



Full wwPDB X-ray Structure Validation Report i

Jun 12, 2024 – 02:39 AM EDT

PDB ID : 1YI8
Title : Crystal structure of tryptophanyl tRNA synthetase II from Deinococcus radiurans in complex with L-Trp
Authors : Buddha, M.R.; Crane, B.R.
Deposited on : 2005-01-11
Resolution : 2.10 Å (reported)

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

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

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

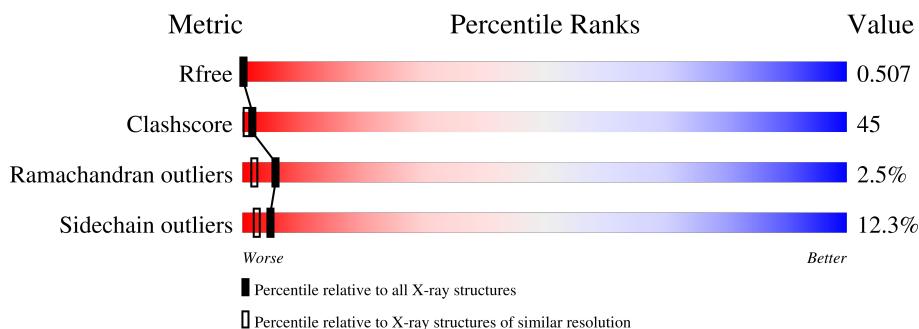
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

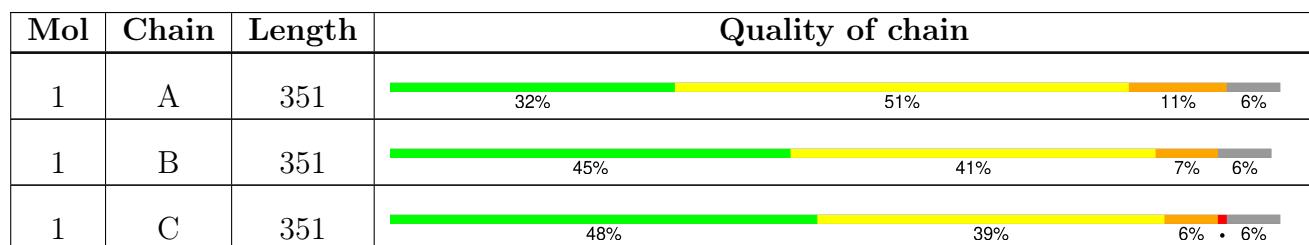
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$



2 Entry composition [\(i\)](#)

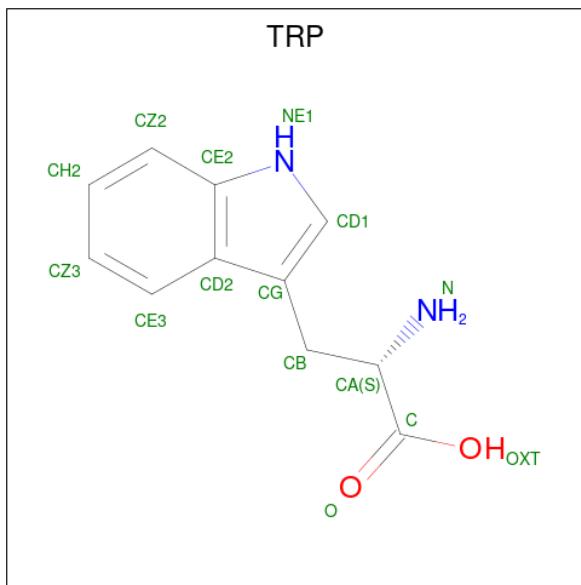
There are 3 unique types of molecules in this entry. The entry contains 8661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	B	331	Total	C 2544	N 1599	O 468	S 471	6	2	0	0
1	A	331	Total	C 2511	N 1581	O 457	S 467	6	0	0	0
1	C	331	Total	C 2532	N 1593	O 462	S 471	6	0	0	0

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C 15	N 11	O 2	S 2	0	0

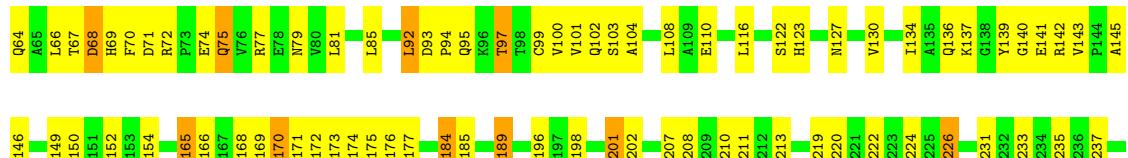
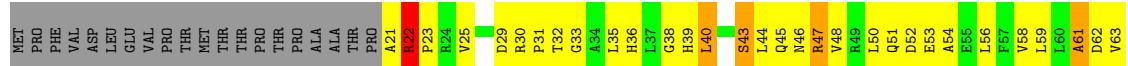
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	308	Total O 308 308	0	0
3	A	375	Total O 375 375	0	0
3	C	376	Total O 376 376	0	0

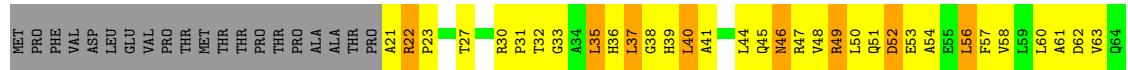
3 Residue-property plots [\(i\)](#)

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. 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. 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: tryptophanyl-tRNA synthetase



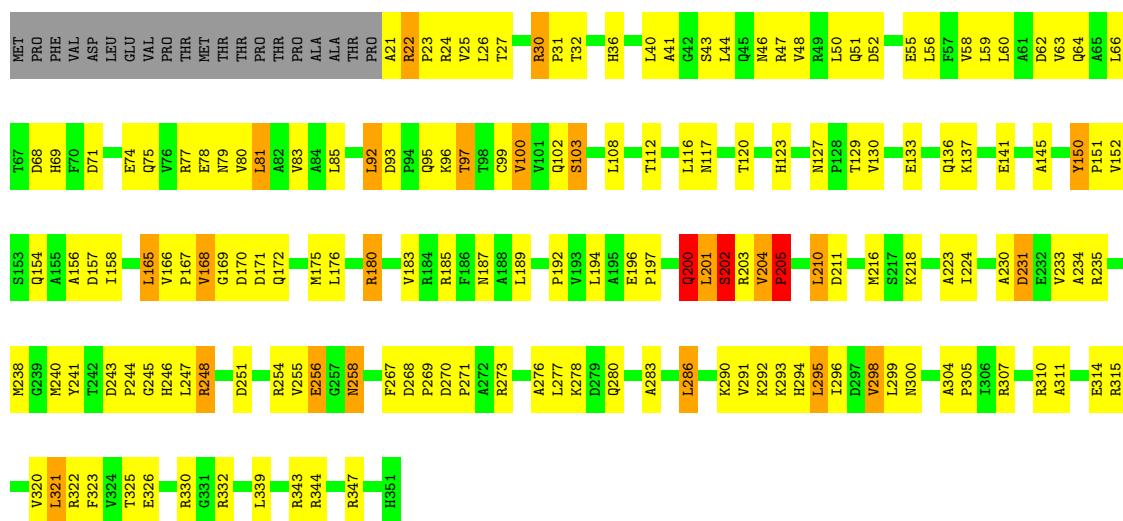
- Molecule 1: tryptophanyl-tRNA synthetase





- Molecule 1: tryptophanyl-tRNA synthetase

Chain C:



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.80Å 58.50Å 88.90Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 30.02 – 2.12	Depositor EDS
% Data completeness (in resolution range)	88.7 (50.00-2.10) 89.4 (30.02-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ ¹	1.45 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R , R_{free}	0.260 , 0.280 0.497 , 0.507	Depositor DCC
R_{free} test set	5520 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 39.0	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	8661	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	0/2558	0.68	0/3478
1	B	0.39	0/2591	0.68	0/3519
1	C	0.48	0/2579	0.73	3/3505 (0.1%)
All	All	0.41	0/7728	0.70	3/10502 (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
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	200	GLN	N-CA-C	-5.49	96.19	111.00
1	C	202	SER	N-CA-C	5.07	124.69	111.00
1	C	169	GLY	N-CA-C	-5.06	100.45	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	150	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	2511	0	2507	297	15
1	B	2544	0	2568	206	7
1	C	2532	0	2546	197	8
2	C	15	0	9	4	0
3	A	375	0	0	16	6
3	B	308	0	0	7	6
3	C	376	0	0	16	18
All	All	8661	0	7630	684	32

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 45.

