY:HA2	1:A:341:ARG:CZ	2.34	0.58
2:B:72:HIS:HB2	2:B:100:ILE:O	2.02	0.58
2:B:98:TYR:N	2:B:99:PRO:CD	2.67	0.58
2:B:180:ILE:CG2	2:B:184:LEU:HD21	2.33	0.58
2:B:299:LEU:HD12	2:B:299:LEU:O	2.03	0.58
3:C:14:ASN:O	3:C:17:ARG:HD3	2.03	0.58
3:C:280:TYR:C	3:C:280:TYR:CD2	2.77	0.58
2:B:59:PHE:CD1	2:B:186:VAL:HG12	2.38	0.57
3:C:9:VAL:HG21	3:C:25:ARG:NH2	2.19	0.57
3:C:393:GLU:O	3:C:393:GLU:HG3	2.04	0.57
1:A:132:TRP:CG	1:A:471:PRO:HB3	2.39	0.57
1:A:204:THR:HG21	1:A:210:ALA:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:VAL:CG1	2:B:206:ASP:N	2.67	0.57
3:C:56:PRO:O	3:C:57:VAL:CG2	2.52	0.57
1:A:36:LEU:HD11	1:A:473:VAL:HG21	1.87	0.57
1:A:398:GLU:HA	1:A:398:GLU:OE1	2.05	0.57
3:C:6:LYS:NZ	3:C:25:ARG:HH21	2.02	0.57
3:C:42:LEU:O	3:C:44:GLU:N	2.38	0.57
3:C:360:SER:OG	3:C:362:ARG:HB2	2.04	0.57
1:A:398:GLU:HG2	1:A:405:TYR:CZ	2.40	0.57
2:B:266:ARG:NH2	2:B:266:ARG:HB3	2.19	0.57
2:B:423:LYS:HE3	2:B:470:LEU:HD21	1.84	0.57
4:E:33:U:C6	4:E:33:U:H3'	2.40	0.57
1:A:285:ILE:HD12	1:A:285:ILE:N	2.17	0.57
1:A:378:LEU:HG	1:A:442:ARG:CA	2.27	0.57
3:C:4:VAL:HB	3:C:33:GLN:OE1	2.04	0.57
3:C:287:THR:OG1	3:C:288:LEU:HD22	2.04	0.57
1:A:285:ILE:HD13	1:A:288:ILE:CG2	2.33	0.57
2:B:181:VAL:HG13	2:B:186:VAL:CG2	2.30	0.57
2:B:401:PHE:O	2:B:401:PHE:CD1	2.58	0.57
3:C:511:VAL:HG22	3:C:542:LEU:HB3	1.87	0.57
4:E:65:C:H2'	4:E:66:C:H6	1.70	0.57
3:C:525:TRP:CH2	3:C:574:LYS:HA	2.40	0.57
3:C:553:ARG:HG3	3:C:565:LEU:HD13	1.85	0.57
4:E:70:C:H2'	4:E:71:C:C6	2.39	0.57
3:C:377:LEU:HD13	3:C:432:MET:HE2	1.86	0.57
3:C:548:VAL:O	3:C:552:ILE:HG12	2.04	0.57
2:B:421:ASP:O	2:B:422:GLU:C	2.43	0.57
3:C:525:TRP:CZ3	3:C:574:LYS:HA	2.40	0.57
2:B:108:ILE:C	2:B:110:GLY:N	2.57	0.56
2:B:311:MET:SD	2:B:318:GLU:HA	2.45	0.56
3:C:432:MET:HB2	3:C:440:LEU:HD13	1.87	0.56
2:B:15:LEU:HD11	2:B:156:ILE:HG13	1.87	0.56
2:B:86:ASP:HB3	2:B:131:LEU:HB2	1.88	0.56
2:B:243:GLU:O	2:B:244:ARG:HB2	2.05	0.56
2:B:456:GLY:HA3	4:E:19:G:O2'	2.05	0.56
3:C:179:TYR:O	3:C:183:ILE:HG13	2.05	0.56
3:C:465:GLU:OE1	3:C:468:ARG:HD3	2.05	0.56
3:C:584:THR:HA	3:C:587:PHE:HB3	1.88	0.56
4:E:18:G:H1'	4:E:57:G:N2	2.21	0.56
1:A:387:PRO:O	1:A:411:PHE:CD1	2.59	0.56
3:C:465:GLU:O	3:C:469:ILE:HG12	2.05	0.56
1:A:208:ARG:HG2	1:A:238:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:HB2	1:A:381:TYR:CZ	2.40	0.56
2:B:425:ILE:N	2:B:425:ILE:CD1	2.68	0.56
3:C:176:SER:OG	3:C:179:TYR:HD2	1.88	0.56
3:C:270:LYS:HA	3:C:284:ASP:HA	1.85	0.56
3:C:361:LYS:HE3	3:C:362:ARG:NH1	2.20	0.56
2:B:41:VAL:HG12	2:B:42:CYS:N	2.19	0.56
3:C:351:ILE:HD11	3:C:359:LEU:HD12	1.86	0.56
2:B:374:GLN:NE2	2:B:374:GLN:N	2.54	0.56
2:B:393:ALA:HA	2:B:396:ILE:HD11	1.87	0.56
4:E:13:U:H6	4:E:13:U:O5'	1.89	0.56
1:A:251:GLU:HG3	1:A:284:LYS:HG2	1.88	0.56
3:C:189:TRP:CZ2	3:C:372:ARG:HG3	2.41	0.56
4:E:71:C:O2'	4:E:72:A:H5'	2.04	0.56
1:A:300:PRO:CG	1:A:346:ILE:HD11	2.35	0.56
2:B:455:VAL:CG2	2:B:472:ASN:HD21	2.18	0.56
3:C:249:TYR:HD2	3:C:250:PRO:HD2	1.71	0.56
1:A:132:TRP:CD2	1:A:471:PRO:HB3	2.40	0.56
2:B:356:LEU:HD12	4:E:62:C:O3'	2.06	0.56
1:A:286:PRO:HG2	1:A:287:HIS:H	1.72	0.55
3:C:502:PHE:CE2	3:C:550:GLN:HB2	2.41	0.55
1:A:140:GLY:N	1:A:168:GLN:NE2	2.52	0.55
1:A:250:PRO:HB2	1:A:253:ILE:CB	2.27	0.55
3:C:469:ILE:HG22	3:C:563:PRO:CB	2.35	0.55
3:C:519:PHE:CZ	3:C:534:LEU:HD11	2.41	0.55
1:A:434:PRO:HB3	1:A:468:PHE:CZ	2.41	0.55
1:A:461:PRO:O	1:A:462:TYR:HB2	2.05	0.55
1:A:72:LEU:HA	1:A:88:SER:HB2	1.88	0.55
2:B:52:PRO:HB2	3:C:63:LEU:HB3	1.88	0.55
3:C:216:TYR:CE2	3:C:300:PRO:HG3	2.41	0.55
1:A:459:ASN:HD22	1:A:459:ASN:N	2.05	0.55
3:C:318:VAL:O	3:C:319:PHE:HD1	1.88	0.55
3:C:361:LYS:HE3	3:C:362:ARG:HH12	1.71	0.55
2:B:12:HIS:CD2	2:B:155:LEU:HD13	2.38	0.55
4:E:21:A:H61	4:E:46:G:H2'	1.70	0.55
1:A:37:ASP:HB3	1:A:38:PRO:HD3	1.89	0.55
2:B:189:GLY:O	2:B:196:LEU:HD12	2.07	0.55
2:B:364:ILE:HG22	2:B:365:GLU:O	2.06	0.55
3:C:236:LYS:HG3	3:C:258:HIS:CD2	2.41	0.55
3:C:306:VAL:O	3:C:309:ASP:N	2.38	0.55
3:C:362:ARG:H	3:C:362:ARG:CD	2.19	0.55
3:C:482:ASP:O	3:C:559:LYS:HE3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:HD2	1:A:327:MET:SD	2.47	0.55
1:A:384:ILE:HG22	1:A:385:LEU:N	2.21	0.55
2:B:259:THR:OG1	2:B:261:ILE:HG13	2.07	0.55
1:A:162:THR:HG21	1:A:193:PHE:CE2	2.42	0.55
1:A:300:PRO:O	1:A:347:GLY:HA3	2.07	0.55
1:A:328:TYR:CE1	2:B:83:PHE:HB3	2.37	0.55
1:A:392:THR:CG2	1:A:433:LEU:HB2	2.36	0.55
2:B:202:ILE:HD11	2:B:216:VAL:HB	1.89	0.55
2:B:421:ASP:O	2:B:422:GLU:O	2.24	0.55
3:C:25:ARG:C	3:C:27:SER:H	2.10	0.55
3:C:234:TYR:HB2	3:C:259:PRO:HG2	1.89	0.55
3:C:391:ARG:HG2	4:E:14:A:OP1	2.05	0.55
1:A:120:THR:CG2	1:A:128:THR:HB	2.34	0.54
2:B:79:ARG:CZ	2:B:91:TYR:CE1	2.89	0.54
2:B:172:VAL:HA	2:B:175:GLU:HB2	1.89	0.54
1:A:458:LYS:HG3	1:A:459:ASN:ND2	2.20	0.54
2:B:63:THR:HG22	2:B:186:VAL:HG21	1.89	0.54
2:B:126:GLU:CG	2:B:152:GLY:HA2	2.37	0.54
2:B:263:VAL:CG1	2:B:264:SER:H	2.21	0.54
3:C:434:ARG:O	3:C:434:ARG:HG2	2.06	0.54
3:C:553:ARG:HD2	3:C:560:LEU:O	2.08	0.54
1:A:73:GLY:O	1:A:74:MET:HG3	2.06	0.54
1:A:392:THR:HG21	1:A:431:ASN:HB2	1.88	0.54
2:B:59:PHE:CE1	2:B:186:VAL:HA	2.43	0.54
2:B:365:GLU:O	2:B:366:ILE:C	2.46	0.54
2:B:378:ASP:O	2:B:379:LEU:C	2.43	0.54
1:A:94:VAL:O	1:A:98:MET:HG2	2.08	0.54
1:A:314:LYS:HD3	1:A:314:LYS:N	2.23	0.54
2:B:338:VAL:CG1	2:B:339:LYS:N	2.71	0.54
2:B:406:MET:O	2:B:409:GLN:HB3	2.08	0.54
3:C:189:TRP:CE2	3:C:372:ARG:HG3	2.42	0.54
2:B:15:LEU:HD21	2:B:156:ILE:HD11	1.90	0.54
2:B:143:TYR:HD1	3:C:90:LYS:HG3	1.71	0.54
2:B:204:VAL:HG12	2:B:238:ILE:HD13	1.90	0.54
2:B:475:ILE:O	2:B:477:LYS:N	2.40	0.54
2:B:181:VAL:C	2:B:183:TYR:N	2.58	0.54
2:B:225:ARG:H	2:B:225:ARG:HE	1.55	0.54
3:C:148:THR:HG21	6:C:1001:GSU:C2	2.35	0.54
3:C:361:LYS:HG2	3:C:362:ARG:HH11	1.71	0.54
3:C:383:ASN:HD21	3:C:397:ILE:HA	1.73	0.54
2:B:340:VAL:HG11	2:B:373:PRO:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ILE:HB	2:B:410:ILE:HD11	1.89	0.54
2:B:457:TYR:HD2	2:B:457:TYR:C	2.10	0.54
3:C:236:LYS:HG3	3:C:258:HIS:NE2	2.23	0.54
3:C:466:THR:HG21	3:C:487:PHE:HD2	1.72	0.54
1:A:35:ARG:O	1:A:38:PRO:HD2	2.08	0.54
2:B:131:LEU:C	2:B:131:LEU:HD13	2.28	0.54
2:B:457:TYR:C	2:B:457:TYR:CD2	2.80	0.54
3:C:144:GLY:O	3:C:148:THR:HG23	2.08	0.54
2:B:403:THR:C	2:B:405:LYS:H	2.11	0.53
3:C:458:VAL:HG23	3:C:459:ASP:H	1.72	0.53
1:A:7:ARG:O	1:A:152:GLY:HA3	2.08	0.53
2:B:462:THR:C	2:B:463:LYS:O	2.46	0.53
3:C:6:LYS:O	3:C:6:LYS:HD3	2.08	0.53
3:C:579:LYS:O	3:C:582:GLU:N	2.42	0.53
1:A:33:ILE:HG12	1:A:153:MET:SD	2.48	0.53
1:A:138:PRO:O	1:A:169:PRO:HA	2.09	0.53
1:A:428:GLY:O	1:A:429:PHE:HB2	2.08	0.53
3:C:19:GLU:O	3:C:20:LEU:HG	2.08	0.53
3:C:216:TYR:CD2	3:C:300:PRO:HG3	2.43	0.53
1:A:349:PHE:HE2	3:C:8:LEU:HD21	1.72	0.53
2:B:263:VAL:CG1	2:B:264:SER:N	2.71	0.53
2:B:466:ALA:O	2:B:467:ASN:HB2	2.08	0.53
3:C:404:LEU:O	3:C:406:SER:N	2.41	0.53
2:B:380:PHE:HD1	2:B:380:PHE:H	1.57	0.53
3:C:278:LYS:HE3	3:C:322:GLU:OE2	2.07	0.53
3:C:302:TYR:OH	6:C:1001:GSU:HG2	2.09	0.53
2:B:391:LYS:HE3	4:E:19:G:O6	2.09	0.53
2:B:466:ALA:O	2:B:467:ASN:CB	2.56	0.53
3:C:459:ASP:HB3	3:C:462:TYR:HB3	1.90	0.53
2:B:139:THR:HG23	2:B:140:ARG:H	1.73	0.53
3:C:165:LEU:HD21	3:C:184:LEU:HD22	1.91	0.53
1:A:132:TRP:HH2	1:A:468:PHE:HE2	1.55	0.53
2:B:57:ILE:HG22	2:B:58:ARG:N	2.24	0.53
2:B:59:PHE:CG	2:B:186:VAL:HG12	2.44	0.52
2:B:344:PRO:HG2	2:B:345:LYS:H	1.74	0.52
2:B:203:SER:HB2	2:B:213:SER:HB2	1.89	0.52
2:B:380:PHE:O	2:B:382:LEU:N	2.42	0.52
3:C:502:PHE:HE2	3:C:550:GLN:HB2	1.73	0.52
3:C:525:TRP:O	3:C:525:TRP:CG	2.63	0.52
1:A:47:ARG:HD3	1:A:74:MET:SD	2.50	0.52
1:A:298:ILE:HG22	1:A:299:ALA:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:SER:HB3	2:B:248:VAL:CG1	2.39	0.52
2:B:241:ALA:C	2:B:243:GLU:N	2.63	0.52
1:A:181:THR:O	1:A:183:GLY:N	2.43	0.52
1:A:191:VAL:HG22	2:B:46:PRO:HB2	1.91	0.52
1:A:366:VAL:O	1:A:370:ILE:HG13	2.09	0.52
1:A:367:ARG:O	1:A:367:ARG:HG2	2.08	0.52
2:B:213:SER:HB3	2:B:248:VAL:CG2	2.39	0.52
2:B:284:PRO:HD3	3:C:54:TYR:OH	2.09	0.52
3:C:249:TYR:HE2	3:C:254:LYS:HD2	1.74	0.52
4:E:33:U:C6	4:E:33:U:C3'	2.92	0.52
1:A:298:ILE:O	1:A:301:ALA:HB3	2.09	0.52
2:B:74:TYR:HD2	2:B:286:VAL:HG12	1.74	0.52
2:B:107:GLU:HG3	2:B:115:LYS:O	2.09	0.52
2:B:140:ARG:CZ	2:B:141:ALA:HA	2.40	0.52
3:C:216:TYR:OH	3:C:309:ASP:OD1	2.28	0.52
3:C:408:ASP:C	3:C:410:LYS:H	2.13	0.52
1:A:360:PHE:HE2	1:A:364:MET:CE	2.22	0.52
2:B:277:PHE:CD1	2:B:277:PHE:C	2.83	0.52
3:C:39:VAL:O	3:C:42:LEU:HD23	2.09	0.52
1:A:10:THR:HG23	1:A:13:GLU:HB2	1.91	0.52
1:A:161:ASP:OD2	1:A:165:SER:N	2.42	0.52
3:C:377:LEU:HD13	3:C:432:MET:CE	2.39	0.52
1:A:119:SER:CB	1:A:394:PHE:HZ	2.21	0.52
3:C:56:PRO:C	3:C:57:VAL:HG22	2.29	0.52
3:C:437:LEU:H	3:C:437:LEU:HD13	1.74	0.52
3:C:38:TYR:O	3:C:38:TYR:CD1	2.63	0.52
3:C:520:LYS:HA	3:C:578:LEU:HD21	1.91	0.52
1:A:167:ARG:NH1	1:A:438:GLN:OE1	2.43	0.51
1:A:171:SER:HB2	1:A:424:SER:OG	2.10	0.51
2:B:80:LYS:HE2	2:B:276:TYR:OH	2.11	0.51
3:C:47:VAL:HG22	3:C:47:VAL:O	2.10	0.51
1:A:204:THR:OG1	1:A:205:LYS:N	2.43	0.51
2:B:363:ASN:O	2:B:364:ILE:HG12	2.09	0.51
2:B:457:TYR:HD2	2:B:457:TYR:O	1.92	0.51
2:B:473:ARG:HG2	2:B:473:ARG:NH2	2.25	0.51
3:C:398:PHE:CD1	3:C:403:LYS:HB2	2.44	0.51
1:A:16:LYS:HD3	1:A:16:LYS:N	2.25	0.51
1:A:406:TYR:CE2	3:C:35:ILE:HD11	2.45	0.51
2:B:89:LYS:HB3	2:B:91:TYR:CE2	2.45	0.51
2:B:351:ILE:O	2:B:356:LEU:HB2	2.10	0.51
1:A:116:MET:HE3	1:A:343:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:TYR:OH	3:C:44:GLU:HB2	2.11	0.51
2:B:341:VAL:HG12	2:B:341:VAL:O	2.09	0.51
3:C:5:THR:CG2	3:C:8:LEU:H	2.24	0.51
3:C:123:ARG:HG3	3:C:123:ARG:HH11	1.76	0.51
3:C:150:LEU:HD12	3:C:154:MET:HG3	1.92	0.51
1:A:181:THR:HG23	1:A:421:PRO:HD3	1.91	0.51
