



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:44 PM GMT

PDB ID : 1YI8
Title : Crystal structure of tryptophanyl trRNA synthetase II from *Deinococcus radiodurans* 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

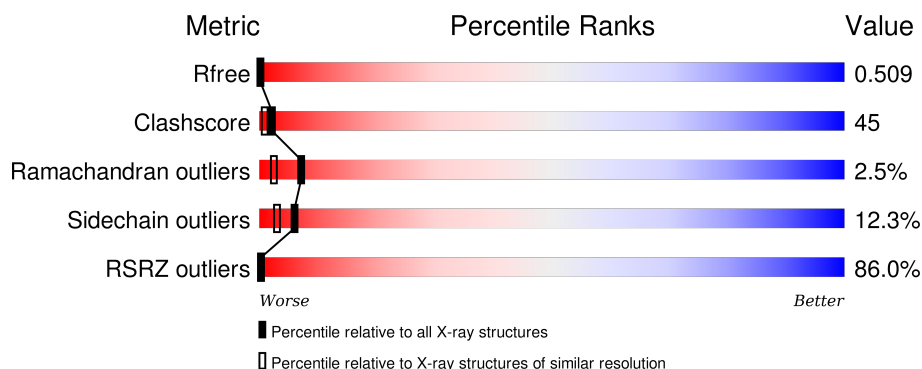
1 Overall quality at a glance ⓘ

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	351	<div> <div>86%</div> <div> <div>32%</div> <div>51%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	351	<div> <div>79%</div> <div> <div>45%</div> <div>41%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	351	<div> <div>79%</div> <div> <div>48%</div> <div>39%</div> <div>6%</div> <div>6%</div> </div> </div>

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
2	TRP	C	3000	-	-	-	X

2 Entry composition [i](#)

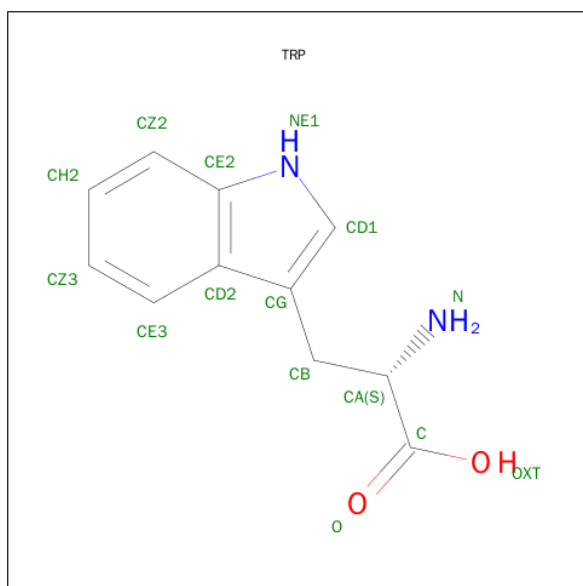
There are 3 unique types of molecules in this entry. The entry contains 8661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	N	O	S	2	0	0
			2544	1599	468	471	6			
1	A	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2532	1593	462	471	6			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