All (684) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG23	1:A:172:GLN:HB2	1.20	1.15
1:A:226:LEU:HB3	1:A:306:ILE:HD11	1.34	1.09
1:A:207:LEU:HD23	1:A:216:MET:HE1	1.38	1.04
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.21	1.03
1:B:51:GLN:HE21	1:B:97:THR:HG22	1.18	1.02
1:C:120:THR:HG23	1:C:123:HIS:H	1.22	1.01
1:A:35:LEU:HD11	1:A:86:ASP:HB3	1.39	1.01
1:B:254:ARG:HD3	1:B:256:GLU:HG2	1.46	0.98
1:B:280:GLN:HB2	1:B:286:LEU:HD12	1.45	0.97
1:C:51:GLN:HE22	1:C:93:ASP:H	1.05	0.97
1:C:77:ARG:O	1:C:80:VAL:HG12	1.66	0.96
1:B:50:LEU:HD11	1:B:56:LEU:HD13	1.49	0.92
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.52	0.92
1:C:204:VAL:HG12	1:C:205:PRO:HD2	1.49	0.92
1:A:73:PRO:O	1:A:76:VAL:HG12	1.70	0.91
1:B:295:LEU:O	1:B:298:VAL:HG12	1.72	0.90
1:B:44:LEU:O	1:B:48:VAL:HG23	1.72	0.90
1:B:47:ARG:HA	1:B:50:LEU:HG	1.54	0.89
1:C:216:MET:HE3	1:C:224:ILE:H	1.38	0.88
1:B:51:GLN:HE22	1:B:93:ASP:N	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD12	1:B:286:LEU:HD11	1.55	0.88
1:C:254:ARG:HD3	1:C:256:GLU:HG2	1.56	0.87
1:A:63:VAL:HG13	1:A:102:GLN:HG2	1.55	0.87
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.56	0.86
1:C:26:LEU:HD23	1:C:158:ILE:HD13	1.55	0.85
1:B:51:GLN:HE22	1:B:93:ASP:H	0.89	0.85
1:A:35:LEU:CD1	1:A:86:ASP:HB3	2.07	0.84
1:A:193:VAL:HG21	1:A:341:GLN:HB3	1.58	0.84
1:A:226:LEU:HD12	1:A:226:LEU:H	1.43	0.84
1:B:213:GLN:OE1	1:B:220:LEU:HD13	1.79	0.82
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.59	0.82
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.60	0.82
1:C:180:ARG:HD3	1:C:197:PRO:O	1.80	0.82
1:B:43:SER:O	1:B:47:ARG:HD2	1.79	0.81
1:A:207:LEU:CD1	1:A:208:PRO:HD2	2.10	0.81
1:A:60:LEU:O	1:A:62:ASP:N	2.13	0.81
1:A:139:TYR:O	1:A:142:ARG:HG3	1.81	0.80
1:C:180:ARG:HG3	1:C:180:ARG:NH1	1.97	0.80
1:C:22:ARG:HB2	1:C:23:PRO:CD	2.11	0.79
1:B:68:ASP:HB3	1:B:69:HIS:HD2	1.47	0.79
1:C:211:ASP:HB3	3:C:1003:HOH:O	1.82	0.79
1:A:108:LEU:O	1:A:112:THR:HG23	1.81	0.78
1:B:184:ARG:HG2	1:B:184:ARG:HH21	1.48	0.78
1:C:168:VAL:HG22	1:C:172:GLN:HB2	1.66	0.78
1:A:27:THR:O	1:A:58:VAL:HA	1.84	0.78
1:B:36:HIS:HD2	1:B:38:GLY:H	1.30	0.77
1:A:333:GLU:O	1:A:337:GLN:HG2	1.85	0.77
1:A:303:LEU:O	1:A:307:ARG:HB2	1.84	0.77
1:C:93:ASP:HB3	1:C:96:LYS:HB2	1.67	0.77
1:A:184:ARG:HD2	1:A:196:GLU:OE1	1.84	0.77
1:A:168:VAL:CG2	1:A:172:GLN:HB2	2.10	0.77
1:A:49:ARG:HA	3:A:1677:HOH:O	1.84	0.76
1:A:201:LEU:HD23	1:A:202:SER:H	1.50	0.76
1:C:154:GLN:NE2	2:C:3000:TRP:OXT	2.18	0.76
1:B:51:GLN:NE2	1:B:93:ASP:H	1.75	0.76
1:A:110:GLU:O	1:A:113:VAL:HG12	1.86	0.76
1:A:85:LEU:HD13	1:A:310:ARG:NH2	2.00	0.75
1:B:268:ASP:OD2	1:B:274:VAL:HG23	1.87	0.75
1:C:92:LEU:HG	1:C:97:THR:HG21	1.69	0.75
1:B:51:GLN:NE2	1:B:97:THR:HG22	1.99	0.75
1:A:255:VAL:HG22	1:A:261:PHE:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:VAL:HG21	1:C:307:ARG:HH21	1.52	0.74
1:B:349:PHE:CD2	1:C:80:VAL:HG11	2.23	0.74
1:A:202:SER:OG	1:A:205:PRO:HB3	1.87	0.74
1:C:56:LEU:HD11	1:C:58:VAL:HG13	1.70	0.73
1:A:291:VAL:HG13	1:A:292:LYS:N	2.02	0.73
1:A:254:ARG:HB2	1:A:256:GLU:OE1	1.88	0.73
1:A:30:ARG:HH22	1:A:68:ASP:HB3	1.53	0.72
1:B:22:ARG:HH21	1:B:53:GLU:HG3	1.53	0.72
1:A:127:ASN:HB3	1:A:130:VAL:CG1	2.19	0.72
1:A:201:LEU:CD2	1:A:202:SER:H	2.02	0.72
1:C:24:ARG:HD3	1:C:55:GLU:OE2	1.90	0.72
1:C:40:LEU:HA	1:C:44:LEU:HD12	1.72	0.72
1:A:44:LEU:O	1:A:48:VAL:HG23	1.90	0.72
1:C:273:ARG:HD2	3:C:1520:HOH:O	1.89	0.72
1:A:49:ARG:HD2	3:A:1677:HOH:O	1.90	0.72
1:C:22:ARG:HB2	1:C:23:PRO:HD3	1.71	0.72
1:B:240:MET:HE3	1:B:260:VAL:HG12	1.72	0.71
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.20	0.71
1:B:254:ARG:CD	1:B:256:GLU:HG2	2.18	0.71
1:A:291:VAL:HG13	1:A:292:LYS:H	1.55	0.71
1:B:127:ASN:HB3	1:B:130:VAL:HG12	1.71	0.71
1:B:68:ASP:OD1	1:B:137:LYS:HE2	1.90	0.71
1:A:169:GLY:H	1:A:172:GLN:HG3	1.54	0.71
1:A:180:ARG:HG2	1:A:196:GLU:HG2	1.73	0.71
1:A:254:ARG:HH11	1:A:256:GLU:HB2	1.56	0.71
1:A:229:SER:O	1:A:233:VAL:HG23	1.91	0.71
1:C:211:ASP:OD1	1:C:211:ASP:O	2.09	0.71
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.71	0.71
1:C:290:LYS:HE2	1:C:290:LYS:HA	1.73	0.70
1:A:173:LEU:N	1:A:174:PRO:HD2	2.05	0.70
1:B:240:MET:CE	1:B:260:VAL:HG12	2.22	0.70
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.57	0.70
1:B:277:LEU:CD1	1:B:286:LEU:HD11	2.22	0.69
1:A:230:ALA:HB1	1:A:300:ASN:HD21	1.57	0.69
1:C:108:LEU:O	1:C:112:THR:HG23	1.93	0.69
1:A:273:ARG:O	1:A:277:LEU:HD23	1.91	0.69
1:A:291:VAL:CG1	1:A:292:LYS:H	2.05	0.69
1:B:262:THR:HG21	3:B:1431:HOH:O	1.93	0.69
1:A:112:THR:O	1:A:116:LEU:HG	1.93	0.69
1:B:146:GLY:HA3	1:C:117:ASN:ND2	2.08	0.69
1:A:216:MET:HG3	1:A:223:ALA:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:HB2	3:A:1490:HOH:O	1.92	0.68
1:B:254:ARG:HD3	1:B:256:GLU:CG	2.22	0.68
1:A:63:VAL:HG13	1:A:102:GLN:CG	2.23	0.68
1:A:305:PRO:HG2	1:A:306:ILE:H	1.59	0.68
1:B:51:GLN:HE21	1:B:97:THR:CG2	1.99	0.68
1:A:168:VAL:HG22	1:A:169:GLY:O	1.93	0.68
1:A:259:PRO:HA	1:A:262:THR:CG2	2.24	0.68
1:A:168:VAL:HG11	1:A:199:ALA:HB1	1.76	0.67
1:B:259:PRO:HA	1:B:262:THR:CG2	2.25	0.67
1:A:241:TYR:O	1:A:259:PRO:HD2	1.94	0.67
1:A:288:ASP:HA	1:A:291:VAL:HG12	1.75	0.67
1:C:171:ASP:HB2	1:C:172:GLN:NE2	2.09	0.67
1:C:166:VAL:HG21	1:C:176:LEU:HD23	1.76	0.67
1:B:43:SER:C	1:B:47:ARG:HD2	2.15	0.66
1:A:85:LEU:HD13	1:A:310:ARG:HH22	1.58	0.66
1:A:215:LYS:NZ	1:A:217:SER:OG	2.29	0.66
1:A:317:PRO:O	1:A:320:VAL:HG12	1.96	0.66
1:C:234:ALA:O	1:C:238:MET:HG2	1.94	0.66
1:B:273:ARG:O	1:B:276:ALA:HB3	1.96	0.66
1:B:127:ASN:HB3	1:B:130:VAL:CG1	2.25	0.66
1:A:63:VAL:CG1	1:A:102:GLN:HG2	2.25	0.66
1:C:56:LEU:HD12	1:C:97:THR:HB	1.78	0.66
1:B:22:ARG:CB	1:B:23:PRO:HD3	2.26	0.65
1:B:237:VAL:HG13	1:B:240:MET:HE2	1.78	0.65
1:B:53:GLU:OE1	1:B:53:GLU:HA	1.96	0.65
1:B:122:SER:OG	1:C:141:GLU:HB3	1.97	0.65
1:A:52:ASP:HB3	1:A:96:LYS:NZ	2.12	0.65
1:C:254:ARG:CD	1:C:256:GLU:HG2	2.24	0.65
1:A:254:ARG:HD2	1:A:256:GLU:HB2	1.79	0.65
1:B:322:ARG:HG2	1:B:322:ARG:HH21	1.62	0.65
1:A:261:PHE:HA	3:A:1622:HOH:O	1.97	0.65
1:A:41:ALA:CB	1:A:207:LEU:HD22	2.27	0.65
1:B:35:LEU:HD13	1:B:44:LEU:HD11	1.77	0.64
1:A:130:VAL:O	1:A:134:ILE:HG13	1.97	0.64
1:C:51:GLN:HE22	1:C:93:ASP:N	1.88	0.64
1:B:22:ARG:CG	1:B:23:PRO:HD3	2.28	0.64
1:A:170:ASP:OD1	1:A:203:ARG:NH2	2.31	0.64
1:A:226:LEU:HD23	1:A:306:ILE:CD1	2.27	0.64
1:C:120:THR:CG2	1:C:123:HIS:H	2.04	0.64
1:C:166:VAL:HG23	1:C:166:VAL:O	1.97	0.64
1:B:295:LEU:O	1:B:295:LEU:HD23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:CYS:SG	1:A:324:VAL:HG12	2.38	0.64
1:A:133:GLU:O	1:A:137:LYS:HG3	1.98	0.63
1:B:40:LEU:HA	1:B:44:LEU:HB2	1.80	0.63
1:A:185:ARG:HD2	1:A:189:LEU:HD22	1.80	0.63
1:B:296:ILE:HG13	1:B:297:ASP:N	2.11	0.63
1:A:139:TYR:CD2	1:A:143:VAL:HG13	2.33	0.63
1:B:233:VAL:O	1:B:237:VAL:HG23	1.98	0.63
1:A:173:LEU:O	1:A:177:GLU:HB2	1.99	0.63
1:B:40:LEU:HD23	1:B:226:LEU:HD21	1.81	0.63
1:A:40:LEU:HA	1:A:44:LEU:HB3	1.79	0.63
1:A:72:ARG:HG2	3:A:1665:HOH:O	1.97	0.63
1:A:130:VAL:HG11	3:A:1543:HOH:O	1.98	0.63
1:C:294:HIS:O	1:C:298:VAL:HG12	1.99	0.63
1:A:30:ARG:HD2	1:A:65:ALA:HA	1.80	0.62
1:A:259:PRO:O	1:A:263:PHE:HB2	1.98	0.62
1:A:160:ALA:HA	1:A:338:THR:HG21	1.82	0.62
1:C:231:ASP:OD1	1:C:235:ARG:NE	2.32	0.62
1:A:256:GLU:H	1:A:256:GLU:CD	2.02	0.62
1:B:101:VAL:HG13	1:B:104:ALA:HB3	1.81	0.62
1:B:255:VAL:HG21	1:B:278:LYS:HG3	1.81	0.62
1:C:112:THR:HG22	1:C:156:ALA:CB	2.30	0.62
1:C:254:ARG:HD2	1:C:256:GLU:O	1.99	0.62
1:B:68:ASP:HB3	1:B:69:HIS:CD2	2.31	0.62
1:A:269:PRO:HD2	1:A:273:ARG:NH1	2.15	0.62
1:A:253:GLY:O	1:A:282:ARG:HA	1.98	0.62