1:A:246:LYS:HE2	1:A:279:LYS:NZ	2.26	0.51
2:B:226:PHE:HE2	2:B:257:MET:HB2	1.75	0.51
3:C:79:LYS:O	3:C:79:LYS:CG	2.58	0.51
3:C:536:ASP:HA	3:C:539:GLU:HB2	1.91	0.51
1:A:80:SER:HB2	1:A:113:GLU:HG3	1.93	0.51
3:C:320:ARG:HD2	3:C:324:HIS:CB	2.41	0.51
3:C:382:MET:HB3	3:C:400:ILE:HD12	1.93	0.51
2:B:218:VAL:HA	2:B:253:ARG:O	2.11	0.51
2:B:378:ASP:OD1	2:B:406:MET:HG3	2.10	0.51
3:C:132:ARG:HG2	3:C:315:ILE:CD1	2.39	0.51
1:A:251:GLU:HG3	1:A:284:LYS:HA	1.93	0.51
2:B:20:LYS:CG	2:B:27:ALA:HB2	2.41	0.51
2:B:285:VAL:CG1	2:B:285:VAL:O	2.58	0.51
1:A:132:TRP:CE2	1:A:434:PRO:HG2	2.44	0.51
2:B:366:ILE:N	2:B:366:ILE:HD12	2.25	0.51
3:C:306:VAL:O	3:C:307:VAL:C	2.48	0.51
3:C:361:LYS:CG	3:C:362:ARG:HH11	2.24	0.51
2:B:81:ASN:O	2:B:82:TYR:HB3	2.11	0.51
2:B:340:VAL:HG22	2:B:340:VAL:O	2.11	0.51
1:A:179:LYS:NZ	1:A:416:ASN:ND2	2.59	0.50
2:B:93:ILE:HD13	2:B:126:GLU:OE2	2.11	0.50
2:B:97:PHE:O	2:B:98:TYR:CB	2.56	0.50
2:B:200:ALA:HB3	2:B:218:VAL:CG2	2.41	0.50
2:B:337:CYS:O	2:B:340:VAL:HG12	2.12	0.50
3:C:19:GLU:HG2	3:C:20:LEU:H	1.76	0.50
4:E:34:C:H2'	4:E:35:U:C6	2.46	0.50
1:A:9:LEU:CD1	1:A:13:GLU:HB3	2.40	0.50
1:A:229:ASN:HD22	1:A:229:ASN:H	1.58	0.50
1:A:319:ILE:O	1:A:321:GLU:N	2.41	0.50
1:A:427:PHE:CD2	1:A:460:SER:HB2	2.46	0.50
2:B:87:LEU:HD11	2:B:92:GLN:HB2	1.93	0.50
3:C:362:ARG:O	3:C:363:HIS:C	2.50	0.50
2:B:5:PRO:HB3	2:B:235:PHE:CE2	2.46	0.50
2:B:122:LEU:HD21	2:B:158:ILE:HG12	1.93	0.50
3:C:218:GLU:O	3:C:221:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HD2	1:A:142:SER:HB3	1.93	0.50
1:A:438:GLN:HG2	1:A:439:VAL:N	2.27	0.50
2:B:292:LEU:C	2:B:294:GLU:H	2.15	0.50
3:C:249:TYR:OH	3:C:254:LYS:HD3	2.11	0.50
1:A:300:PRO:HG2	1:A:346:ILE:HD11	1.93	0.50
2:B:29:VAL:HG21	2:B:149:ASN:HB3	1.93	0.50
2:B:88:PRO:O	2:B:90:GLY:N	2.44	0.50
2:B:420:ASN:C	2:B:420:ASN:ND2	2.58	0.50
3:C:54:TYR:CE2	3:C:55:THR:HG22	2.46	0.50
1:A:47:ARG:HG3	1:A:48:GLU:N	2.26	0.50
3:C:495:GLU:C	3:C:497:ASP:H	2.14	0.50
4:E:53:G:O2'	4:E:54:U:H5'	2.12	0.50
1:A:72:LEU:C	1:A:72:LEU:HD23	2.32	0.50
2:B:113:GLY:O	2:B:114:ARG:HB2	2.12	0.50
2:B:424:LEU:HD12	2:B:425:ILE:HD12	1.93	0.50
2:B:468:PRO:HG3	4:E:56:C:C4	2.47	0.50
1:A:10:THR:HG23	1:A:13:GLU:H	1.76	0.50
2:B:220:ASN:O	2:B:221:MET:HB3	2.12	0.50
3:C:5:THR:CG2	3:C:8:LEU:HD13	2.40	0.50
3:C:150:LEU:CD1	3:C:154:MET:HG3	2.42	0.50
3:C:292:ILE:HG12	4:E:74:C:H5'	1.93	0.50
3:C:303:ASN:HD22	3:C:331:GLN:HE21	1.59	0.50
1:A:26:PRO:CG	1:A:52:VAL:HG21	2.42	0.49
3:C:326:SER:HB2	4:E:71:C:O4'	2.12	0.49
3:C:455:ILE:HG12	3:C:455:ILE:O	2.12	0.49
1:A:92:ALA:CB	1:A:189:GLY:HA3	2.43	0.49
2:B:136:ASP:HB2	2:B:139:THR:CG2	2.41	0.49
2:B:335:GLU:O	2:B:338:VAL:HG12	2.11	0.49
1:A:329:MET:HB3	3:C:19:GLU:H	1.77	0.49
2:B:41:VAL:HA	2:B:48:ALA:HB1	1.94	0.49
2:B:462:THR:O	2:B:463:LYS:O	2.28	0.49
3:C:165:LEU:HD23	3:C:194:TRP:CD2	2.47	0.49
3:C:245:THR:O	3:C:246:THR:C	2.51	0.49
3:C:371:PHE:O	3:C:376:ILE:HB	2.12	0.49
1:A:305:SER:HA	1:A:308:ALA:HB2	1.94	0.49
3:C:320:ARG:HH22	3:C:345:PHE:HE1	1.59	0.49
1:A:27:GLN:C	1:A:29:SER:H	2.15	0.49
1:A:378:LEU:O	1:A:442:ARG:NH2	2.46	0.49
3:C:6:LYS:HZ2	3:C:25:ARG:HH21	1.58	0.49
2:B:266:ARG:HB3	2:B:266:ARG:HH21	1.78	0.49
2:B:299:LEU:HD12	2:B:299:LEU:C	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:70:C:H2'	4:E:71:C:H6	1.78	0.49
2:B:233:TYR:CD1	2:B:233:TYR:C	2.86	0.49
2:B:340:VAL:HG11	2:B:373:PRO:CB	2.43	0.49
2:B:295:VAL:HA	2:B:298:GLU:CG	2.41	0.49
1:A:349:PHE:HE1	1:A:359:TYR:HE1	1.61	0.49
1:A:59:TRP:O	1:A:61:ILE:HG13	2.13	0.49
1:A:64:ALA:O	1:A:157:ALA:HA	2.13	0.49
1:A:132:TRP:O	1:A:133:ASP:CB	2.61	0.49
2:B:38:ILE:HD11	3:C:74:ARG:HB3	1.94	0.49
2:B:369:SER:O	2:B:371:LEU:N	2.42	0.49
2:B:439:ALA:O	2:B:442:ASP:HB2	2.12	0.49
3:C:462:TYR:CD2	3:C:463:PHE:N	2.81	0.49
1:A:178:TYR:HB3	1:A:202:PRO:HD2	1.94	0.48
1:A:195:SER:HB2	2:B:280:PRO:HB2	1.95	0.48
1:A:199:GLN:HA	1:A:199:GLN:OE1	2.12	0.48
1:A:295:TYR:HD2	1:A:296:TYR:CD2	2.31	0.48
1:A:295:TYR:CG	1:A:413:ILE:HD12	2.48	0.48
2:B:322:LYS:HD3	2:B:322:LYS:C	2.33	0.48
4:E:71:C:H2'	4:E:72:A:O4'	2.13	0.48
1:A:11:ILE:O	1:A:14:CYS:HB2	2.13	0.48
1:A:240:GLU:HB3	1:A:451:ARG:HD2	1.95	0.48
2:B:354:GLU:HB3	2:B:397:PHE:CD2	2.48	0.48
2:B:391:LYS:HD2	2:B:459:MET:HE2	1.95	0.48
1:A:273:LEU:HD12	1:A:278:ALA:HB3	1.94	0.48
1:A:312:GLY:O	1:A:318:ARG:HD3	2.13	0.48
2:B:22:PHE:HB3	2:B:50:PRO:HB3	1.95	0.48
2:B:166:SER:C	2:B:168:ARG:H	2.16	0.48
2:B:184:LEU:HD23	2:B:184:LEU:H	1.79	0.48
3:C:324:HIS:CD2	6:C:1001:GSU:HG3	2.48	0.48
1:A:319:ILE:HG12	1:A:331:THR:HA	1.94	0.48
1:A:428:GLY:O	1:A:468:PHE:HE1	1.96	0.48
2:B:166:SER:C	2:B:168:ARG:N	2.65	0.48
2:B:226:PHE:HE2	2:B:257:MET:CA	2.27	0.48
2:B:398:PRO:O	2:B:400:VAL:N	2.46	0.48
2:B:418:GLN:O	2:B:418:GLN:HG2	2.13	0.48
3:C:234:TYR:O	3:C:258:HIS:HD2	1.95	0.48
4:E:57:G:H2'	4:E:58:A:H5'	1.95	0.48
1:A:132:TRP:CH2	1:A:434:PRO:HG2	2.48	0.48
3:C:347:HIS:N	3:C:347:HIS:CD2	2.81	0.48
2:B:348:SER:O	2:B:349:ASN:C	2.51	0.48
2:B:392:ILE:CD1	2:B:395:GLU:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:O	3:C:58:GLU:HG2	2.14	0.48
3:C:273:PHE:HD1	3:C:274:GLU:O	1.95	0.48
3:C:382:MET:SD	3:C:382:MET:N	2.86	0.48
1:A:348:THR:HG22	2:B:275:ARG:NH1	2.28	0.48
2:B:148:MET:O	2:B:149:ASN:C	2.52	0.48
2:B:213:SER:HB3	2:B:248:VAL:HG11	1.95	0.48
3:C:321:GLY:C	3:C:323:ASP:N	2.65	0.48
3:C:458:VAL:CG2	3:C:459:ASP:H	2.25	0.48
3:C:499:VAL:HA	3:C:503:LEU:HB2	1.94	0.48
1:A:346:ILE:HG13	1:A:347:GLY:N	2.29	0.48
2:B:22:PHE:CZ	2:B:93:ILE:HG21	2.49	0.48
2:B:54:GLU:OE2	3:C:65:LYS:HE3	2.14	0.48
2:B:316:LEU:HD21	2:B:334:PHE:CZ	2.49	0.48
2:B:341:VAL:O	2:B:343:ARG:N	2.41	0.48
4:E:68:U:H2'	4:E:69:C:C6	2.48	0.48
1:A:27:GLN:HE22	1:A:49:ASN:ND2	2.12	0.48
1:A:129:ARG:HD3	1:A:134:LEU:HB3	1.94	0.48
2:B:27:ALA:HB1	2:B:153:VAL:HG12	1.96	0.48
2:B:423:LYS:HE3	2:B:470:LEU:CD2	2.43	0.48
3:C:303:ASN:ND2	3:C:331:GLN:HE21	2.12	0.48
3:C:307:VAL:HG11	3:C:334:ILE:CG2	2.43	0.48
3:C:369:GLU:O	3:C:372:ARG:HB3	2.14	0.48
1:A:179:LYS:HZ1	1:A:416:ASN:ND2	2.12	0.48
1:A:190:LEU:HB2	1:A:200:ILE:HD11	1.95	0.48
1:A:272:LEU:HD13	1:A:275:ARG:HD2	1.96	0.48
1:A:340:VAL:O	1:A:341:ARG:C	2.51	0.48
2:B:381:LYS:HA	2:B:384:ASP:HB2	1.95	0.48
2:B:404:GLY:O	2:B:405:LYS:C	2.51	0.48
2:B:447:LYS:O	2:B:448:LYS:C	2.52	0.48
3:C:136:SER:O	3:C:138:THR:N	2.44	0.48
3:C:166:ARG:HD3	3:C:313:MET:SD	2.54	0.48
1:A:392:THR:CG2	1:A:431:ASN:HB2	2.45	0.47
2:B:312:ARG:C	2:B:313:GLU:OE2	2.53	0.47
1:A:12:GLU:OE1	1:A:208:ARG:NH1	2.46	0.47
2:B:43:THR:HG23	2:B:43:THR:O	2.14	0.47
2:B:344:PRO:CG	2:B:345:LYS:H	2.27	0.47
2:B:253:ARG:HA	2:B:263:VAL:O	2.15	0.47
2:B:433:MET:HG2	2:B:440:VAL:HG11	1.96	0.47
3:C:21:SER:O	3:C:23:ASP:N	2.48	0.47
3:C:534:LEU:C	3:C:536:ASP:H	2.17	0.47
3:C:536:ASP:C	3:C:538:SER:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HG21	1:A:193:PHE:CD2	2.49	0.47
2:B:19:THR:CG2	2:B:23:CYS:O	2.59	0.47
2:B:60:ALA:HB2	2:B:124:LEU:HD21	1.96	0.47
2:B:310:PHE:O	2:B:314:TYR:HB2	2.14	0.47
2:B:443:TYR:HB3	2:B:479:LEU:HD22	1.96	0.47
1:A:6:PHE:C	1:A:8:LYS:N	2.66	0.47
2:B:140:ARG:HH22	2:B:141:ALA:HA	1.76	0.47
2:B:250:ARG:NH1	2:B:250:ARG:HB3	2.30	0.47
2:B:443:TYR:HD2	2:B:479:LEU:HD22	1.77	0.47
2:B:454:PHE:O	2:B:458:VAL:HG23	2.14	0.47
3:C:136:SER:C	3:C:138:THR:H	2.17	0.47
3:C:332:LEU:HD23	3:C:332:LEU:HA	1.72	0.47
3:C:445:ILE:O	3:C:448:ALA:HB3	2.14	0.47
1:A:246:LYS:C	1:A:247:PHE:HD1	2.18	0.47
1:A:329:MET:HB3	3:C:19:GLU:N	2.29	0.47
2:B:15:LEU:HD21	2:B:156:ILE:CD1	2.45	0.47
2:B:213:SER:CB	2:B:248:VAL:HG11	2.45	0.47
3:C:498:TYR:CZ	3:C:554:GLY:O	2.67	0.47
3:C:519:PHE:O	3:C:522:LEU:HB2	2.15	0.47
3:C:582:GLU:C	3:C:584:THR:H	2.17	0.47
1:A:54:LYS:O	1:A:55:LYS:O	2.33	0.47
1:A:181:THR:HG21	1:A:444:PHE:N	2.20	0.47
1:A:209:ASP:HA	1:A:212:ILE:CG2	2.40	0.47
1:A:300:PRO:HG3	1:A:346:ILE:HD11	1.97	0.47
1:A:348:THR:HG22	2:B:275:ARG:HH11	1.79	0.47
2:B:226:PHE:CD2	2:B:255:TRP:NE1	2.81	0.47
2:B:291:TYR:C	2:B:291:TYR:CD2	2.88	0.47
2:B:362:ARG:HD2	2:B:364:ILE:CD1	2.42	0.47
2:B:397:PHE:N	2:B:398:PRO:HD2	2.29	0.47
2:B:423:LYS:HE3	2:B:470:LEU:CG	2.44	0.47
3:C:132:ARG:NH1	6:C:1001:GSU:CD	2.65	0.47
3:C:165:LEU:HD21	3:C:184:LEU:HD21	1.96	0.47
3:C:422:GLN:H	3:C:422:GLN:NE2	1.97	0.47
1:A:440:ILE:CG2	1:A:441:GLY:N	2.78	0.47
3:C:320:ARG:HD2	3:C:324:HIS:HB3	1.96	0.47
2:B:76:ARG:NH1	2:B:76:ARG:CG	2.78	0.47
2:B:89:LYS:HD2	2:B:91:TYR:HE2	1.78	0.47
2:B:448:LYS:O	2:B:449:LYS:C	2.53	0.47
3:C:186:SER:O	3:C:189:TRP:HB3	2.15	0.47
4:E:28:C:C2'	4:E:29:G:H5'	2.45	0.47
1:A:295:TYR:C	1:A:295:TYR:CD2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:THR:CG2	6:C:1001:GSU:C2	2.92	0.47
3:C:249:TYR:HD2	3:C:250:PRO:CD	2.28	0.47
3:C:438:GLU:O	3:C:441:LYS:HB3	2.15	0.47
3:C:571:VAL:O	3:C:571:VAL:HG22	2.15	0.47
1:A:72:LEU:HD23	1:A:73:GLY:N	2.30	0.46
2:B:29:VAL:HG23	2:B:32:LEU:HD22	1.96	0.46
2:B:124:LEU:HD23	2:B:156:ILE:HG12	1.97	0.46
3:C:25:ARG:C	3:C:27:SER:N	2.69	0.46
3:C:244:PHE:HD1	3:C:244:PHE:H	1.62	0.46
3:C:534:LEU:O	3:C:536:ASP:N	2.44	0.46
3:C:552:ILE:O	3:C:556:VAL:HG22	2.15	0.46
3:C:575:GLU:CD	3:C:575:GLU:H	2.19	0.46
1:A:281:GLU:C	1:A:282:ARG:HD3	2.35	0.46
2:B:87:LEU:HD23	2:B:87:LEU:O	2.15	0.46
1:A:47:ARG:CG	1:A:50:VAL:HG23	2.46	0.46
1:A:100:GLU:O	1:A:101:ALA:HB2	2.15	0.46
2:B:89:LYS:HD2	2:B:91:TYR:CE2	2.50	0.46
2:B:221:MET:O	2:B:221:MET:HG3	2.15	0.46
2:B:341:VAL:HG12	2:B:343:ARG:CG	2.40	0.46
3:C:10:LEU:O	3:C:12:LEU:N	2.48	0.46
3:C:155:PHE:CD2	3:C:319:PHE:CE2	3.03	0.46
3:C:327:ASN:O	3:C:331:GLN:HG3	2.16	0.46
1:A:443:ARG:HG2	1:A:444:PHE:CD2	2.51	0.46
2:B:355:VAL:HG12	2:B:356:LEU:N	2.30	0.46
2:B:360:ASN:C	2:B:362:ARG:N	2.68	0.46