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

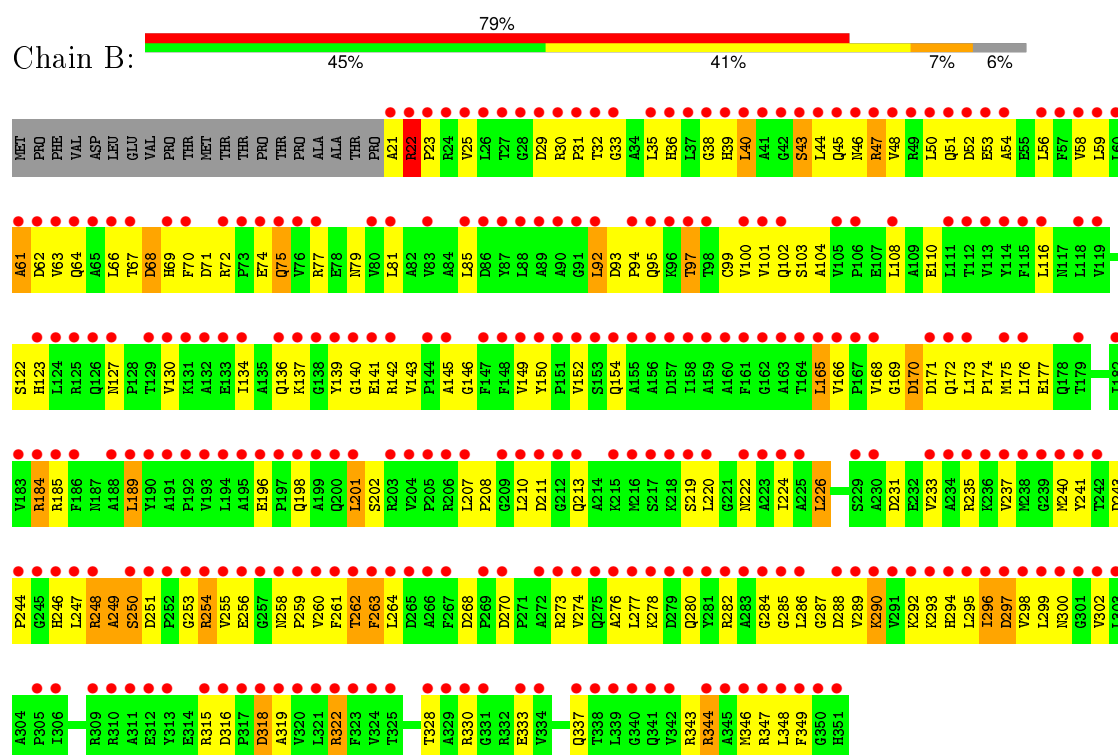
- Molecule 3 is water.