1:B:289:VAL:O	1:B:293:LYS:HG3	2.00	0.62
1:A:79:ASN:HA	1:A:82:ALA:HB3	1.82	0.62
1:C:56:LEU:CD1	1:C:58:VAL:HG13	2.30	0.61
1:C:64:GLN:H	1:C:102:GLN:HE22	1.47	0.61
1:A:207:LEU:CG	1:A:208:PRO:HD2	2.30	0.61
1:C:295:LEU:HD22	1:C:299:LEU:HG	1.82	0.61
1:C:326:GLU:HG2	3:C:1650:HOH:O	2.00	0.61
1:C:175:MET:SD	1:C:175:MET:C	2.79	0.61
1:B:146:GLY:HA3	1:C:117:ASN:HD22	1.64	0.61
1:A:269:PRO:HA	3:A:1293:HOH:O	2.01	0.61
1:B:248:ARG:HD3	1:B:248:ARG:N	2.15	0.61
1:A:208:PRO:HG2	1:A:263:PHE:CE2	2.35	0.61
1:B:22:ARG:HB2	1:B:23:PRO:HD3	1.81	0.60
1:A:52:ASP:OD2	1:A:52:ASP:N	2.30	0.60
1:A:299:LEU:O	1:A:303:LEU:HD13	2.01	0.60
1:B:173:LEU:N	1:B:174:PRO:HD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:CG1	1:A:292:LYS:N	2.61	0.60
1:A:190:TYR:O	1:A:191:ALA:C	2.39	0.60
1:B:22:ARG:HH21	1:B:53:GLU:CG	2.15	0.60
1:A:289:VAL:O	1:A:293:LYS:HB2	2.02	0.60
1:C:203:ARG:C	1:C:204:VAL:HG23	2.22	0.60
1:B:62:ASP:O	1:B:66:LEU:HD23	2.02	0.60
1:C:201:LEU:HD23	1:C:202:SER:H	1.67	0.60
1:A:232:GLU:O	1:A:236:LYS:HB2	2.02	0.59
1:A:255:VAL:HG22	1:A:261:PHE:CD1	2.36	0.59
1:B:40:LEU:O	1:B:45:GLN:HG2	2.03	0.59
1:B:140:GLY:O	1:B:143:VAL:HG23	2.02	0.59
1:B:268:ASP:OD1	1:B:273:ARG:NH2	2.36	0.59
1:A:176:LEU:O	1:A:176:LEU:HD13	2.02	0.59
1:A:294:HIS:HA	1:A:297:ASP:OD2	2.03	0.59
1:A:261:PHE:CE1	1:A:278:LYS:HG2	2.37	0.59
1:A:295:LEU:O	1:A:299:LEU:HG	2.03	0.59
1:B:64:GLN:H	1:B:102:GLN:HE22	1.51	0.59
1:A:210:LEU:HB2	1:A:222:ASN:OD1	2.02	0.59
1:A:229:SER:OG	1:A:232:GLU:HB2	2.01	0.59
1:B:127:ASN:CB	1:B:130:VAL:HG12	2.32	0.59
1:A:21:ALA:HB3	1:A:53:GLU:O	2.03	0.59
1:A:142:ARG:O	1:A:142:ARG:HD3	2.03	0.59
1:A:254:ARG:HH11	1:A:256:GLU:CB	2.16	0.59
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.17	0.59
1:C:310:ARG:O	1:C:314:GLU:HG2	2.03	0.59
1:A:35:LEU:O	1:A:226:LEU:CD1	2.51	0.58
1:A:35:LEU:HD12	1:A:226:LEU:HD13	1.85	0.58
1:A:304:ALA:N	1:A:305:PRO:HD2	2.18	0.58
1:C:79:ASN:O	1:C:83:VAL:HG22	2.02	0.58
1:C:210:LEU:HD12	1:C:240:MET:HG2	1.84	0.58
1:C:254:ARG:CG	1:C:256:GLU:HG2	2.33	0.58
1:C:310:ARG:O	1:C:314:GLU:CG	2.52	0.58
1:A:273:ARG:O	1:A:276:ALA:HB3	2.04	0.58
2:C:3000:TRP:OXT	2:C:3000:TRP:CG	2.57	0.58
1:A:237:VAL:O	1:A:240:MET:N	2.30	0.58
1:A:208:PRO:HG3	1:A:262:THR:HG23	1.85	0.58
1:B:137:LYS:HD3	1:B:139:TYR:CE2	2.39	0.58
1:C:36:HIS:HB2	1:C:216:MET:CE	2.34	0.57
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.86	0.57
1:C:293:LYS:HG2	3:C:1361:HOH:O	2.04	0.57
1:B:23:PRO:HD2	1:B:54:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD12	1:A:226:LEU:N	2.16	0.57
1:A:305:PRO:HG2	1:A:306:ILE:HG22	1.86	0.57
1:C:48:VAL:O	1:C:51:GLN:HG2	2.04	0.57
1:A:22:ARG:N	1:A:23:PRO:CD	2.67	0.57
1:B:184:ARG:HG2	1:B:184:ARG:NH2	2.17	0.57
1:A:211:ASP:C	1:A:213:GLN:H	2.08	0.57
1:C:218:LYS:HB2	3:C:1206:HOH:O	2.04	0.57
1:A:98:THR:CG2	1:A:330:ARG:HD2	2.34	0.57
1:C:171:ASP:HB2	1:C:172:GLN:HE22	1.69	0.57
1:A:56:LEU:HD22	1:A:57:PHE:N	2.20	0.57
1:A:136:GLN:O	1:A:136:GLN:HG3	2.03	0.57
1:B:231:ASP:O	1:B:235:ARG:HG3	2.05	0.57
1:A:259:PRO:HA	1:A:262:THR:HG22	1.86	0.57
1:A:277:LEU:HD12	1:A:286:LEU:HD11	1.87	0.57
1:A:321:LEU:O	1:A:325:THR:HG23	2.04	0.57
1:B:207:LEU:HD12	1:B:208:PRO:HD2	1.87	0.57
1:C:56:LEU:HD11	1:C:58:VAL:CG1	2.35	0.57
1:B:177:GLU:HG3	3:B:1946:HOH:O	2.05	0.56
1:A:98:THR:OG1	1:A:330:ARG:HD2	2.05	0.56
1:A:296:ILE:HG13	1:A:297:ASP:N	2.20	0.56
1:C:40:LEU:HA	1:C:44:LEU:HB2	1.87	0.56
1:C:133:GLU:O	1:C:136:GLN:HG3	2.04	0.56
1:B:263:PHE:HB3	1:B:295:LEU:HD11	1.86	0.56
1:C:187:ASN:HB3	1:C:192:PRO:HA	1.86	0.56
1:B:36:HIS:CD2	1:B:38:GLY:H	2.19	0.56
1:C:56:LEU:HD13	1:C:56:LEU:C	2.26	0.56
1:B:277:LEU:HD22	1:B:277:LEU:H	1.69	0.56
1:A:246:HIS:NE2	1:A:251:ASP:O	2.33	0.56
1:A:36:HIS:H	1:A:39:HIS:HD2	1.52	0.56
1:C:74:GLU:HB2	3:C:1034:HOH:O	2.05	0.56
1:C:180:ARG:HD2	1:C:196:GLU:HG3	1.87	0.56
1:A:277:LEU:HA	1:A:280:GLN:NE2	2.21	0.56
1:A:302:VAL:O	1:A:305:PRO:HD2	2.06	0.56
1:B:75:GLN:O	1:B:79:ASN:ND2	2.38	0.56
1:A:240:MET:CE	1:A:259:PRO:HB2	2.36	0.56
1:B:44:LEU:HA	1:B:47:ARG:CD	2.35	0.56
1:B:189:LEU:HD21	1:C:71:ASP:HA	1.87	0.55
1:C:166:VAL:HG21	1:C:176:LEU:CD2	2.37	0.55
1:C:216:MET:HE2	1:C:223:ALA:HB1	1.87	0.55
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.07	0.55
1:A:149:VAL:O	1:A:149:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.21	0.55
1:C:204:VAL:HG21	3:C:1173:HOH:O	2.05	0.55
1:B:248:ARG:HD3	1:B:248:ARG:H	1.71	0.55
1:A:112:THR:HG22	1:A:156:ALA:CB	2.36	0.55
1:A:216:MET:HA	1:A:222:ASN:O	2.07	0.55
1:C:254:ARG:HG2	1:C:255:VAL:N	2.20	0.55
1:A:37:LEU:HG	1:A:224:ILE:HG12	1.88	0.55
1:A:201:LEU:CD2	1:A:202:SER:N	2.70	0.55
1:C:233:VAL:HG21	1:C:307:ARG:NH2	2.22	0.55
1:C:256:GLU:H	1:C:256:GLU:CD	2.08	0.55
1:B:349:PHE:CE2	1:C:81:LEU:HD13	2.42	0.55
1:A:58:VAL:HG13	1:A:58:VAL:O	2.05	0.55
1:A:76:VAL:HG13	1:A:77:ARG:N	2.22	0.55
1:A:218:LYS:HA	1:A:218:LYS:CE	2.34	0.55
1:C:40:LEU:HD12	1:C:44:LEU:HB2	1.87	0.55
1:C:62:ASP:OD2	1:C:103:SER:OG	2.24	0.55
1:C:183:VAL:HG13	1:C:194:LEU:HB2	1.89	0.55
1:B:64:GLN:HE22	1:B:154:GLN:CG	2.20	0.55
1:C:59:LEU:HD12	1:C:100:VAL:HG22	1.87	0.55
1:B:237:VAL:HG13	1:B:240:MET:CE	2.36	0.55
1:B:134:ILE:HD13	1:B:143:VAL:HG21	1.88	0.54
1:A:35:LEU:O	1:A:226:LEU:HD12	2.07	0.54
1:A:260:VAL:O	1:A:264:LEU:HB2	2.07	0.54
1:C:127:ASN:HB3	1:C:130:VAL:HG22	1.89	0.54
1:A:220:LEU:C	1:A:222:ASN:H	2.10	0.54
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.07	0.54
1:C:175:MET:HB2	3:C:1018:HOH:O	2.07	0.54
1:B:247:LEU:HB2	1:B:248:ARG:HH21	1.72	0.54
1:A:247:LEU:HD22	3:A:1323:HOH:O	2.07	0.54
1:A:288:ASP:O	1:A:292:LYS:HG3	2.07	0.54
1:C:64:GLN:OE1	1:C:154:GLN:HG3	2.08	0.54
1:C:51:GLN:NE2	1:C:93:ASP:H	1.89	0.54
1:A:193:VAL:HG22	1:A:193:VAL:O	2.08	0.54
1:A:220:LEU:C	1:A:222:ASN:N	2.60	0.54
1:C:339:LEU:O	1:C:343:ARG:HG3	2.08	0.54
1:C:27:THR:HB	3:C:1219:HOH:O	2.07	0.54
1:A:107:GLU:HB3	1:A:339:LEU:HG	1.90	0.54
1:C:187:ASN:CB	1:C:192:PRO:HA	2.37	0.54
1:C:295:LEU:O	1:C:298:VAL:HG13	2.07	0.54
1:B:58:VAL:HG23	1:B:58:VAL:O	2.07	0.54
1:B:168:VAL:HG22	1:B:169:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLN:HG2	3:C:1945:HOH:O	2.07	0.54
1:B:295:LEU:HD23	1:B:295:LEU:C	2.28	0.54
1:B:296:ILE:HD12	1:B:300:ASN:ND2	2.23	0.54
1:B:22:ARG:NH2	1:B:53:GLU:HG3	2.22	0.53
1:B:66:LEU:C	1:B:68:ASP:H	2.10	0.53
1:A:248:ARG:HD3	1:A:248:ARG:N	2.23	0.53
1:C:40:LEU:CA	1:C:44:LEU:HD12	2.37	0.53
1:A:249:ALA:HB2	1:A:287:GLY:HA3	1.90	0.53
1:B:344:ARG:CG	1:B:344:ARG:HH11	2.21	0.53
1:B:259:PRO:HA	1:B:262:THR:HG23	1.89	0.53
1:A:242:THR:HB	1:A:258:ASN:HD21	1.73	0.53
1:C:243:ASP:OD2	1:C:246:HIS:HB2	2.08	0.53
1:C:180:ARG:HE	1:C:196:GLU:CD	2.12	0.53
1:B:23:PRO:O	1:B:54:ALA:HB1	2.09	0.53
1:B:74:GLU:OE1	1:C:347:ARG:NH1	2.42	0.53
1:B:255:VAL:HG13	1:B:261:PHE:CD2	2.43	0.53
1:A:255:VAL:HG13	1:A:261:PHE:CD1	2.44	0.53
1:B:211:ASP:HB3	1:B:213:GLN:HG3	1.90	0.53
1:C:120:THR:HG22	1:C:123:HIS:HB2	1.90	0.53
1:C:22:ARG:CB	1:C:23:PRO:CD	2.86	0.52
1:A:215:LYS:HB3	3:A:2052:HOH:O	2.08	0.52
1:A:237:VAL:HG13	1:A:295:LEU:HD23	1.91	0.52
1:C:286:LEU:HD12	1:C:291:VAL:HG23	1.91	0.52
1:B:299:LEU:HA	1:B:302:VAL:CG1	2.40	0.52
1:A:180:ARG:O	1:A:184:ARG:HD3	2.10	0.52
1:C:180:ARG:NH1	1:C:180:ARG:CG	2.68	0.52
1:B:202:SER:HB3	3:B:1285:HOH:O	2.09	0.52
1:B:253:GLY:O	1:B:282:ARG:HA	2.09	0.52
1:B:296:ILE:CD1	1:B:300:ASN:ND2	2.73	0.52
1:C:21:ALA:HB2	3:C:1220:HOH:O	2.09	0.52
1:B:102:GLN:HG3	1:B:108:LEU:HD12	1.92	0.52
1:A:180:ARG:HB3	1:A:184:ARG:HH11	1.75	0.52
1:A:207:LEU:HG	1:A:208:PRO:HD2	1.91	0.52
1:A:250:SER:O	1:A:284:GLY:HA2	2.09	0.52