3:C:185:GLU:HA	3:C:185:GLU:OE1	2.16	0.46
3:C:526:ASN:O	3:C:530:ILE:HB	2.16	0.46
1:A:185:VAL:N	1:A:199:GLN:HE22	2.11	0.46
1:A:285:ILE:H	1:A:285:ILE:CD1	2.12	0.46
1:A:464:GLU:O	1:A:465:ASN:HB2	2.14	0.46
2:B:213:SER:HB3	2:B:248:VAL:HG21	1.97	0.46
3:C:328:THR:N	3:C:329:PRO:CD	2.79	0.46
3:C:426:TRP:HE3	3:C:427:VAL:HG12	1.80	0.46
3:C:556:VAL:HG21	3:C:569:ILE:HD11	1.98	0.46
4:E:33:U:H3'	4:E:33:U:H6	1.78	0.46
2:B:7:ILE:HB	2:B:164:ILE:HG22	1.97	0.46
2:B:250:ARG:O	2:B:251:GLU:CB	2.64	0.46
2:B:467:ASN:O	2:B:468:PRO:C	2.54	0.46
3:C:428:ASN:HD21	3:C:476:THR:HA	1.78	0.46
1:A:33:ILE:HG12	1:A:153:MET:HG2	1.98	0.46
1:A:135:GLU:O	1:A:396:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:O	1:A:396:ILE:N	2.48	0.46
1:A:251:GLU:CG	1:A:284:LYS:HA	2.46	0.46
1:A:426:PRO:HA	1:A:436:GLY:HA3	1.98	0.46
2:B:350:TRP:CH2	2:B:393:ALA:O	2.67	0.46
3:C:38:TYR:CD1	3:C:38:TYR:C	2.88	0.46
3:C:273:PHE:CD1	3:C:274:GLU:O	2.69	0.46
3:C:311:HIS:CD2	3:C:340:TRP:CE3	3.04	0.46
2:B:338:VAL:CG1	2:B:339:LYS:H	2.29	0.46
2:B:374:GLN:NE2	2:B:374:GLN:H	2.13	0.46
2:B:441:GLN:O	2:B:444:LYS:HB3	2.16	0.46
3:C:129:VAL:HB	3:C:161:GLY:HA3	1.97	0.46
3:C:238:ASP:O	3:C:240:SER:N	2.49	0.46
3:C:277:LEU:HD12	3:C:278:LYS:HZ3	1.79	0.46
3:C:321:GLY:O	3:C:324:HIS:N	2.45	0.46
3:C:399:THR:HB	3:C:401:GLU:H	1.80	0.46
4:E:34:C:H2'	4:E:35:U:H6	1.81	0.46
1:A:18:SER:HB3	1:A:21:GLU:HB2	1.97	0.46
1:A:247:PHE:HD2	1:A:385:LEU:HD23	1.81	0.46
2:B:124:LEU:CD2	2:B:156:ILE:HG12	2.46	0.46
3:C:325:LEU:C	3:C:327:ASN:N	2.66	0.46
4:E:43:C:O2'	4:E:44:U:H5'	2.16	0.46
1:A:26:PRO:O	1:A:29:SER:HB3	2.16	0.46
1:A:93:THR:OG1	1:A:186:SER:CB	2.63	0.46
2:B:200:ALA:HB3	2:B:218:VAL:HG22	1.98	0.46
2:B:437:PRO:HA	2:B:440:VAL:CG1	2.43	0.46
3:C:4:VAL:O	3:C:4:VAL:HG13	2.16	0.46
3:C:133:PHE:CE1	3:C:149:ALA:HB2	2.51	0.46
3:C:136:SER:OG	3:C:138:THR:HG23	2.16	0.46
4:E:53:G:C2'	4:E:54:U:H5'	2.46	0.46
1:A:138:PRO:HA	1:A:173:CYS:SG	2.55	0.45
1:A:226:THR:HG22	2:B:283:PRO:HD3	1.97	0.45
2:B:98:TYR:N	2:B:99:PRO:HD3	2.30	0.45
3:C:238:ASP:C	3:C:240:SER:H	2.18	0.45
1:A:70:LEU:HA	1:A:76:THR:OG1	2.16	0.45
1:A:246:LYS:HB2	1:A:381:TYR:HB3	1.98	0.45
2:B:382:LEU:HG	2:B:388:ILE:HD12	1.99	0.45
2:B:387:LYS:O	2:B:388:ILE:HG13	2.16	0.45
2:B:419:ILE:HG12	2:B:465:LYS:HD3	1.97	0.45
3:C:8:LEU:O	3:C:12:LEU:HB2	2.16	0.45
3:C:250:PRO:O	3:C:251:HIS:C	2.54	0.45
3:C:391:ARG:HD3	4:E:14:A:OP1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:C	1:A:84:GLU:O	2.54	0.45
1:A:263:SER:HA	1:A:266:PHE:HB3	1.98	0.45
2:B:255:TRP:O	2:B:255:TRP:CD1	2.70	0.45
2:B:360:ASN:C	2:B:362:ARG:H	2.20	0.45
3:C:273:PHE:CE2	3:C:283:PHE:HE2	2.33	0.45
3:C:463:PHE:C	3:C:465:GLU:H	2.19	0.45
1:A:53:GLU:HB2	1:A:54:LYS:H	1.59	0.45
1:A:175:VAL:HB	1:A:204:THR:O	2.16	0.45
1:A:238:ILE:HG23	1:A:239:GLU:N	2.28	0.45
2:B:250:ARG:HB3	2:B:250:ARG:HH11	1.81	0.45
2:B:341:VAL:CG1	2:B:343:ARG:HG2	2.40	0.45
3:C:54:TYR:H	3:C:54:TYR:HD2	1.64	0.45
3:C:225:GLU:HG3	3:C:226:ASP:N	2.32	0.45
4:E:33:U:H6	4:E:33:U:H5'	1.81	0.45
1:A:78:CYS:SG	1:A:191:VAL:HG11	2.56	0.45
1:A:416:ASN:C	1:A:418:ALA:H	2.19	0.45
2:B:40:PRO:HD3	3:C:71:PHE:CD2	2.51	0.45
2:B:219:LYS:O	2:B:220:ASN:HB3	2.17	0.45
3:C:165:LEU:HD23	3:C:194:TRP:CE2	2.52	0.45
4:E:21:A:C2	4:E:46:G:C2	3.05	0.45
4:E:31:A:H2'	4:E:32:C:O4'	2.17	0.45
1:A:65:ILE:HG22	1:A:105:VAL:HG11	1.98	0.45
1:A:80:SER:CB	1:A:113:GLU:HG3	2.46	0.45
1:A:264:GLU:C	1:A:266:PHE:H	2.19	0.45
1:A:443:ARG:HG2	1:A:444:PHE:CE2	2.52	0.45
3:C:228:ARG:HD2	3:C:228:ARG:HA	1.72	0.45
3:C:306:VAL:HB	3:C:307:VAL:H	1.43	0.45
3:C:528:GLU:C	3:C:530:ILE:H	2.20	0.45
3:C:567:GLU:O	3:C:570:GLU:HG3	2.16	0.45
2:B:70:LYS:H	2:B:70:LYS:HG2	1.43	0.45
2:B:266:ARG:O	2:B:268:LYS:HE3	2.16	0.45
2:B:443:TYR:CD2	2:B:479:LEU:HB3	2.52	0.45
3:C:19:GLU:HG2	3:C:20:LEU:N	2.32	0.45
3:C:121:LYS:HG2	3:C:122:ILE:H	1.82	0.45
4:E:66:C:C2	4:E:67:C:C5	3.05	0.45
1:A:245:MET:SD	1:A:451:ARG:NH1	2.89	0.45
1:A:354:ALA:O	1:A:355:TYR:CG	2.70	0.45
1:A:440:ILE:HG22	1:A:441:GLY:N	2.32	0.45
2:B:338:VAL:O	2:B:339:LYS:C	2.55	0.45
2:B:433:MET:HG2	2:B:440:VAL:CG1	2.46	0.45
3:C:485:TYR:CE1	3:C:489:ASN:ND2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:35:U:C2'	4:E:36:G:H5'	2.47	0.45
1:A:222:GLU:O	2:B:51:VAL:HG11	2.17	0.45
1:A:407:LEU:C	1:A:409:ASP:N	2.71	0.45
2:B:199:ASP:OD2	2:B:219:LYS:HG2	2.17	0.45
2:B:221:MET:SD	2:B:227:VAL:HG23	2.57	0.45
3:C:350:LEU:HD12	3:C:358:PRO:HG3	1.99	0.45
3:C:410:LYS:HB3	3:C:410:LYS:HE2	1.79	0.45
3:C:473:LYS:CD	4:E:36:G:H21	2.14	0.45
3:C:525:TRP:CH2	3:C:577:THR:HG21	2.52	0.45
1:A:84:GLU:O	1:A:85:ASN:ND2	2.50	0.45
1:A:413:ILE:O	1:A:416:ASN:HB2	2.16	0.45
2:B:225:ARG:HB3	4:E:1:U:O2'	2.17	0.45
2:B:347:LEU:HD23	2:B:380:PHE:CZ	2.51	0.45
2:B:449:LYS:HG3	2:B:452:GLY:HA3	1.99	0.45
2:B:468:PRO:HB3	4:E:56:C:C6	2.52	0.45
3:C:126:PHE:O	3:C:127:GLU:C	2.55	0.45
3:C:137:PRO:HD3	3:C:167:ILE:HG22	1.99	0.45
3:C:177:ARG:HH22	3:C:208:ARG:NH2	2.15	0.45
1:A:14:CYS:SG	1:A:25:LEU:HD13	2.56	0.44
1:A:178:TYR:CZ	1:A:450:PHE:CE2	3.05	0.44
2:B:337:CYS:SG	2:B:373:PRO:HG3	2.57	0.44
3:C:496:LYS:NZ	3:C:496:LYS:HB3	2.31	0.44
3:C:512:LEU:O	3:C:515:ALA:HB3	2.16	0.44
1:A:36:LEU:HD21	1:A:473:VAL:HG11	1.99	0.44
3:C:177:ARG:HH12	3:C:208:ARG:CD	2.31	0.44
3:C:277:LEU:CD1	3:C:278:LYS:HZ2	2.31	0.44
1:A:65:ILE:CG2	1:A:105:VAL:HG11	2.47	0.44
1:A:70:LEU:HG	1:A:90:PHE:CE2	2.53	0.44
1:A:94:VAL:HG21	1:A:200:ILE:HD13	2.00	0.44
1:A:288:ILE:HD13	1:A:288:ILE:O	2.17	0.44
1:A:392:THR:O	1:A:393:ALA:HB2	2.17	0.44
1:A:409:ASP:HB3	1:A:412:THR:OG1	2.18	0.44
2:B:72:HIS:O	2:B:73:LYS:C	2.55	0.44
2:B:108:ILE:HD11	2:B:117:VAL:HG21	1.98	0.44
2:B:199:ASP:CG	2:B:219:LYS:HG2	2.37	0.44
3:C:270:LYS:HG2	3:C:284:ASP:HB2	1.99	0.44
3:C:580:ARG:O	3:C:584:THR:HG22	2.17	0.44
1:A:297:VAL:HG13	1:A:350:THR:HG21	1.97	0.44
3:C:241:LYS:HZ1	3:C:243:LEU:HD11	1.83	0.44
3:C:276:LEU:CD1	3:C:345:PHE:O	2.66	0.44
1:A:33:ILE:HG12	1:A:153:MET:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:OD1	1:A:76:THR:HA	2.18	0.44
1:A:71:THR:O	1:A:72:LEU:C	2.55	0.44
1:A:190:LEU:O	1:A:192:ALA:N	2.51	0.44
3:C:173:GLU:C	3:C:175:SER:H	2.21	0.44
4:E:67:C:H2'	4:E:68:U:C6	2.51	0.44
1:A:235:LEU:O	1:A:236:SER:HB2	2.17	0.44
1:A:446:ASP:O	1:A:448:LYS:N	2.51	0.44
1:A:461:PRO:O	1:A:462:TYR:CB	2.66	0.44
2:B:340:VAL:HG13	2:B:341:VAL:HG23	1.98	0.44
1:A:6:PHE:CZ	1:A:28:LEU:O	2.71	0.44
2:B:241:ALA:O	2:B:246:GLU:HB3	2.18	0.44
2:B:398:PRO:C	2:B:400:VAL:N	2.71	0.44
2:B:443:TYR:HD1	2:B:450:ALA:HB3	1.83	0.44
1:A:272:LEU:HD13	1:A:272:LEU:HA	1.88	0.44
2:B:51:VAL:O	2:B:51:VAL:CG2	2.60	0.44
3:C:64:ARG:HG3	3:C:64:ARG:O	2.16	0.44
3:C:86:ASP:N	3:C:86:ASP:OD1	2.48	0.44
3:C:187:LEU:CD1	3:C:192:LEU:HD12	2.48	0.44
1:A:290:TYR:O	1:A:292:VAL:N	2.51	0.44
2:B:430:LYS:C	2:B:432:ALA:N	2.70	0.44
3:C:26:GLU:HA	3:C:29:MET:HE2	2.00	0.44
3:C:121:LYS:HE3	3:C:122:ILE:O	2.18	0.44
3:C:335:TYR:CE1	3:C:342:ALA:HA	2.53	0.44
3:C:421:TYR:C	3:C:421:TYR:CD2	2.91	0.44
1:A:349:PHE:CE2	3:C:8:LEU:HD21	2.51	0.43
2:B:161:GLU:C	2:B:163:ASP:H	2.21	0.43
3:C:245:THR:O	3:C:246:THR:O	2.36	0.43
3:C:300:PRO:HB2	3:C:305:ALA:HB2	1.99	0.43
3:C:461:ARG:HA	3:C:464:SER:HB2	2.00	0.43
1:A:44:ILE:HD11	1:A:110:ASN:ND2	2.30	0.43
1:A:280:VAL:HG23	1:A:280:VAL:O	2.17	0.43
1:A:368:ARG:HD2	3:C:51:GLU:O	2.18	0.43
3:C:20:LEU:HA	3:C:20:LEU:HD23	1.80	0.43
3:C:511:VAL:C	3:C:513:GLU:N	2.69	0.43
1:A:9:LEU:HD12	1:A:13:GLU:HB3	2.00	0.43
1:A:282:ARG:HD3	1:A:282:ARG:N	2.33	0.43
1:A:419:GLY:O	1:A:420:LEU:O	2.36	0.43
1:A:427:PHE:HE2	1:A:460:SER:HB2	1.79	0.43
2:B:226:PHE:HE2	2:B:257:MET:CB	2.31	0.43
2:B:403:THR:HG21	2:B:405:LYS:CE	2.48	0.43
2:B:480:GLU:OE1	2:B:480:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:408:ASP:C	3:C:410:LYS:N	2.72	0.43
4:E:49:G:N2	4:E:66:C:H1'	2.33	0.43
1:A:415:ALA:HA	1:A:420:LEU:HB2	2.01	0.43
4:E:68:U:H2'	4:E:69:C:H6	1.83	0.43
3:C:42:LEU:C	3:C:44:GLU:H	2.21	0.43
3:C:382:MET:CB	3:C:400:ILE:HD12	2.49	0.43
3:C:412:ILE:HG13	3:C:413:SER:O	2.17	0.43
2:B:49:LEU:HA	2:B:50:PRO:HD3	1.73	0.43
2:B:333:PHE:CG	2:B:366:ILE:HG21	2.53	0.43
2:B:363:ASN:O	2:B:364:ILE:CG1	2.67	0.43
3:C:76:LEU:O	3:C:80:ASN:HB2	2.18	0.43
3:C:128:LEU:O	3:C:130:ARG:HG3	2.19	0.43
3:C:281:MET:CE	4:E:5:A:OP1	2.67	0.43
1:A:208:ARG:O	1:A:212:ILE:HB	2.18	0.43
1:A:242:VAL:CG2	1:A:273:LEU:HD11	2.48	0.43
1:A:429:PHE:O	1:A:432:ASN:HA	2.19	0.43
3:C:404:LEU:HD12	3:C:404:LEU:HA	1.85	0.43
3:C:503:LEU:C	3:C:505:ARG:H	2.22	0.43
1:A:90:PHE:CD1	1:A:188:TYR:CE2	3.06	0.43
1:A:132:TRP:HB3	1:A:471:PRO:HB3	2.01	0.43
2:B:406:MET:O	2:B:407:PRO:C	2.57	0.43
2:B:459:MET:O	2:B:460:ARG:C	2.57	0.43
3:C:371:PHE:HE1	3:C:421:TYR:HD1	1.67	0.43
3:C:544:SER:O	3:C:548:VAL:HG23	2.19	0.43
4:E:54:U:C5	4:E:55:U:C5	3.07	0.43
4:E:67:C:O2'	4:E:68:U:H5'	2.18	0.43
1:A:57:LYS:HB3	1:A:58:PHE:HD2	1.83	0.43
1:A:434:PRO:HB3	1:A:468:PHE:HZ	1.81	0.43
2:B:79:ARG:NE	2:B:279:GLU:OE2	2.52	0.43
2:B:223:SER:HB3	2:B:226:PHE:HB2	2.01	0.43
3:C:204:PHE:O	3:C:212:ARG:NH2	2.52	0.43
1:A:188:TYR:CE1	1:A:223:ASN:HB3	2.53	0.43
1:A:249:VAL:HG13	1:A:250:PRO:HD2	1.99	0.43
2:B:181:VAL:HG12	2:B:187:SER:HB3	1.98	0.43
3:C:329:PRO:O	3:C:330:LYS:C	2.57	0.43
3:C:355:ASP:OD1	3:C:357:THR:HG21	2.18	0.43
3:C:444:PHE:O	3:C:447:TRP:HB3	2.19	0.43
2:B:41:VAL:HG22	2:B:48:ALA:HB1	2.00	0.42
2:B:310:PHE:N	2:B:310:PHE:CD1	2.87	0.42
2:B:337:CYS:HA	2:B:373:PRO:HB3	2.01	0.42
2:B:459:MET:HE1	2:B:465:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:PRO:HB3	4:E:56:C:C5	2.54	0.42
1:A:6:PHE:C	1:A:8:LYS:H	2.21	0.42
1:A:6:PHE:O	1:A:8:LYS:N	2.52	0.42
1:A:116:MET:SD	1:A:193:PHE:CD1	3.12	0.42