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

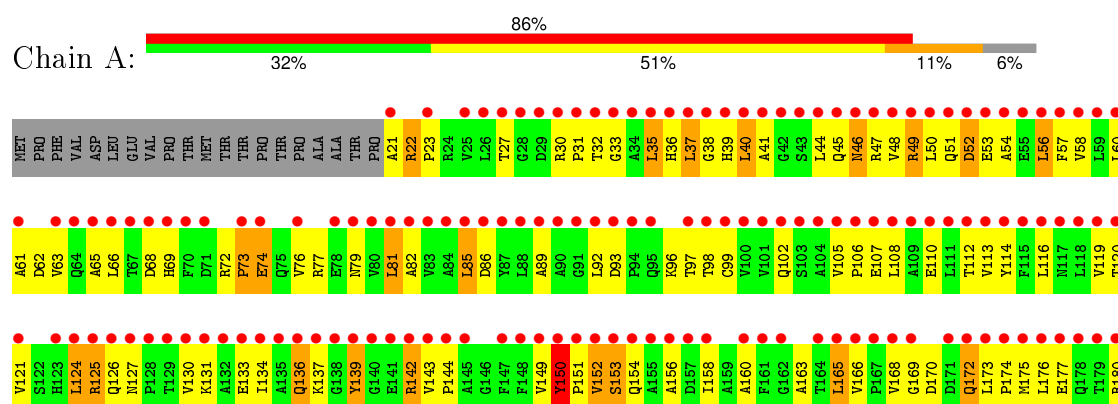
3 Residue-property plots

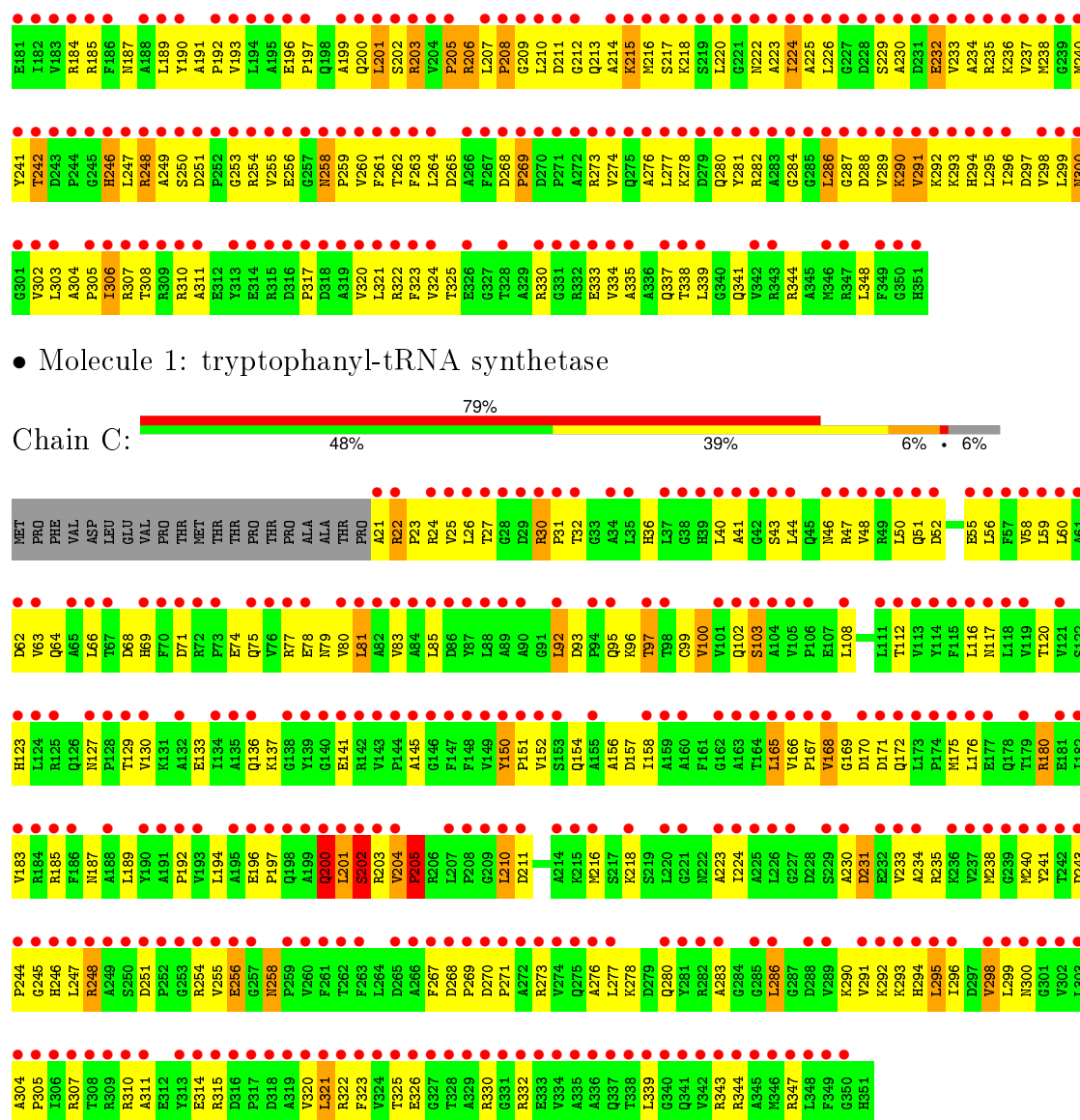
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: tryptophanyl-tRNA synthetase



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• Molecule 1: tryptophanyl-tRNA synthetase

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.280 0.495 , 0.509	Depositor DCC
R_{free} test set	5517 reflections (10.14%)	DCC
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 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54416 reflections	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	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(°)	Ideal(°)
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 ⓘ