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.25	0.52
1:B:32:THR:O	1:B:75:GLN:NE2	2.43	0.52
1:A:288:ASP:O	1:A:291:VAL:HG12	2.09	0.52
1:A:116:LEU:HD23	1:A:152:VAL:HG21	1.91	0.52
1:A:261:PHE:CD1	1:A:278:LYS:HG2	2.44	0.52
1:B:299:LEU:HA	1:B:302:VAL:HG12	1.92	0.51
1:A:232:GLU:HB3	3:A:1447:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	1:C:145:ALA:HB3	2.10	0.51
1:B:189:LEU:CD2	1:C:71:ASP:HA	2.40	0.51
1:A:255:VAL:HG11	1:A:278:LYS:HE2	1.92	0.51
1:B:211:ASP:OD1	1:B:222:ASN:HB3	2.11	0.51
1:A:23:PRO:O	1:A:54:ALA:HB1	2.09	0.51
1:B:292:LYS:O	1:B:296:ILE:CG2	2.58	0.51
1:A:260:VAL:HG13	1:A:295:LEU:CD2	2.40	0.51
1:B:298:VAL:O	1:B:302:VAL:HG12	2.11	0.51
1:A:234:ALA:HA	1:A:296:ILE:CG2	2.41	0.51
1:A:293:LYS:O	1:A:296:ILE:HG12	2.10	0.51
1:C:165:LEU:HD22	1:C:200:GLN:HB2	1.93	0.51
1:C:295:LEU:CD2	1:C:299:LEU:HG	2.40	0.51
1:B:248:ARG:NE	1:B:251:ASP:OD2	2.44	0.51
1:A:41:ALA:HB2	1:A:207:LEU:HD22	1.92	0.51
1:A:66:LEU:HD21	1:A:76:VAL:HG11	1.92	0.51
1:A:208:PRO:HG2	1:A:263:PHE:HE2	1.74	0.51
1:B:333:GLU:HG3	1:B:337:GLN:HE21	1.74	0.51
1:C:41:ALA:HB2	1:C:267:PHE:CZ	2.46	0.51
1:C:77:ARG:O	1:C:80:VAL:CG1	2.51	0.51
1:C:322:ARG:HD3	3:C:1047:HOH:O	2.10	0.51
1:B:333:GLU:OE2	1:B:333:GLU:HA	2.11	0.50
1:A:215:LYS:O	1:A:222:ASN:ND2	2.44	0.50
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.21	0.50
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.36	0.50
1:A:63:VAL:HG13	1:A:102:GLN:CD	2.32	0.50
1:A:150:TYR:CE2	1:A:154:GLN:NE2	2.80	0.50
1:C:120:THR:HG23	1:C:123:HIS:N	2.07	0.50
1:A:193:VAL:HG21	1:A:341:GLN:CB	2.36	0.50
1:A:74:GLU:HG2	3:A:1380:HOH:O	2.11	0.50
1:A:290:LYS:HE2	1:A:290:LYS:HA	1.93	0.50
1:C:210:LEU:HD12	1:C:240:MET:CG	2.42	0.50
1:B:273:ARG:NH2	1:B:294:HIS:NE2	2.59	0.50
1:A:150:TYR:O	1:A:154:GLN:HG3	2.11	0.50
1:A:276:ALA:O	1:A:280:GLN:HG3	2.12	0.50
1:C:127:ASN:OD1	1:C:129:THR:HG22	2.12	0.50
1:B:30:ARG:HH22	1:B:68:ASP:HB2	1.76	0.50
1:B:184:ARG:HH21	1:B:184:ARG:CG	2.20	0.50
1:A:110:GLU:O	1:A:113:VAL:CG1	2.58	0.50
1:A:205:PRO:O	1:A:206:ARG:C	2.50	0.50
1:B:316:ASP:OD2	1:B:319:ALA:HB2	2.11	0.49
1:A:173:LEU:N	1:A:174:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG13	1:A:295:LEU:HD22	1.92	0.49
1:B:254:ARG:HH11	1:B:256:GLU:CG	2.25	0.49
1:C:256:GLU:HB2	3:C:1723:HOH:O	2.11	0.49
1:B:295:LEU:HA	1:B:298:VAL:HG12	1.94	0.49
1:A:290:LYS:HE2	1:A:290:LYS:CA	2.43	0.49
1:C:133:GLU:O	1:C:137:LYS:HD3	2.12	0.49
1:B:145:ALA:HB3	1:C:116:LEU:O	2.13	0.49
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.77	0.49
1:B:315:ARG:O	1:B:315:ARG:HG2	2.12	0.49
1:B:349:PHE:CD2	1:C:80:VAL:CG1	2.95	0.49
1:A:237:VAL:O	1:A:240:MET:HB2	2.11	0.49
1:B:25:VAL:HG22	1:B:165:LEU:HB3	1.94	0.49
1:B:292:LYS:O	1:B:296:ILE:HG23	2.12	0.49
1:C:241:TYR:OH	1:C:244:PRO:HD3	2.13	0.49
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.94	0.49
1:A:218:LYS:NZ	1:A:225:ALA:HB2	2.28	0.49
1:C:23:PRO:HB3	3:C:1304:HOH:O	2.12	0.49
1:A:49:ARG:O	1:A:52:ASP:OD2	2.31	0.49
1:B:23:PRO:HD2	1:B:54:ALA:CB	2.41	0.49
1:B:43:SER:O	1:B:46:ASN:N	2.46	0.49
1:C:60:LEU:HD22	1:C:83:VAL:HG21	1.95	0.49
1:C:254:ARG:CD	1:C:256:GLU:O	2.61	0.49
1:A:143:VAL:HG12	1:A:144:PRO:HD2	1.95	0.48
1:A:175:MET:SD	1:A:176:LEU:N	2.86	0.48
1:A:211:ASP:O	1:A:213:GLN:N	2.42	0.48
1:A:292:LYS:O	1:A:295:LEU:N	2.47	0.48
1:B:29:ASP:O	1:B:31:PRO:HD3	2.14	0.48
1:B:50:LEU:C	1:B:50:LEU:HD12	2.34	0.48
1:C:255:VAL:HG21	1:C:278:LYS:HG2	1.95	0.48
1:B:237:VAL:CG1	1:B:240:MET:HE2	2.43	0.48
1:A:125:ARG:HG3	1:A:125:ARG:HH21	1.78	0.48
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.94	0.48
1:B:211:ASP:OD1	1:B:213:GLN:NE2	2.47	0.48
1:A:98:THR:OG1	1:A:330:ARG:NH1	2.43	0.48
1:A:112:THR:HG22	1:A:153:SER:HA	1.95	0.48
1:A:158:ILE:HG23	1:A:163:ALA:HB3	1.95	0.48
1:A:105:VAL:HG13	1:A:108:LEU:HG	1.94	0.48
1:A:185:ARG:O	1:A:189:LEU:HB2	2.14	0.48
1:A:308:THR:O	1:A:311:ALA:HB3	2.12	0.48
1:B:270:ASP:O	1:B:273:ARG:HB3	2.14	0.48
1:B:277:LEU:HD13	1:B:280:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD22	1:C:83:VAL:CG2	2.43	0.48
1:B:264:LEU:HG	1:B:295:LEU:HD12	1.96	0.48
1:A:175:MET:SD	1:A:175:MET:C	2.92	0.48
1:C:292:LYS:O	1:C:296:ILE:HG13	2.14	0.48
1:B:68:ASP:OD1	1:B:137:LYS:CE	2.62	0.47
1:B:101:VAL:HG13	1:B:101:VAL:O	2.14	0.47
1:B:255:VAL:HG22	1:B:261:PHE:CE2	2.48	0.47
1:A:212:GLY:O	1:A:213:GLN:C	2.53	0.47
1:A:253:GLY:HA3	1:A:281:TYR:CE2	2.49	0.47
1:B:127:ASN:CG	1:B:130:VAL:HG12	2.34	0.47
1:B:315:ARG:HG3	3:B:1367:HOH:O	2.13	0.47
1:A:45:GLN:O	1:A:48:VAL:HB	2.14	0.47
1:C:276:ALA:O	1:C:280:GLN:HG3	2.13	0.47
1:C:344:ARG:HD3	3:C:1217:HOH:O	2.15	0.47
1:B:36:HIS:CE1	1:B:39:HIS:CE1	3.03	0.47
1:B:77:ARG:NE	1:C:347:ARG:NH2	2.62	0.47
1:B:249:ALA:O	1:B:250:SER:C	2.53	0.47
1:C:63:VAL:H	1:C:102:GLN:HE21	1.61	0.47
1:A:32:THR:HG23	1:A:69:HIS:HE1	1.79	0.47
1:A:215:LYS:NZ	1:A:215:LYS:HB2	2.29	0.47
1:C:154:GLN:CD	2:C:3000:TRP:OXT	2.52	0.47
1:C:201:LEU:HD23	1:C:202:SER:N	2.27	0.47
1:B:92:LEU:HD12	1:B:92:LEU:HA	1.78	0.47
1:C:36:HIS:CE1	1:C:216:MET:HG2	2.50	0.47
1:B:22:ARG:HB2	1:B:23:PRO:CD	2.45	0.47
1:B:64:GLN:H	1:B:102:GLN:NE2	2.12	0.47
1:B:66:LEU:C	1:B:68:ASP:N	2.68	0.47
1:B:149:VAL:O	1:B:149:VAL:CG1	2.63	0.47
1:A:36:HIS:HD2	1:A:38:GLY:H	1.61	0.47
1:A:130:VAL:HG13	1:A:131:LYS:N	2.28	0.47
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.78	0.47
1:A:288:ASP:CA	1:A:291:VAL:HG12	2.42	0.47
1:B:62:ASP:OD1	1:B:103:SER:OG	2.26	0.47
1:B:316:ASP:OD1	1:B:318:ASP:OD2	2.33	0.47
1:A:241:TYR:O	1:A:259:PRO:CD	2.60	0.47
1:B:71:ASP:OD1	1:B:72:ARG:CD	2.63	0.47
1:A:209:GLY:O	1:A:210:LEU:C	2.53	0.47
1:C:241:TYR:CZ	1:C:244:PRO:HD3	2.50	0.47
1:A:98:THR:HG23	1:A:330:ARG:HD2	1.96	0.46
1:B:241:TYR:O	1:B:259:PRO:HG2	2.14	0.46
1:A:234:ALA:HA	1:A:296:ILE:HG22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:OE1	1:B:343:ARG:HD3	2.15	0.46
1:C:320:VAL:O	1:C:323:PHE:HB3	2.15	0.46
1:A:56:LEU:HD13	1:A:97:THR:HG23	1.98	0.46
1:A:288:ASP:HA	1:A:291:VAL:CG1	2.43	0.46
1:A:296:ILE:HG13	1:A:297:ASP:H	1.81	0.46
1:B:274:VAL:C	1:B:276:ALA:N	2.69	0.46
1:A:32:THR:HG22	1:A:32:THR:O	2.15	0.46
1:A:33:GLY:HA2	1:A:79:ASN:ND2	2.31	0.46
1:A:99:CYS:HB2	1:A:323:PHE:CZ	2.50	0.46
1:A:242:THR:HB	1:A:258:ASN:ND2	2.30	0.46
1:C:258:ASN:C	1:C:258:ASN:HD22	2.18	0.46
1:C:310:ARG:O	1:C:314:GLU:HG3	2.15	0.46
1:B:22:ARG:CD	1:B:23:PRO:HD3	2.46	0.46
1:A:32:THR:HG23	1:A:69:HIS:CE1	2.51	0.46
1:A:36:HIS:O	1:A:38:GLY:N	2.49	0.46
1:A:277:LEU:HD13	1:A:280:GLN:NE2	2.31	0.46
1:A:46:ASN:ND2	1:A:50:LEU:HG	2.30	0.46
1:A:255:VAL:HG21	1:A:278:LYS:HD3	1.98	0.46
1:A:290:LYS:HE2	1:A:290:LYS:N	2.30	0.46
1:B:333:GLU:O	1:B:337:GLN:HG3	2.16	0.46
1:A:30:ARG:O	1:A:32:THR:N	2.48	0.46
1:A:335:ALA:O	1:A:339:LEU:HD23	2.16	0.46
1:B:263:PHE:CB	1:B:295:LEU:HD11	2.46	0.46
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.30	0.46
1:C:311:ALA:CA	1:C:314:GLU:HG3	2.43	0.46
1:A:256:GLU:CD	1:A:256:GLU:N	2.70	0.46
1:C:25:VAL:HG13	1:C:167:PRO:HD3	1.96	0.46
1:B:166:VAL:HB	1:B:176:LEU:HD21	1.98	0.45
1:A:344:ARG:HD3	3:A:1031:HOH:O	2.16	0.45
1:C:187:ASN:CG	1:C:192:PRO:HA	2.36	0.45
1:B:22:ARG:CB	1:B:23:PRO:CD	2.94	0.45
1:B:330:ARG:O	1:B:333:GLU:HB3	2.16	0.45
1:B:287:GLY:O	1:B:290:LYS:N	2.49	0.45
1:A:51:GLN:HE22	1:A:92:LEU:HA	1.80	0.45
1:A:180:ARG:HB3	1:A:184:ARG:NH1	2.31	0.45
1:C:270:ASP:OD2	1:C:273:ARG:CZ	2.64	0.45
1:B:51:GLN:NE2	1:B:97:THR:CG2	2.71	0.45
1:B:184:ARG:NH2	1:B:184:ARG:CG	2.76	0.45
1:A:255:VAL:HG13	1:A:261:PHE:HB3	1.99	0.45
1:C:30:ARG:HD2	1:C:64:GLN:HE21	1.81	0.45