2:B:240:LYS:HE3	2:B:240:LYS:HB3	1.78	0.42
2:B:292:LEU:C	2:B:292:LEU:HD23	2.40	0.42
2:B:309:ARG:O	2:B:310:PHE:C	2.57	0.42
3:C:455:ILE:O	3:C:455:ILE:CG1	2.64	0.42
4:E:33:U:C6	4:E:33:U:H5'	2.54	0.42
2:B:98:TYR:H	2:B:99:PRO:CD	2.32	0.42
2:B:139:THR:HG23	2:B:140:ARG:N	2.34	0.42
2:B:364:ILE:HG22	2:B:365:GLU:H	1.81	0.42
3:C:33:GLN:HE21	3:C:33:GLN:CA	2.31	0.42
3:C:277:LEU:HD12	3:C:278:LYS:HZ2	1.81	0.42
4:E:36:G:H8	4:E:36:G:OP2	2.02	0.42
1:A:228:VAL:HG12	3:C:58:GLU:OE2	2.20	0.42
1:A:242:VAL:CG1	1:A:452:ILE:HG12	2.49	0.42
2:B:180:ILE:O	2:B:184:LEU:HD23	2.20	0.42
2:B:267:GLY:O	2:B:268:LYS:HB2	2.19	0.42
2:B:358:GLU:OE1	2:B:362:ARG:NH1	2.52	0.42
2:B:393:ALA:HA	2:B:396:ILE:CD1	2.49	0.42
4:E:66:C:H2'	4:E:67:C:H6	1.85	0.42
2:B:21:ALA:HA	2:B:56:MET:HE3	2.01	0.42
2:B:167:PRO:O	2:B:228:GLU:HG3	2.20	0.42
3:C:318:VAL:C	3:C:319:PHE:HD1	2.22	0.42
1:A:27:GLN:HE22	1:A:49:ASN:HD21	1.67	0.42
1:A:339:GLU:O	1:A:340:VAL:C	2.58	0.42
2:B:213:SER:OG	2:B:248:VAL:HG11	2.20	0.42
2:B:374:GLN:O	2:B:406:MET:CE	2.68	0.42
2:B:411:VAL:HG13	2:B:416:LEU:HB2	2.02	0.42
3:C:5:THR:HG23	3:C:6:LYS:N	2.34	0.42
3:C:295:LYS:HG3	3:C:299:PHE:O	2.20	0.42
3:C:329:PRO:O	3:C:332:LEU:N	2.52	0.42
3:C:422:GLN:N	3:C:422:GLN:NE2	2.61	0.42
1:A:7:ARG:HE	1:A:7:ARG:HB2	1.63	0.42
1:A:133:ASP:C	1:A:135:GLU:H	2.22	0.42
1:A:229:ASN:HD22	1:A:229:ASN:N	2.16	0.42
1:A:303:ALA:C	1:A:305:SER:H	2.23	0.42
2:B:444:LYS:O	2:B:444:LYS:HG2	2.18	0.42
3:C:244:PHE:N	3:C:244:PHE:CD1	2.88	0.42
3:C:404:LEU:C	3:C:406:SER:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:LYS:CE	4:E:36:G:N2	2.83	0.42
3:C:507:GLU:O	3:C:511:VAL:HG23	2.19	0.42
4:E:65:C:O2'	4:E:66:C:H5'	2.19	0.42
1:A:16:LYS:HD3	1:A:16:LYS:H	1.85	0.42
1:A:167:ARG:HH11	1:A:422:ALA:HB3	1.83	0.42
1:A:423:ILE:HG22	1:A:424:SER:N	2.35	0.42
2:B:9:LEU:HD11	2:B:173:PHE:CE2	2.55	0.42
2:B:201:ASN:HB3	2:B:215:ARG:HG2	2.02	0.42
2:B:259:THR:OG1	2:B:260:LYS:N	2.49	0.42
2:B:359:LEU:HD21	2:B:366:ILE:HG13	2.02	0.42
3:C:224:VAL:HG22	3:C:229:ALA:HB3	2.02	0.42
3:C:544:SER:O	3:C:545:LYS:C	2.55	0.42
1:A:176:VAL:HG21	1:A:207:VAL:HG22	2.00	0.42
1:A:253:ILE:HD12	1:A:411:PHE:CE2	2.55	0.42
1:A:414:PRO:HA	1:A:417:LEU:HG	2.01	0.42
2:B:305:GLU:C	2:B:307:ALA:N	2.70	0.42
3:C:174:ARG:HH21	3:C:362:ARG:HH12	1.65	0.42
3:C:573:GLY:HA3	3:C:575:GLU:HG2	2.02	0.42
1:A:90:PHE:N	1:A:90:PHE:CD2	2.88	0.42
1:A:197:LEU:HB3	1:A:416:ASN:HB3	2.01	0.42
1:A:281:GLU:H	1:A:281:GLU:HG2	1.73	0.42
2:B:9:LEU:HD12	2:B:9:LEU:H	1.85	0.42
2:B:284:PRO:CG	3:C:59:ASP:HB2	2.47	0.42
2:B:400:VAL:HG23	2:B:410:ILE:HD13	2.01	0.42
3:C:222:LYS:HE2	3:C:222:LYS:O	2.20	0.42
3:C:311:HIS:CD2	3:C:340:TRP:CE2	3.08	0.42
3:C:317:HIS:CD2	3:C:344:VAL:CG2	3.01	0.42
1:A:274:GLU:OE2	1:A:280:VAL:HG22	2.20	0.41
1:A:367:ARG:NH2	3:C:56:PRO:HD3	2.35	0.41
2:B:57:ILE:CG2	2:B:58:ARG:N	2.83	0.41
2:B:436:ASN:N	2:B:437:PRO:CD	2.82	0.41
3:C:38:TYR:O	3:C:38:TYR:HD1	2.02	0.41
3:C:518:ALA:CB	3:C:537:LEU:HD12	2.50	0.41
3:C:581:LEU:HD13	3:C:581:LEU:HA	1.95	0.41
4:E:60:U:H5"	4:E:61:C:C5	2.55	0.41
1:A:59:TRP:HE3	1:A:60:GLY:N	2.18	0.41
1:A:184:LEU:HD22	1:A:232:VAL:HG21	2.01	0.41
1:A:214:MET:C	1:A:216:ILE:H	2.23	0.41
1:A:252:GLU:HA	1:A:255:GLU:HB2	2.02	0.41
1:A:292:VAL:HG21	1:A:406:TYR:O	2.19	0.41
1:A:319:ILE:HG12	1:A:331:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASP:HB3	1:A:448:LYS:HD3	2.01	0.41
2:B:436:ASN:H	2:B:437:PRO:HD3	1.84	0.41
3:C:137:PRO:HD3	3:C:167:ILE:CG2	2.50	0.41
3:C:352:LEU:HD23	3:C:352:LEU:N	2.35	0.41
3:C:525:TRP:HH2	3:C:577:THR:HG21	1.85	0.41
4:E:2:G:C2	4:E:72:A:C2	3.09	0.41
4:E:75:C:H2'	4:E:76:A:O4'	2.20	0.41
1:A:69:ILE:HD13	1:A:200:ILE:HD13	2.02	0.41
1:A:473:VAL:O	1:A:475:ALA:N	2.53	0.41
2:B:7:ILE:HG22	2:B:164:ILE:HB	2.00	0.41
2:B:15:LEU:N	2:B:15:LEU:HD12	2.36	0.41
2:B:134:GLU:HB2	2:B:143:TYR:CD2	2.54	0.41
2:B:206:ASP:HB3	2:B:207:THR:H	1.49	0.41
2:B:291:TYR:O	2:B:294:GLU:CB	2.68	0.41
2:B:463:LYS:C	2:B:464:GLY:O	2.57	0.41
3:C:520:LYS:HB2	3:C:578:LEU:HD11	2.01	0.41
1:A:12:GLU:O	1:A:15:LEU:HB2	2.20	0.41
1:A:178:TYR:CD1	1:A:180:PRO:HD3	2.55	0.41
1:A:252:GLU:CG	1:A:255:GLU:HB2	2.49	0.41
1:A:314:LYS:N	1:A:314:LYS:CD	2.83	0.41
2:B:29:VAL:HG23	2:B:32:LEU:CB	2.50	0.41
2:B:366:ILE:HD12	2:B:366:ILE:H	1.85	0.41
2:B:371:LEU:HD13	2:B:401:PHE:HD2	1.86	0.41
2:B:424:LEU:HA	2:B:427:GLU:HG3	1.99	0.41
3:C:218:GLU:CG	3:C:219:TYR:N	2.82	0.41
3:C:301:THR:HG22	3:C:302:TYR:N	2.35	0.41
3:C:321:GLY:C	3:C:323:ASP:H	2.23	0.41
3:C:432:MET:HA	3:C:435:ILE:HD11	2.02	0.41
4:E:6:G:C2'	4:E:7:G:C5'	2.90	0.41
1:A:116:MET:HE2	1:A:340:VAL:HA	2.01	0.41
1:A:181:THR:HB	1:A:444:PHE:HD1	1.85	0.41
2:B:7:ILE:HA	2:B:201:ASN:O	2.21	0.41
2:B:343:ARG:HD3	2:B:380:PHE:HD2	1.86	0.41
2:B:433:MET:SD	2:B:433:MET:C	2.99	0.41
3:C:142:HIS:HD2	3:C:145:GLY:H	1.66	0.41
3:C:463:PHE:HD1	3:C:488:MET:HE3	1.84	0.41
1:A:9:LEU:H	1:A:205:LYS:NZ	2.19	0.41
1:A:389:SER:HB2	1:A:435:VAL:HG11	2.02	0.41
1:A:468:PHE:HA	1:A:469:PRO:HD3	1.77	0.41
1:A:472:GLU:H	1:A:472:GLU:HG2	1.51	0.41
2:B:241:ALA:C	2:B:246:GLU:HB3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:ASN:OD1	2:B:342:ASN:N	2.53	0.41
3:C:310:ASP:O	3:C:315:ILE:HG13	2.21	0.41
3:C:476:THR:OG1	3:C:479:GLN:HG3	2.21	0.41
3:C:495:GLU:C	3:C:497:ASP:N	2.74	0.41
4:E:66:C:H2'	4:E:67:C:C6	2.56	0.41
1:A:245:MET:HG2	1:A:382:ASP:OD2	2.20	0.41
1:A:252:GLU:O	1:A:252:GLU:HG2	2.21	0.41
1:A:266:PHE:O	1:A:269:ALA:N	2.52	0.41
1:A:305:SER:CB	2:B:81:ASN:HD21	2.34	0.41
1:A:358:ALA:O	1:A:362:LYS:HB2	2.20	0.41
2:B:91:TYR:C	2:B:91:TYR:CD2	2.94	0.41
2:B:122:LEU:CD2	2:B:158:ILE:HG12	2.51	0.41
2:B:292:LEU:HD23	2:B:292:LEU:O	2.21	0.41
2:B:423:LYS:HZ1	2:B:470:LEU:HD11	1.84	0.41
3:C:453:LYS:HB3	3:C:481:TYR:CZ	2.55	0.41
3:C:582:GLU:O	3:C:584:THR:N	2.48	0.41
1:A:28:LEU:HA	1:A:31:GLU:HB3	2.02	0.41
1:A:41:LYS:HG3	1:A:126:PHE:CE2	2.56	0.41
1:A:82:ILE:HB	1:A:335:GLY:HA3	2.02	0.41
1:A:119:SER:O	1:A:120:THR:OG1	2.35	0.41
1:A:246:LYS:HA	1:A:279:LYS:HB2	2.02	0.41
1:A:276:LEU:HD22	1:A:459:ASN:OD1	2.20	0.41
2:B:471:THR:HG22	2:B:472:ASN:N	2.35	0.41
1:A:254:TYR:O	1:A:255:GLU:HG2	2.21	0.41
1:A:258:ILE:H	1:A:258:ILE:HG13	1.56	0.41
1:A:286:PRO:CG	1:A:287:HIS:H	2.33	0.41
1:A:422:ALA:HB1	1:A:438:GLN:OE1	2.20	0.41
2:B:6:VAL:HG22	2:B:162:PRO:O	2.20	0.41
2:B:39:CYS:O	2:B:40:PRO:C	2.59	0.41
2:B:51:VAL:HG21	3:C:64:ARG:HH21	1.83	0.41
2:B:72:HIS:HE1	2:B:102:THR:CG2	2.34	0.41
2:B:74:TYR:CE2	2:B:284:PRO:HB2	2.56	0.41
2:B:180:ILE:O	2:B:183:TYR:CB	2.67	0.41
2:B:284:PRO:O	3:C:60:SER:O	2.38	0.41
2:B:358:GLU:C	2:B:360:ASN:H	2.23	0.41
2:B:398:PRO:C	2:B:400:VAL:H	2.23	0.41
2:B:403:THR:HG21	2:B:405:LYS:HE2	2.02	0.41
2:B:405:LYS:HB3	2:B:410:ILE:HG22	2.02	0.41
2:B:423:LYS:HE3	2:B:470:LEU:HG	2.02	0.41
2:B:425:ILE:HG21	2:B:471:THR:HA	2.02	0.41
3:C:3:LYS:HD3	3:C:3:LYS:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:VAL:HB	3:C:46:ASP:H	1.70	0.41
3:C:170:THR:CG2	3:C:300:PRO:HG2	2.48	0.41
3:C:297:ASN:OD1	3:C:299:PHE:HB2	2.21	0.41
3:C:442:ARG:O	3:C:446:GLU:HG3	2.21	0.41
3:C:530:ILE:HD13	3:C:569:ILE:O	2.21	0.41
3:C:562:THR:HB	3:C:563:PRO:HD2	2.02	0.41
1:A:168:GLN:HE21	1:A:168:GLN:HB3	1.56	0.41
1:A:185:VAL:H	1:A:199:GLN:NE2	2.16	0.41
1:A:252:GLU:HA	1:A:255:GLU:CG	2.42	0.41
2:B:71:ILE:HD13	2:B:292:LEU:HD11	2.02	0.41
2:B:277:PHE:C	2:B:277:PHE:HD1	2.24	0.41
2:B:326:SER:HB2	2:B:327:SER:H	1.58	0.41
2:B:362:ARG:O	2:B:362:ARG:HG2	2.20	0.41
3:C:154:MET:HE3	3:C:407:PHE:CE1	2.56	0.41
3:C:526:ASN:ND2	3:C:527:MET:H	2.19	0.41
4:E:28:C:H2'	4:E:29:G:H5'	2.03	0.41
4:E:58:A:C5	4:E:61:C:C5	3.09	0.41
2:B:43:THR:HG21	3:C:77:ILE:HD13	2.03	0.40
2:B:228:GLU:O	2:B:232:GLU:HB2	2.20	0.40
2:B:310:PHE:O	2:B:311:MET:O	2.39	0.40
2:B:392:ILE:HD13	2:B:392:ILE:HA	1.70	0.40
3:C:273:PHE:HE2	3:C:283:PHE:CE2	2.34	0.40
1:A:110:ASN:CG	1:A:111:LEU:H	2.25	0.40
1:A:198:ASP:O	1:A:199:GLN:HG2	2.21	0.40
1:A:252:GLU:C	1:A:254:TYR:N	2.74	0.40
2:B:335:GLU:C	2:B:337:CYS:N	2.73	0.40
2:B:344:PRO:CD	2:B:345:LYS:HG2	2.49	0.40
2:B:465:LYS:O	2:B:467:ASN:N	2.53	0.40
2:B:475:ILE:C	2:B:477:LYS:N	2.74	0.40
3:C:233:VAL:HG21	3:C:244:PHE:HE1	1.87	0.40
3:C:408:ASP:OD2	3:C:410:LYS:HG3	2.21	0.40
4:E:61:C:O2	4:E:61:C:C2'	2.66	0.40
1:A:430:SER:C	1:A:432:ASN:N	2.75	0.40
2:B:94:SER:HB3	2:B:125:GLU:HG2	2.04	0.40
2:B:98:TYR:O	2:B:99:PRO:C	2.58	0.40
2:B:374:GLN:H	2:B:374:GLN:CD	2.24	0.40
3:C:213:LEU:HD12	3:C:213:LEU:N	2.31	0.40
3:C:477:LEU:HD23	3:C:477:LEU:HA	1.92	0.40
1:A:113:GLU:HG2	1:A:340:VAL:HG21	2.03	0.40
1:A:266:PHE:CE2	1:A:270:LEU:HD11	2.56	0.40
1:A:355:TYR:O	1:A:358:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:OG1	1:A:438:GLN:HB2	2.21	0.40
1:A:403:LEU:H	1:A:403:LEU:CD1	2.32	0.40
1:A:470:LEU:HA	1:A:471:PRO:HD2	1.87	0.40
2:B:7:ILE:HG13	2:B:202:ILE:HG22	2.03	0.40
2:B:433:MET:CG	2:B:440:VAL:HG11	2.51	0.40
3:C:48:GLU:O	3:C:49:GLY:C	2.60	0.40
3:C:134:ALA:HB1	3:C:168:GLU:HG3	2.04	0.40
3:C:199:ASP:OD1	3:C:200:ILE:N	2.54	0.40
3:C:309:ASP:O	3:C:313:MET:HB2	2.21	0.40
1:A:249:VAL:HB	1:A:282:ARG:HG3	2.03	0.40
2:B:347:LEU:HD23	2:B:347:LEU:HA	1.54	0.40
3:C:35:ILE:CG2	3:C:36:LEU:N	2.85	0.40
3:C:174:ARG:HH22	3:C:361:LYS:HE3	1.86	0.40
3:C:206:PRO:HG2	3:C:211:GLU:O	2.20	0.40
3:C:241:LYS:HZ2	3:C:243:LEU:HD11	1.86	0.40
3:C:267:LEU:HD13	3:C:267:LEU:HA	1.75	0.40
3:C:328:THR:N	3:C:329:PRO:HD2	2.37	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	470/475 (99%)	305 (65%)	113 (24%)	52 (11%)	0 2
2	B	480/482 (100%)	306 (64%)	102 (21%)	72 (15%)	0 1
3	C	560/592 (95%)	396 (71%)	105 (19%)	59 (10%)	0 3
All	All	1510/1549 (98%)	1007 (67%)	320 (21%)	183 (12%)	0 2