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:H	1:A:226:LEU:HD12	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:C:180:ARG:HD3	1:C:197:PRO:O	1.80	0.82
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.60	0.82
1:A:207:LEU:CD1	1:A:208:PRO:HD2	2.10	0.81
1:B:43:SER:O	1:B:47:ARG:HD2	1.79	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:NH1	1:C:180:ARG:HG3	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:A:127:ASN:HB3	1:A:130:VAL:CG1	2.19	0.72
1:B:22:ARG:HH21	1:B:53:GLU:HG3	1.53	0.72
1:A:201:LEU:CD2	1:A:202:SER:H	2.02	0.72
1:C:40:LEU:HA	1:C:44:LEU:HD12	1.72	0.72
1:C:24:ARG:HD3	1:C:55:GLU:OE2	1.90	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:C:22:ARG:HB2	1:C:23:PRO:HD3	1.71	0.72
1:A:49:ARG:HD2	3:A:1677:HOH:O	1.90	0.72
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.20	0.71
1:B:240:MET:HE3	1:B:260:VAL:HG12	1.72	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:A:169:GLY:H	1:A:172:GLN:HG3	1.54	0.71
1:B:68:ASP:OD1	1:B:137:LYS:HE2	1.90	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:HA	1:C:290:LYS:HE2	1.73	0.70
1:A:173:LEU:N	1:A:174:PRO:HD2	2.05	0.70
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.57	0.70
1:B:240:MET:CE	1:B:260:VAL:HG12	2.22	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:A:112:THR:O	1:A:116:LEU:HG	1.93	0.69
1:B:262:THR:HG21	3:B:1431:HOH:O	1.93	0.69
1:A:216:MET:HG3	1:A:223:ALA:HA	1.73	0.69
1:B:146:GLY:HA3	1:C:117:ASN:ND2	2.08	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:A:63:VAL:CG1	1:A:102:GLN:HG2	2.25	0.66
1:B:127:ASN:HB3	1:B:130:VAL:CG1	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:C:254:ARG:CD	1:C:256:GLU:HG2	2.24	0.65
1:A:52:ASP:HB3	1:A:96:LYS:NZ	2.12	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:254:ARG:HD2	1:A:256:GLU:HB2	1.79	0.65
1:A:261:PHE:HA	3:A:1622:HOH:O	1.97	0.65
1:B:322:ARG:HH21	1:B:322:ARG:HG2	1.62	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: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: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: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:A:139:TYR:CD2	1:A:143:VAL:HG13	2.33	0.63
1:B:296:ILE:HG13	1:B:297:ASP:N	2.11	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: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:A:40:LEU:HA	1:A:44:LEU:HB3	1.79	0.63
1:C:294:HIS:O	1:C:298:VAL:HG12	1.99	0.63
1:A:259:PRO:O	1:A:263:PHE:HB2	1.98	0.62
1:A:30:ARG:HD2	1:A:65:ALA:HA	1.80	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:C:254:ARG:HD2	1:C:256:GLU:O	1.99	0.62
1:C:112:THR:HG22	1:C:156:ALA:CB	2.30	0.62
1:B:255:VAL:HG21	1:B:278:LYS:HG3	1.81	0.62
1:B:101:VAL:HG13	1:B:104:ALA:HB3	1.81	0.62
1:A:269:PRO:HD2	1:A:273:ARG:NH1	2.15	0.62
1:B:68:ASP:HB3	1:B:69:HIS:CD2	2.31	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:A:269:PRO:HA	3:A:1293:HOH:O	2.01	0.61
1:B:146:GLY:HA3	1:C:117:ASN:HD22	1.64	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:A:52:ASP:OD2	1:A:52:ASP:N	2.30	0.60