1:C:210:LEU:HD21	1:C:224:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLY:O	1:C:247:LEU:HD13	2.16	0.45
1:C:246:HIS:C	1:C:247:LEU:HD12	2.37	0.45
1:B:219:SER:HA	3:B:1401:HOH:O	2.16	0.45
1:B:264:LEU:O	1:B:268:ASP:HB3	2.17	0.45
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.76	0.45
1:A:21:ALA:HB1	1:A:23:PRO:HD2	1.98	0.45
1:A:46:ASN:O	1:A:50:LEU:N	2.33	0.45
1:A:187:ASN:OD1	1:A:192:PRO:HA	2.16	0.45
1:A:294:HIS:O	1:A:298:VAL:HG23	2.16	0.45
1:A:296:ILE:O	1:A:300:ASN:HB2	2.15	0.45
1:A:303:LEU:HB3	1:A:307:ARG:NH2	2.31	0.45
1:A:249:ALA:CB	1:A:287:GLY:HA3	2.47	0.45
1:A:265:ASP:HB3	1:A:274:VAL:HG11	1.97	0.45
1:A:322:ARG:HA	1:A:325:THR:HG1	1.82	0.45
1:B:74:GLU:OE2	1:C:347:ARG:NH1	2.50	0.45
1:A:211:ASP:C	1:A:213:GLN:N	2.70	0.45
1:A:226:LEU:HD23	1:A:306:ILE:HD12	1.98	0.45
1:A:277:LEU:O	1:A:281:TYR:N	2.50	0.45
1:A:302:VAL:HG13	1:A:303:LEU:HD13	1.97	0.45
1:B:270:ASP:HB2	1:B:273:ARG:CZ	2.47	0.45
1:C:112:THR:HG22	1:C:156:ALA:HB3	1.98	0.45
1:B:74:GLU:CD	1:C:347:ARG:NH1	2.70	0.44
1:B:169:GLY:O	1:B:170:ASP:C	2.55	0.44
1:B:175:MET:SD	1:B:175:MET:C	2.95	0.44
1:C:51:GLN:NE2	1:C:97:THR:CG2	2.79	0.44
1:C:271:PRO:HG2	3:C:1373:HOH:O	2.17	0.44
1:B:122:SER:HG	1:C:141:GLU:HB3	1.83	0.44
1:A:130:VAL:CG1	1:A:131:LYS:N	2.79	0.44
1:B:140:GLY:O	1:B:143:VAL:CG2	2.66	0.44
1:B:165:LEU:HD23	1:B:198:GLN:O	2.18	0.44
1:A:68:ASP:OD2	1:A:137:LYS:NZ	2.45	0.44
1:A:105:VAL:HA	1:A:106:PRO:HD2	1.80	0.44
1:A:293:LYS:HD2	1:A:296:ILE:HD11	1.99	0.44
1:C:185:ARG:O	1:C:189:LEU:HB2	2.16	0.44
1:A:136:GLN:O	1:A:136:GLN:CG	2.66	0.44
1:C:36:HIS:CG	1:C:216:MET:HE2	2.52	0.44
1:C:321:LEU:HD22	1:C:325:THR:HG23	2.00	0.44
1:C:30:ARG:HA	1:C:31:PRO:HD3	1.79	0.44
1:A:205:PRO:HG2	1:A:206:ARG:H	1.82	0.44
1:C:62:ASP:OD2	1:C:103:SER:CB	2.66	0.44
1:C:201:LEU:HD22	1:C:202:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG22	1:A:120:THR:N	2.32	0.44
1:A:149:VAL:O	1:A:152:VAL:HG13	2.17	0.44
1:C:58:VAL:CG2	1:C:99:CYS:HA	2.47	0.44
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.80	0.44
1:B:123:HIS:HE1	3:B:1334:HOH:O	2.01	0.43
1:A:52:ASP:HB3	1:A:96:LYS:HZ1	1.82	0.43
1:A:52:ASP:HB3	1:A:96:LYS:HZ3	1.83	0.43
1:A:76:VAL:CG1	1:A:77:ARG:N	2.81	0.43
1:A:143:VAL:HG12	1:A:144:PRO:CD	2.49	0.43
1:A:180:ARG:HG2	1:A:197:PRO:HD2	1.99	0.43
1:C:154:GLN:NE2	2:C:3000:TRP:CD2	2.86	0.43
1:C:154:GLN:O	1:C:158:ILE:HG12	2.18	0.43
1:C:166:VAL:O	1:C:166:VAL:CG2	2.66	0.43
1:C:268:ASP:HA	1:C:269:PRO:HD2	1.87	0.43
1:B:346:MET:CE	1:B:348:LEU:HD11	2.49	0.43
1:A:237:VAL:HA	1:A:240:MET:HG3	2.00	0.43
1:C:68:ASP:OD2	1:C:69:HIS:CD2	2.69	0.43
1:A:168:VAL:CG1	1:A:199:ALA:HB1	2.46	0.43
1:A:294:HIS:HD2	1:A:297:ASP:OD2	2.02	0.43
1:B:255:VAL:HG13	1:B:261:PHE:CB	2.48	0.43
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.77	0.43
1:C:203:ARG:C	1:C:204:VAL:O	2.57	0.43
1:A:250:SER:O	1:A:284:GLY:CA	2.66	0.43
1:A:293:LYS:O	1:A:296:ILE:CG1	2.66	0.43
1:C:204:VAL:HG12	1:C:205:PRO:CD	2.36	0.43
1:A:210:LEU:HD22	1:A:240:MET:HG2	2.01	0.43
1:A:269:PRO:HD2	1:A:273:ARG:HH12	1.84	0.43
1:A:291:VAL:O	1:A:292:LYS:C	2.56	0.43
1:C:62:ASP:O	1:C:66:LEU:HG	2.18	0.43
1:B:93:ASP:HA	1:B:94:PRO:HD3	1.86	0.43
1:B:101:VAL:HG12	1:B:328:THR:OG1	2.18	0.43
1:A:210:LEU:HD22	1:A:240:MET:CG	2.49	0.42
1:A:254:ARG:CD	1:A:256:GLU:HB2	2.47	0.42
1:A:334:VAL:HA	1:A:337:GLN:HG3	2.01	0.42
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.87	0.42
1:A:21:ALA:HB1	1:A:23:PRO:CD	2.48	0.42
1:A:121:VAL:O	1:A:125:ARG:HB2	2.19	0.42
1:A:173:LEU:HD13	3:A:2045:HOH:O	2.18	0.42
1:B:58:VAL:HG23	1:B:99:CYS:HA	2.00	0.42
1:A:208:PRO:HG3	1:A:262:THR:CG2	2.48	0.42
1:B:254:ARG:NH1	1:B:256:GLU:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:H	1:A:102:GLN:HB3	1.84	0.42
1:A:105:VAL:HG13	1:A:105:VAL:O	2.19	0.42
1:A:105:VAL:HG13	1:A:108:LEU:CD1	2.49	0.42
1:A:150:TYR:N	1:A:151:PRO:CD	2.83	0.42
1:C:52:ASP:OD2	1:C:96:LYS:NZ	2.49	0.42
1:B:277:LEU:HA	1:B:286:LEU:HD11	2.01	0.42
1:A:58:VAL:O	1:A:58:VAL:CG1	2.67	0.42
1:A:191:ALA:HA	1:A:192:PRO:HD3	1.80	0.42
1:A:241:TYR:O	1:A:241:TYR:CD1	2.73	0.42
1:B:30:ARG:HH22	1:B:68:ASP:CB	2.33	0.42
1:A:274:VAL:C	1:A:276:ALA:H	2.22	0.42
1:C:108:LEU:HD13	1:C:157:ASP:OD1	2.19	0.42
1:C:230:ALA:HB1	1:C:300:ASN:HD21	1.85	0.42
1:B:21:ALA:HA	1:B:54:ALA:HA	2.01	0.42
1:B:258:ASN:HA	1:B:259:PRO:HD2	1.97	0.42
1:B:346:MET:HE3	1:B:348:LEU:HD11	2.02	0.42
1:C:231:ASP:OD1	1:C:235:ARG:CZ	2.68	0.42
1:B:211:ASP:CB	1:B:213:GLN:HG3	2.50	0.42
1:A:214:ALA:C	1:A:215:LYS:HG3	2.40	0.42
1:C:180:ARG:CD	1:C:197:PRO:O	2.61	0.42
1:B:277:LEU:HA	1:B:286:LEU:CD1	2.50	0.42
1:A:119:VAL:HG21	1:A:124:LEU:HD13	2.02	0.42
1:B:59:LEU:HD12	1:B:100:VAL:O	2.19	0.42
1:A:165:LEU:HD22	1:A:166:VAL:N	2.35	0.42
1:C:25:VAL:HG22	1:C:165:LEU:HB3	2.01	0.42
1:C:243:ASP:HA	1:C:244:PRO:HD2	1.87	0.42
1:A:22:ARG:N	1:A:23:PRO:HD2	2.34	0.41
1:A:216:MET:CG	1:A:223:ALA:HA	2.47	0.41
1:C:248:ARG:O	1:C:251:ASP:HB2	2.20	0.41
1:B:273:ARG:O	1:B:277:LEU:HD22	2.20	0.41
1:B:278:LYS:HG2	1:B:282:ARG:NH2	2.34	0.41
1:B:344:ARG:CG	1:B:344:ARG:NH1	2.80	0.41
1:A:203:ARG:HD2	3:A:1508:HOH:O	2.20	0.41
1:A:305:PRO:HG2	1:A:306:ILE:N	2.31	0.41
1:C:32:THR:O	1:C:32:THR:HG22	2.19	0.41
1:C:64:GLN:H	1:C:102:GLN:NE2	2.15	0.41
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.51	0.41
1:B:142:ARG:HA	1:C:120:THR:OG1	2.20	0.41
1:B:244:PRO:C	1:B:246:HIS:H	2.24	0.41
1:A:47:ARG:O	1:A:51:GLN:N	2.51	0.41
1:A:110:GLU:HG2	1:A:114:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HD3	3:A:1187:HOH:O	2.20	0.41
1:C:129:THR:O	1:C:133:GLU:HG3	2.21	0.41
1:C:170:ASP:OD1	1:C:170:ASP:N	2.53	0.41
1:B:66:LEU:HD12	1:B:70:PHE:HA	2.01	0.41
1:B:255:VAL:HG22	1:B:261:PHE:CD2	2.56	0.41
1:C:304:ALA:N	1:C:305:PRO:HD2	2.35	0.41
1:A:201:LEU:HD22	1:A:202:SER:N	2.35	0.41
1:C:255:VAL:O	1:C:258:ASN:HB3	2.20	0.41
1:A:51:GLN:OE1	1:A:93:ASP:N	2.43	0.41
1:A:72:ARG:N	1:A:73:PRO:CD	2.83	0.41
1:C:25:VAL:HG11	1:C:50:LEU:HD13	2.02	0.41
1:C:293:LYS:HD2	1:C:293:LYS:HA	1.93	0.41
1:A:32:THR:CG2	1:A:69:HIS:HE1	2.33	0.41
1:A:125:ARG:HG3	1:A:125:ARG:NH2	2.35	0.41
1:A:89:ALA:O	1:A:306:ILE:HB	2.20	0.41
1:B:63:VAL:H	1:B:102:GLN:HE21	1.67	0.41
1:B:243:ASP:OD1	1:B:244:PRO:O	2.39	0.41
1:B:246:HIS:CE1	1:B:288:ASP:OD2	2.73	0.41
1:A:105:VAL:O	1:A:108:LEU:HG	2.21	0.41
1:A:230:ALA:CB	1:A:300:ASN:HD21	2.28	0.41
1:B:137:LYS:HE3	3:B:1218:HOH:O	2.19	0.41
1:B:210:LEU:HD21	1:B:224:ILE:HG13	2.03	0.41
1:A:36:HIS:O	1:A:39:HIS:N	2.51	0.41
1:C:58:VAL:HG23	1:C:99:CYS:HA	2.02	0.41
1:C:102:GLN:HG3	1:C:108:LEU:HD12	2.02	0.41
1:B:67:THR:HG22	1:C:117:ASN:HD21	1.85	0.40
1:B:184:ARG:HE	1:B:196:GLU:CD	2.23	0.40
1:B:61:ALA:HB1	1:B:64:GLN:HB3	2.04	0.40
1:B:295:LEU:C	1:B:298:VAL:HG12	2.39	0.40
1:A:36:HIS:CE1	1:A:39:HIS:NE2	2.89	0.40
1:B:33:GLY:HA2	1:B:79:ASN:OD1	2.21	0.40
1:B:93:ASP:O	1:B:97:THR:CG2	2.69	0.40
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.57	0.40
1:A:277:LEU:HA	1:A:280:GLN:HE21	1.87	0.40
1:A:302:VAL:HG13	1:A:303:LEU:CD1	2.51	0.40
1:C:270:ASP:OD2	1:C:273:ARG:NH1	2.54	0.40
1:B:260:VAL:HG23	1:B:261:PHE:N	2.37	0.40
1:A:41:ALA:HB1	1:A:207:LEU:HD13	2.04	0.40
1:A:260:VAL:HA	1:A:295:LEU:HD22	2.02	0.40
1:C:62:ASP:OD2	1:C:103:SER:HB2	2.21	0.40
1:C:150:TYR:N	1:C:151:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:O	1:B:51:GLN:HB2	2.20	0.40
1:B:254:ARG:NH1	1:B:256:GLU:CG	2.84	0.40
1:B:322:ARG:HG2	1:B:322:ARG:NH2	2.32	0.40
1:A:261:PHE:HZ	1:A:281:TYR:CG	2.40	0.40
1:A:264:LEU:HD22	3:A:1622:HOH:O	2.22	0.40
1:C:32:THR:HG23	1:C:75:GLN:NE2	2.36	0.40
1:C:43:SER:O	1:C:47:ARG:HD3	2.21	0.40
1:C:58:VAL:HG23	1:C:58:VAL:O	2.21	0.40