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	55	LYS
1	A	101	ALA
1	A	120	THR
1	A	133	ASP
1	A	257	ASP
1	A	286	PRO
1	A	291	SER
1	A	393	ALA
1	A	408	MET
1	A	410	ILE
1	A	420	LEU
1	A	427	PHE
1	A	429	PHE
1	A	474	LYS
2	B	20	LYS
2	B	73	LYS
2	B	98	TYR
2	B	103	GLU
2	B	213	SER
2	B	214	ASN
2	B	221	MET
2	B	244	ARG
2	B	251	GLU
2	B	259	THR
2	B	260	LYS
2	B	291	TYR
2	B	311	MET
2	B	348	SER
2	B	382	LEU
2	B	418	GLN
2	B	421	ASP
2	B	449	LYS
2	B	465	LYS
2	B	467	ASN
3	C	4	VAL
3	C	25	ARG
3	C	49	GLY
3	C	50	VAL
3	C	56	PRO
3	C	57	VAL
3	C	247	TYR
3	C	306	VAL

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Mol	Chain	Res	Type
3	C	307	VAL
3	C	322	GLU
3	C	326	SER
3	C	362	ARG
3	C	405	GLN
3	C	493	GLU
3	C	523	ASN
3	C	526	ASN
3	C	570	GLU
1	A	118	SER
1	A	182	TYR
1	A	191	VAL
1	A	242	VAL
1	A	340	VAL
1	A	356	TYR
1	A	392	THR
2	B	110	GLY
2	B	138	ILE
2	B	141	ALA
2	B	204	VAL
2	B	205	VAL
2	B	206	ASP
2	B	211	ARG
2	B	215	ARG
2	B	268	LYS
2	B	272	SER
2	B	327	SER
2	B	342	ASN
2	B	345	LYS
2	B	367	THR
2	B	370	LYS
2	B	380	PHE
2	B	381	LYS
2	B	405	LYS
2	B	422	GLU
2	B	463	LYS
3	C	10	LEU
3	C	22	GLU
3	C	43	ASN
3	C	80	ASN
3	C	86	ASP
3	C	284	ASP