1:B:22:ARG:HB2	1:B:23:PRO:HD3	1.81	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:C:203:ARG:C	1:C:204:VAL:HG23	2.22	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: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:255:VAL:HG22	1:A:261:PHE:CD1	2.36	0.59
1:A:232:GLU:O	1:A:236:LYS:HB2	2.02	0.59
1:B:40:LEU:O	1:B:45:GLN:HG2	2.03	0.59
1:B:268:ASP:OD1	1:B:273:ARG:NH2	2.36	0.59
1:B:140:GLY:O	1:B:143:VAL:HG23	2.02	0.59
1:A:294:HIS:HA	1:A:297:ASP:OD2	2.03	0.59
1:A:176:LEU:HD13	1:A:176:LEU:O	2.02	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: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:64:GLN:H	1:B:102:GLN:HE22	1.51	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:310:ARG:O	1:C:314:GLU:HG2	2.03	0.59
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.17	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:210:LEU:HD12	1:C:240:MET:HG2	1.84	0.58
1:C:79:ASN:O	1:C:83:VAL:HG22	2.02	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:CG	2:C:3000:TRP:OXT	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:293:LYS:HG2	3:C:1361:HOH:O	2.04	0.57
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.86	0.57
1:A:226:LEU:HD12	1:A:226:LEU:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:23:PRO:HD2	1:B:54:ALA:HB2	1.85	0.57
1:A:22:ARG:N	1:A:23:PRO:CD	2.67	0.57
1:B:184:ARG:NH2	1:B:184:ARG:HG2	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:C:171:ASP:HB2	1:C:172:GLN:HE22	1.69	0.57
1:A:98:THR:CG2	1:A:330:ARG:HD2	2.34	0.57
1:A:136:GLN:HG3	1:A:136:GLN:O	2.03	0.57
1:A:56:LEU:HD22	1:A:57:PHE:N	2.20	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:231:ASP:O	1:B:235:ARG:HG3	2.05	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:C:40:LEU:HA	1:C:44:LEU:HB2	1.87	0.56
1:A:296:ILE:HG13	1:A:297:ASP:N	2.20	0.56
1:A:98:THR:OG1	1:A:330:ARG:HD2	2.05	0.56
1:B:177:GLU:HG3	3:B:1946:HOH:O	2.05	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:C:56:LEU:HD13	1:C:56:LEU:C	2.26	0.56
1:B:36:HIS:CD2	1:B:38:GLY:H	2.19	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:C:180:ARG:HD2	1:C:196:GLU:HG3	1.87	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: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:A:240:MET:CE	1:A:259:PRO:HB2	2.36	0.56
1:B:75:GLN:O	1:B:79:ASN:ND2	2.38	0.56
1:B:44:LEU:HA	1:B:47:ARG:CD	2.35	0.56
1:C:216:MET:HE2	1:C:223:ALA:HB1	1.87	0.55
1:C:166:VAL:HG21	1:C:176:LEU:CD2	2.37	0.55
1:B:189:LEU:HD21	1:C:71:ASP:HA	1.87	0.55
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.07	0.55
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG21	3:C:1173:HOH:O	2.05	0.55
1:A:149:VAL:O	1:A:149:VAL:HG12	2.07	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:112:THR:HG22	1:A:156:ALA:CB	2.36	0.55
1:B:248:ARG:H	1:B:248:ARG:HD3	1.71	0.55
1:C:256:GLU:CD	1:C:256:GLU:H	2.08	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:A:37:LEU:HG	1:A:224:ILE:HG12	1.88	0.55
1:B:349:PHE:CE2	1:C:81:LEU:HD13	2.42	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:A:58:VAL:O	1:A:58:VAL:HG13	2.05	0.55
1:C:40:LEU:HD12	1:C:44:LEU:HB2	1.87	0.55