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:CA	3:C:2021:HOH:O[1_554]	0.49	1.71
3:C:1200:HOH:O	3:C:1789:HOH:O[4_546]	0.74	1.46
1:C:315:ARG:NH1	3:C:1771:HOH:O[4_556]	0.82	1.38
1:A:235:ARG:CZ	3:B:1589:HOH:O[1_554]	0.84	1.36
1:B:322:ARG:NH1	3:A:1468:HOH:O[1_546]	0.88	1.32
1:A:235:ARG:CB	3:C:2021:HOH:O[1_554]	1.14	1.06
1:A:235:ARG:NH2	3:B:1589:HOH:O[1_554]	1.32	0.88
1:A:235:ARG:NH1	3:B:1589:HOH:O[1_554]	1.34	0.86
1:C:315:ARG:NE	3:C:1613:HOH:O[4_556]	1.36	0.84
1:C:315:ARG:CD	3:C:1613:HOH:O[4_556]	1.59	0.61
1:A:235:ARG:CD	3:C:1529:HOH:O[1_554]	1.60	0.60
1:A:235:ARG:NE	3:C:1529:HOH:O[1_554]	1.62	0.58
1:A:235:ARG:N	3:C:2021:HOH:O[1_554]	1.64	0.56
3:A:1790:HOH:O	3:A:1956:HOH:O[2_655]	1.71	0.49
3:C:1118:HOH:O	3:C:1754:HOH:O[4_546]	1.80	0.40
1:B:201:LEU:N	1:A:341:GLN:NE2[2_655]	1.81	0.39
1:C:322:ARG:NH1	3:C:1537:HOH:O[4_546]	1.81	0.39
1:B:201:LEU:O	1:A:341:GLN:OE1[2_655]	1.86	0.34
1:A:235:ARG:C	3:C:2021:HOH:O[1_554]	1.93	0.27
1:B:235:ARG:NH1	1:C:245:GLY:O[4_535]	1.96	0.24
1:A:235:ARG:NE	3:B:1589:HOH:O[1_554]	1.97	0.23
1:B:177:GLU:OE2	1:A:192:PRO:CG[2_655]	1.98	0.22
1:B:322:ARG:CZ	3:A:1468:HOH:O[1_546]	1.99	0.21
1:C:315:ARG:CZ	3:C:1613:HOH:O[4_556]	2.00	0.20
1:A:235:ARG:CG	3:C:1529:HOH:O[1_554]	2.02	0.18
3:B:1248:HOH:O	3:A:1154:HOH:O[2_655]	2.05	0.15
3:C:1588:HOH:O	3:C:1691:HOH:O[1_545]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:OD1	3:A:1031:HOH:O[2_655]	2.12	0.08
1:A:235:ARG:CG	3:C:2021:HOH:O[1_554]	2.12	0.08
1:C:315:ARG:CZ	3:C:1771:HOH:O[4_556]	2.12	0.08
3:B:1371:HOH:O	3:A:1175:HOH:O[2_655]	2.15	0.05
1:C:315:ARG:CA	3:C:1808:HOH:O[4_556]	2.17	0.03