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Mol	Chain	Res	Type
3	C	337	ALA
3	C	346	MET
3	C	363	HIS
3	C	393	GLU
3	C	457	SER
3	C	458	VAL
3	C	476	THR
3	C	528	GLU
3	C	536	ASP
3	C	546	LYS
1	A	7	ARG
1	A	9	LEU
1	A	46	VAL
1	A	75	ARG
1	A	84	GLU
1	A	198	ASP
1	A	394	PHE
1	A	418	ALA
1	A	434	PRO
2	B	88	PRO
2	B	240	LYS
2	B	245	GLY
2	B	275	ARG
2	B	448	LYS
2	B	466	ALA
3	C	21	SER
3	C	59	ASP
3	C	174	ARG
3	C	251	HIS
3	C	496	LYS
1	A	15	LEU
1	A	18	SER
1	A	28	LEU
1	A	250	PRO
1	A	320	LYS
1	A	336	PHE
1	A	341	ARG
1	A	353	ALA
1	A	358	ALA
1	A	400	LYS
1	A	447	GLY
1	A	462	TYR

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Mol	Chain	Res	Type
2	B	71	ILE
2	B	89	LYS
2	B	134	GLU
2	B	149	ASN
2	B	270	GLU
2	B	336	GLU
2	B	399	GLU
3	C	41	LEU
3	C	334	ILE
3	C	535	ARG
1	A	54	LYS
1	A	382	ASP
1	A	399	ILE
1	A	417	LEU
2	B	122	LEU
2	B	139	THR
2	B	217	GLU
2	B	309	ARG
2	B	379	LEU
2	B	436	ASN
2	B	468	PRO
3	C	11	HIS
3	C	23	ASP
3	C	26	GLU
3	C	30	LYS
3	C	239	PRO
3	C	329	PRO
3	C	370	HIS
3	C	495	GLU
3	C	508	ALA
3	C	529	GLU
3	C	583	ARG
1	A	131	PRO
1	A	459	ASN
2	B	127	ASP
2	B	182	ARG
2	B	223	SER
2	B	308	GLU
2	B	326	SER
3	C	137	PRO
3	C	246	THR
3	C	464	SER