1:C:183:VAL:HG13	1:C:194:LEU:HB2	1.89	0.55
1:C:62:ASP:OD2	1:C:103:SER:OG	2.24	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: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:B:134:ILE:HD13	1:B:143:VAL:HG21	1.88	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:175:MET:HB2	3:C:1018:HOH:O	2.07	0.54
1:C:78:GLU:HA	1:C:78:GLU:OE2	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: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:C:51:GLN:NE2	1:C:93:ASP:H	1.89	0.54
1:A:220:LEU:C	1:A:222:ASN:N	2.60	0.54
1:A:193:VAL:HG22	1:A:193:VAL:O	2.08	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:C:295:LEU:O	1:C:298:VAL:HG13	2.07	0.54
1:C:187:ASN:CB	1:C:192:PRO:HA	2.37	0.54
1:A:107:GLU:HB3	1:A:339:LEU:HG	1.90	0.54
1:B:168:VAL:HG22	1:B:169:GLY:O	2.07	0.54
1:C:172:GLN:HG2	3:C:1945:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG23	1:B:58:VAL: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:66:LEU:C	1:B:68:ASP:H	2.10	0.53
1:B:22:ARG:NH2	1:B:53:GLU:HG3	2.22	0.53
1:C:40:LEU:CA	1:C:44:LEU:HD12	2.37	0.53
1:A:248:ARG:N	1:A:248:ARG:HD3	2.23	0.53
1:A:249:ALA:HB2	1:A:287:GLY:HA3	1.90	0.53
1:B:344:ARG:HH11	1:B:344:ARG:CG	2.21	0.53
1:B:259:PRO:HA	1:B:262:THR:HG23	1.89	0.53
1:C:243:ASP:OD2	1:C:246:HIS:HB2	2.08	0.53
1:A:242:THR:HB	1:A:258:ASN:HD21	1.73	0.53
1:C:180:ARG:HE	1:C:196:GLU:CD	2.12	0.53
1:A:255:VAL:HG13	1:A:261:PHE:CD1	2.44	0.53
1:B:23:PRO:O	1:B:54:ALA:HB1	2.09	0.53
1:B:255:VAL:HG13	1:B:261:PHE:CD2	2.43	0.53
1:B:74:GLU:OE1	1:C:347:ARG:NH1	2.42	0.53
1:C:120:THR:HG22	1:C:123:HIS:HB2	1.90	0.53
1:B:211:ASP:HB3	1:B:213:GLN:HG3	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:C:180:ARG:CG	1:C:180:ARG:NH1	2.68	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: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:202:SER:HB3	3:B:1285:HOH:O	2.09	0.52
1:A:207:LEU:HG	1:A:208:PRO:HD2	1.91	0.52
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.25	0.52
1:A:180:ARG:HB3	1:A:184:ARG:HH11	1.75	0.52
1:B:102:GLN:HG3	1:B:108:LEU:HD12	1.92	0.52
1:A:250:SER:O	1:A:284:GLY:HA2	2.09	0.52
1:A:288:ASP:O	1:A:291:VAL:HG12	2.09	0.52
1:B:32:THR:O	1:B:75:GLN:NE2	2.43	0.52
1:A:261:PHE:CD1	1:A:278:LYS:HG2	2.44	0.52
1:A:116:LEU:HD23	1:A:152:VAL:HG21	1.91	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:A:255:VAL:HG11	1:A:278:LYS:HE2	1.92	0.51
1:B:189:LEU:CD2	1:C:71:ASP:HA	2.40	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:A:260:VAL:HG13	1:A:295:LEU:CD2	2.40	0.51
1:B:292:LYS:O	1:B:296:ILE:CG2	2.58	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:295:LEU:CD2	1:C:299:LEU:HG	2.40	0.51
1:C:165:LEU:HD22	1:C:200:GLN:HB2	1.93	0.51
1:A:41:ALA:HB2	1:A:207:LEU:HD22	1.92	0.51
1:A:208:PRO:HG2	1:A:263:PHE:HE2	1.74	0.51
1:A:66:LEU:HD21	1:A:76:VAL:HG11	1.92	0.51
1:B:248:ARG:NE	1:B:251:ASP:OD2	2.44	0.51
1:C:77:ARG:O	1:C:80:VAL:CG1	2.51	0.51
1:C:41:ALA:HB2	1:C:267:PHE:CZ	2.46	0.51
1:B:333:GLU:HG3	1:B:337:GLN:HE21	1.74	0.51
1:C:322:ARG:HD3	3:C:1047:HOH:O	2.10	0.51
1:A:215:LYS:O	1:A:222:ASN:ND2	2.44	0.50