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	329/351 (94%)	278 (84%)	37 (11%)	14 (4%)	2 0
1	B	329/351 (94%)	294 (89%)	28 (8%)	7 (2%)	7 3
1	C	329/351 (94%)	312 (95%)	13 (4%)	4 (1%)	13 8
All	All	987/1053 (94%)	884 (90%)	78 (8%)	25 (2%)	5 2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	A	61	ALA
1	C	22	ARG
1	C	202	SER
1	C	205	PRO
1	B	61	ALA
1	A	37	LEU
1	B	43	SER
1	B	284	GLY
1	A	31	PRO
1	A	205	PRO
1	A	242	THR
1	A	269	PRO
1	B	250	SER

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Mol	Chain	Res	Type
1	A	73	PRO
1	A	74	GLU
1	A	206	ARG
1	A	208	PRO
1	C	283	ALA
1	B	249	ALA
1	A	238	MET
1	B	285	GLY
1	A	258	ASN
1	A	291	VAL
1	A	22	ARG

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	256/282 (91%)	224 (88%)	32 (12%)	4 2
1	B	264/282 (94%)	230 (87%)	34 (13%)	4 2
1	C	262/282 (93%)	232 (88%)	30 (12%)	5 3
All	All	782/846 (92%)	686 (88%)	96 (12%)	4 2