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Mol	Chain	Res	Type
3	C	497	ASP
1	A	164	GLY
2	B	344	PRO
3	C	238	ASP
2	B	341	VAL
2	B	398	PRO
2	B	407	PRO
1	A	180	PRO
2	B	167	PRO
2	B	419	ILE
2	B	164	ILE
3	C	569	ILE
1	A	280	VAL
3	C	279	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/397 (99%)	324 (82%)	70 (18%)	2	7
2	B	430/430 (100%)	349 (81%)	81 (19%)	1	6
3	C	510/530 (96%)	412 (81%)	98 (19%)	1	5
All	All	1334/1357 (98%)	1085 (81%)	249 (19%)	1	6

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	PHE
1	A	7	ARG
1	A	8	LYS
1	A	13	GLU
1	A	16	LYS
1	A	17	LEU
1	A	28	LEU

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Mol	Chain	Res	Type
1	A	33	ILE
1	A	47	ARG
1	A	48	GLU
1	A	49	ASN
1	A	50	VAL
1	A	53	GLU
1	A	63	VAL
1	A	77	THR
1	A	87	GLU
1	A	90	PHE
1	A	94	VAL
1	A	105	VAL
1	A	111	LEU
1	A	125	PHE
1	A	132	TRP
1	A	158	LEU
1	A	162	THR
1	A	167	ARG
1	A	168	GLN
1	A	173	CYS
1	A	179	LYS
1	A	181	THR
1	A	186	SER
1	A	187	ARG
1	A	193	PHE
1	A	199	GLN
1	A	207	VAL
1	A	212	ILE
1	A	216	ILE
1	A	229	ASN
1	A	230	ARG
1	A	232	VAL
1	A	237	GLU
1	A	256	HIS
1	A	258	ILE
1	A	271	LYS
1	A	272	LEU
1	A	273	LEU
1	A	276	LEU
1	A	282	ARG
1	A	284	LYS
1	A	285	ILE

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Mol	Chain	Res	Type
1	A	288	ILE
1	A	291	SER
1	A	295	TYR
1	A	314	LYS
1	A	318	ARG
1	A	324	LEU
1	A	346	ILE
1	A	348	THR
1	A	364	MET
1	A	375	ASN
1	A	380	GLN
1	A	381	TYR
1	A	391	VAL
1	A	396	ILE
1	A	446	ASP
1	A	454	ARG
1	A	458	LYS
1	A	459	ASN
1	A	472	GLU
1	A	473	VAL
2	B	2	ARG
2	B	6	VAL
2	B	9	LEU
2	B	14	GLN
2	B	31	GLU
2	B	38	ILE
2	B	39	CYS
2	B	43	THR
2	B	57	ILE
2	B	61	VAL
2	B	67	LEU
2	B	70	LYS
2	B	71	ILE
2	B	72	HIS
2	B	73	LYS
2	B	77	PHE
2	B	79	ARG
2	B	82	TYR
2	B	87	LEU
2	B	91	TYR
2	B	97	PHE
2	B	103	GLU

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Mol	Chain	Res	Type
2	B	106	LEU
2	B	108	ILE
2	B	114	ARG
2	B	122	LEU
2	B	138	ILE
2	B	140	ARG
2	B	142	SER
2	B	145	LEU
2	B	160	THR
2	B	165	SER
2	B	174	MET
2	B	184	LEU
2	B	196	LEU
2	B	202	ILE
2	B	206	ASP
2	B	214	ASN
2	B	215	ARG
2	B	222	ASN
2	B	223	SER
2	B	225	ARG
2	B	226	PHE
2	B	243	GLU
2	B	248	VAL
2	B	255	TRP
2	B	261	ILE
2	B	266	ARG
2	B	277	PHE
2	B	285	VAL
2	B	291	TYR
2	B	299	LEU
2	B	304	ASP
2	B	306	LYS
2	B	314	TYR
2	B	318	GLU
2	B	320	ASP
2	B	342	ASN
2	B	345	LYS
2	B	347	LEU
2	B	351	ILE
2	B	356	LEU
2	B	357	ARG
2	B	358	GLU

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Mol	Chain	Res	Type
2	B	365	GLU
2	B	366	ILE
2	B	367	THR
2	B	368	GLU
2	B	372	THR
2	B	374	GLN
2	B	395	GLU
2	B	410	ILE
2	B	420	ASN
2	B	422	GLU
2	B	436	ASN
2	B	445	SER
2	B	447	LYS
2	B	457	TYR
2	B	458	VAL
2	B	471	THR
2	B	472	ASN
3	C	5	THR
3	C	7	ASP
3	C	8	LEU
3	C	18	LEU
3	C	22	GLU
3	C	23	ASP
3	C	33	GLN
3	C	35	ILE
3	C	50	VAL
3	C	54	TYR
3	C	63	LEU
3	C	64	ARG
3	C	67	ASP
3	C	79	LYS
3	C	80	ASN
3	C	85	LYS
3	C	86	ASP
3	C	91	VAL
3	C	94	ILE
3	C	123	ARG
3	C	128	LEU
3	C	131	VAL
3	C	132	ARG
3	C	140	HIS
3	C	142	HIS

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Mol	Chain	Res	Type
3	C	148	THR
3	C	170	THR
3	C	173	GLU
3	C	176	SER
3	C	181	GLN
3	C	185	GLU
3	C	188	ARG
3	C	193	ASP
3	C	222	LYS
3	C	225	GLU
3	C	227	LYS
3	C	244	PHE
3	C	245	THR
3	C	246	THR
3	C	260	VAL
3	C	261	THR
3	C	267	LEU
3	C	281	MET
3	C	284	ASP
3	C	285	ASN
3	C	289	GLU
3	C	292	ILE
3	C	306	VAL
3	C	310	ASP
3	C	344	VAL
3	C	346	MET
3	C	348	ILE
3	C	352	LEU
3	C	356	ARG
3	C	357	THR
3	C	361	LYS
3	C	366	THR
3	C	374	GLU
3	C	382	MET
3	C	388	LEU
3	C	390	TRP
3	C	391	ARG
3	C	392	VAL
3	C	399	THR
3	C	400	ILE
3	C	404	LEU
3	C	414	ASN

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Mol	Chain	Res	Type
3	C	415	LYS
3	C	422	GLN
3	C	431	HIS
3	C	435	ILE
3	C	437	LEU
3	C	454	GLU
3	C	455	ILE
3	C	457	SER
3	C	460	GLU
3	C	461	ARG
3	C	462	TYR
3	C	467	LEU
3	C	471	ARG
3	C	478	SER
3	C	484	MET
3	C	491	ASP
3	C	496	LYS
3	C	497	ASP
3	C	507	GLU
3	C	510	ARG
3	C	522	LEU
3	C	535	ARG
3	C	537	LEU
3	C	539	GLU
3	C	546	LYS
3	C	570	GLU
3	C	575	GLU
3	C	578	LEU
3	C	579	LYS
3	C	581	LEU
3	C	584	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	85	ASN
1	A	110	ASN
1	A	168	GLN
1	A	199	GLN
1	A	229	ASN
1	A	375	ASN

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Mol	Chain	Res	Type
1	A	380	GLN
1	A	416	ASN
2	B	12	HIS
2	B	14	GLN
2	B	68	ASN
2	B	72	HIS
2	B	133	HIS
2	B	214	ASN
2	B	374	GLN
2	B	420	ASN
2	B	435	GLN
2	B	472	ASN
3	C	33	GLN
3	C	80	ASN
3	C	142	HIS
3	C	182	GLN
3	C	209	GLN
3	C	258	HIS
3	C	303	ASN
3	C	311	HIS
3	C	347	HIS
3	C	383	ASN
3	C	414	ASN
3	C	422	GLN
3	C	489	ASN
3	C	523	ASN
3	C	526	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	73/74 (98%)	11 (15%)	1 (1%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	8	U
4	E	16	C
4	E	18	G
4	E	22	G
4	E	26	G

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Mol	Chain	Res	Type
4	E	33	U
4	E	36	G
4	E	48	U
4	E	58	A
4	E	60	U
4	E	74	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	E	73	G

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	GSU	C	1001	-	31,34,34	1.30	4 (12%)	34,50,50	1.54	6 (17%)

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
6	GSU	C	1001	-	-	5/19/40/40	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	GSU	S-N10	4.47	1.67	1.59
6	C	1001	GSU	O5'-S	-2.50	1.54	1.59
6	C	1001	GSU	OE1-CD	-2.34	1.22	1.30
6	C	1001	GSU	O4'-C1'	2.24	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1001	GSU	N3-C2-N1	-4.20	122.11	128.68
6	C	1001	GSU	C3'-C2'-C1'	3.30	105.94	100.98
6	C	1001	GSU	C5'-O5'-S	-3.15	110.88	117.37
6	C	1001	GSU	C4-C5-N7	-2.46	106.84	109.40
6	C	1001	GSU	O2S-S-O1S	2.35	124.41	120.76
6	C	1001	GSU	O4'-C1'-C2'	-2.04	103.95	106.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1001	GSU	C5'-O5'-S-N10
6	C	1001	GSU	OE1-CD-CG-CB
6	C	1001	GSU	C-CA-CB-CG
6	C	1001	GSU	OE2-CD-CG-CB
6	C	1001	GSU	N-CA-CB-CG

There are no ring outliers.

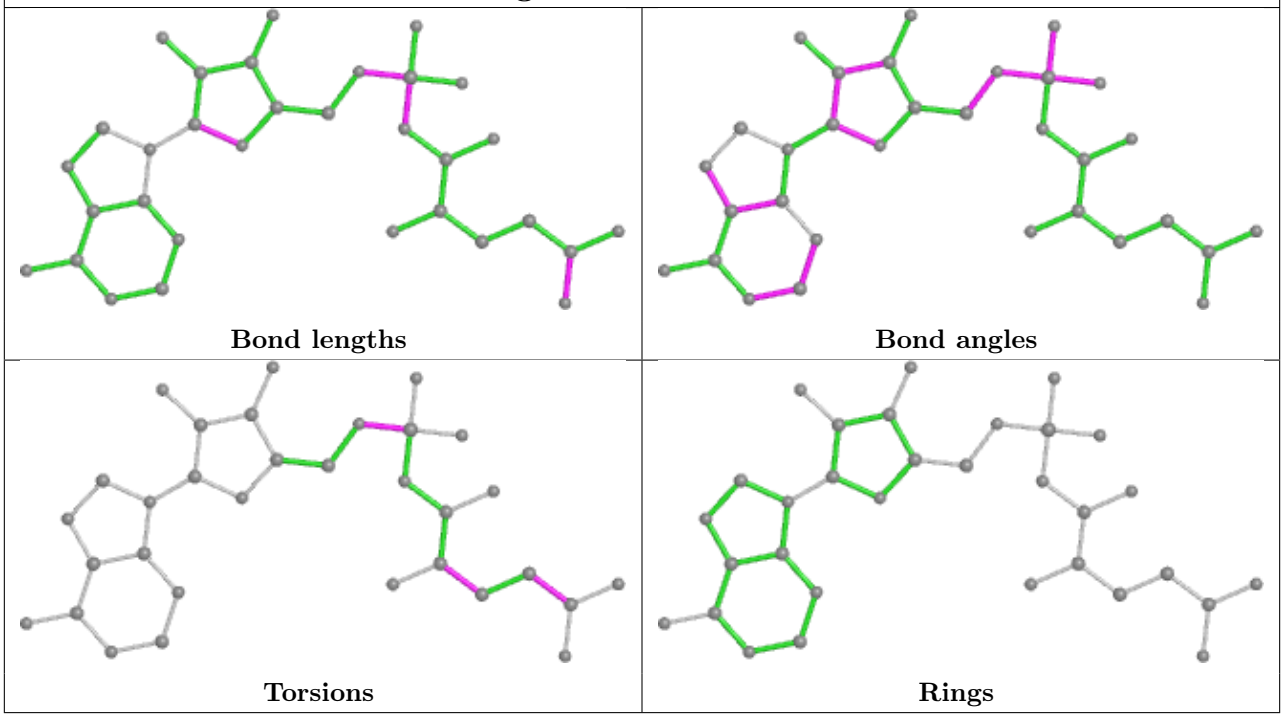
1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1001	GSU	11	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 GSU C 1001



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	472/475 (99%)	0.20	17 (3%) 42 45	83, 143, 190, 241	0
2	B	482/482 (100%)	0.17	22 (4%) 32 35	51, 114, 185, 262	0
3	C	564/592 (95%)	-0.07	8 (1%) 75 78	52, 106, 178, 224	0
4	E	74/74 (100%)	-0.45	0 100 100	70, 91, 146, 167	0
All	All	1592/1623 (98%)	0.06	47 (2%) 50 53	51, 121, 185, 262	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	210	GLY	11.3
2	B	209	THR	10.7
2	B	212	GLN	8.5
1	A	427	PHE	6.6
3	C	529	GLU	5.3
2	B	204	VAL	4.7
1	A	475	ALA	4.3
2	B	211	ARG	4.3
2	B	9	LEU	4.1
2	B	214	ASN	4.1
1	A	231	LYS	3.9
2	B	111	ASP	3.7
2	B	203	SER	3.6
2	B	4	ARG	3.6
3	C	59	ASP	3.6
3	C	537	LEU	3.4
2	B	482	GLU	3.3
1	A	163	GLY	3.3
1	A	117	GLY	3.3
2	B	238	ILE	3.2
2	B	266	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	ALA	3.1
1	A	428	GLY	3.0
2	B	137	SER	2.7
2	B	160	THR	2.6
1	A	238	ILE	2.6
3	C	569	ILE	2.5
1	A	272	LEU	2.4
2	B	464	GLY	2.4
1	A	235	LEU	2.4
2	B	213	SER	2.4
1	A	429	PHE	2.4
1	A	400	LYS	2.4
2	B	262	THR	2.4
2	B	164	ILE	2.3
3	C	520	LYS	2.3
3	C	47	VAL	2.3
1	A	284	LYS	2.2
1	A	162	THR	2.2
3	C	521	ASP	2.2
1	A	164	GLY	2.1
2	B	7	ILE	2.1
2	B	109	ASP	2.1
1	A	129	ARG	2.1
3	C	363	HIS	2.1
2	B	10	GLU	2.0
1	A	165	SER	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)

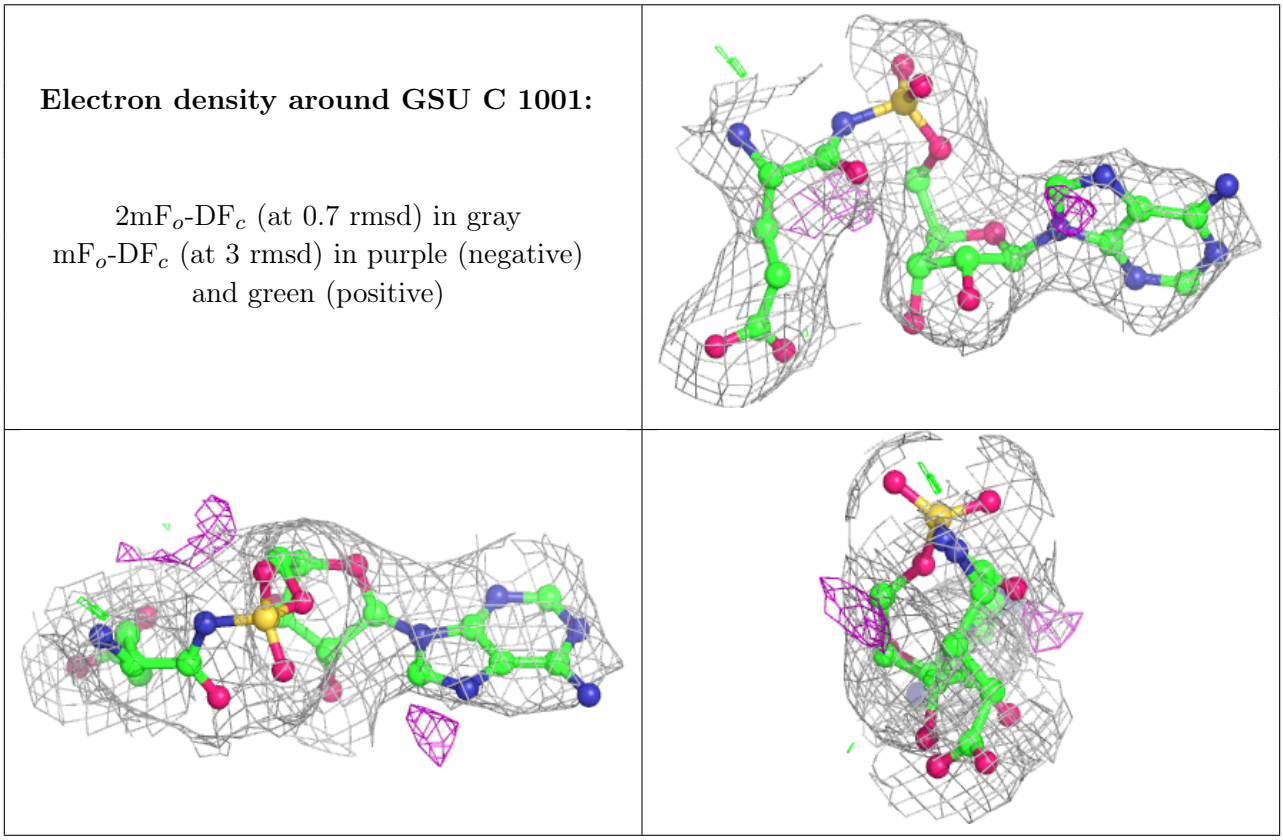
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GSU	C	1001	32/32	0.95	0.21	48,78,102,109	0
5	ZN	B	1001	1/1	0.98	0.20	81,81,81,81	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 GSU C 1001:

$2mF_o$-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.