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	40	LEU
1	B	47	ARG
1	B	52	ASP
1	B	68	ASP
1	B	75	GLN
1	B	81	LEU
1	B	85	LEU
1	B	92	LEU
1	B	95	GLN
1	B	97	THR

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	141	GLU
1	B	150	TYR
1	B	152	VAL
1	B	165	LEU
1	B	170	ASP
1	B	171	ASP
1	B	184	ARG
1	B	185	ARG
1	B	189	LEU
1	B	201	LEU
1	B	226	LEU
1	B	248	ARG
1	B	254	ARG
1	B	262	THR
1	B	263	PHE
1	B	290	LYS
1	B	296	ILE
1	B	297	ASP
1	B	318	ASP
1	B	322	ARG
1	B	344	ARG
1	B	347	ARG
1	A	35	LEU
1	A	40	LEU
1	A	46	ASN
1	A	49	ARG
1	A	52	ASP
1	A	56	LEU
1	A	81	LEU
1	A	85	LEU
1	A	124	LEU
1	A	125	ARG
1	A	126	GLN
1	A	136	GLN
1	A	142	ARG
1	A	150	TYR
1	A	152	VAL
1	A	153	SER
1	A	165	LEU
1	A	172	GLN
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	203	ARG
1	A	215	LYS
1	A	224	ILE
1	A	232	GLU
1	A	246	HIS
1	A	248	ARG
1	A	268	ASP
1	A	286	LEU
1	A	290	LYS
1	A	300	ASN
1	A	306	ILE
1	A	348	LEU
1	C	30	ARG
1	C	46	ASN
1	C	81	LEU
1	C	85	LEU
1	C	92	LEU
1	C	97	THR
1	C	100	VAL
1	C	103	SER
1	C	150	TYR
1	C	152	VAL
1	C	165	LEU
1	C	168	VAL
1	C	180	ARG
1	C	200	GLN
1	C	201	LEU
1	C	202	SER
1	C	204	VAL
1	C	205	PRO
1	C	210	LEU
1	C	231	ASP
1	C	248	ARG
1	C	256	GLU
1	C	258	ASN
1	C	277	LEU
1	C	286	LEU
1	C	295	LEU
1	C	298	VAL
1	C	321	LEU
1	C	330	ARG

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Mol	Chain	Res	Type
1	C	332	ARG

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

Mol	Chain	Res	Type
1	B	36	HIS
1	B	46	ASN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	102	GLN
1	B	117	ASN
1	B	136	GLN
1	B	200	GLN
1	B	280	GLN
1	B	300	ASN
1	B	337	GLN
1	A	36	HIS
1	A	46	ASN
1	A	69	HIS
1	A	154	GLN
1	A	172	GLN
1	A	200	GLN
1	A	258	ASN
1	A	280	GLN
1	A	294	HIS
1	A	300	ASN
1	A	341	GLN
1	C	46	ASN
1	C	51	GLN
1	C	69	HIS
1	C	95	GLN
1	C	102	GLN
1	C	117	ASN
1	C	126	GLN
1	C	200	GLN
1	C	246	HIS
1	C	258	ASN
1	C	300	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

1 ligand is modelled in this entry.

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$
2	TRP	C	3000	-	14,16,16	1.31	2 (14%)	13,22,22	0.82	0

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
2	TRP	C	3000	-	-	2/7/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	TRP	OXT-C	-2.94	1.21	1.30
2	C	3000	TRP	CH2-CZ3	2.06	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3000	TRP	OXT-C-CA-CB
2	C	3000	TRP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	TRP	4	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.