1:B:333:GLU:OE2	1:B:333:GLU:HA	2.11	0.50
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.36	0.50
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.21	0.50
1:C:120:THR:HG23	1:C:123:HIS:N	2.07	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:A:193:VAL:HG21	1:A:341:GLN:CB	2.36	0.50
1:C:210:LEU:HD12	1:C:240:MET:CG	2.42	0.50
1:A:290:LYS:HE2	1:A:290:LYS:HA	1.93	0.50
1:A:74:GLU:HG2	3:A:1380:HOH:O	2.11	0.50
1:B:273:ARG:NH2	1:B:294:HIS:NE2	2.59	0.50
1:A:276:ALA:O	1:A:280:GLN:HG3	2.12	0.50
1:A:150:TYR:O	1:A:154:GLN:HG3	2.11	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:CG	1:B:184:ARG:HH21	2.20	0.50
1:A:205:PRO:O	1:A:206:ARG:C	2.50	0.50
1:A:110:GLU:O	1:A:113:VAL:CG1	2.58	0.50
1:A:260:VAL:HG13	1:A:295:LEU:HD22	1.92	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:B:316:ASP:OD2	1:B:319:ALA:HB2	2.11	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:C:133:GLU:O	1:C:137:LYS:HD3	2.12	0.49
1:A:290:LYS:CA	1:A:290:LYS:HE2	2.43	0.49
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.77	0.49
1:B:145:ALA:HB3	1:C:116:LEU:O	2.13	0.49
1:A:237:VAL:O	1:A:240:MET:HB2	2.11	0.49
1:B:349:PHE:CD2	1:C:80:VAL:CG1	2.95	0.49
1:B:315:ARG:O	1:B:315:ARG:HG2	2.12	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:B:25:VAL:HG22	1:B:165:LEU:HB3	1.94	0.49
1:A:218:LYS:NZ	1:A:225:ALA:HB2	2.28	0.49
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.94	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:43:SER:O	1:B:46:ASN:N	2.46	0.49
1:C:254:ARG:CD	1:C:256:GLU:O	2.61	0.49
1:B:23:PRO:HD2	1:B:54:ALA:CB	2.41	0.49
1:C:60:LEU:HD22	1:C:83:VAL:HG21	1.95	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:292:LYS:O	1:A:295:LEU:N	2.47	0.48
1:A:211:ASP:O	1:A:213:GLN:N	2.42	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:29:ASP:O	1:B:31:PRO:HD3	2.14	0.48
1:B:237:VAL:CG1	1:B:240:MET:HE2	2.43	0.48
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.94	0.48
1:A:125:ARG:HH21	1:A:125:ARG:HG3	1.78	0.48
1:B:211:ASP:OD1	1:B:213:GLN:NE2	2.47	0.48
1:A:112:THR:HG22	1:A:153:SER:HA	1.95	0.48
1:A:98:THR:OG1	1:A:330:ARG:NH1	2.43	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:C	1:A:175:MET:SD	2.92	0.48
1:C:292:LYS:O	1:C:296:ILE:HG13	2.14	0.48
1:A:253:GLY:HA3	1:A:281:TYR:CE2	2.49	0.47
1:B:68:ASP:OD1	1:B:137:LYS:CE	2.62	0.47
1:B:255:VAL:HG22	1:B:261:PHE:CE2	2.48	0.47
1:B:101:VAL:O	1:B:101:VAL:HG13	2.14	0.47
1:A:212:GLY:O	1:A:213:GLN:C	2.53	0.47
1:B:127:ASN:CG	1:B:130:VAL:HG12	2.34	0.47
1:A:45:GLN:O	1:A:48:VAL:HB	2.14	0.47
1:B:315:ARG:HG3	3:B:1367:HOH:O	2.13	0.47
1:C:344:ARG:HD3	3:C:1217:HOH:O	2.15	0.47
1:C:276:ALA:O	1:C:280:GLN:HG3	2.13	0.47
1:C:63:VAL:H	1:C:102:GLN:HE21	1.61	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: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:A:32:THR:HG23	1:A:69:HIS:HE1	1.79	0.47
1:C:201:LEU:HD23	1:C:202:SER:N	2.27	0.47
1:C:36:HIS:CE1	1:C:216:MET:HG2	2.50	0.47
1:B:92:LEU:HA	1:B:92:LEU:HD12	1.78	0.47
1:A:130:VAL:HG13	1:A:131:LYS:N	2.28	0.47
1:B:66:LEU:C	1:B:68:ASP:N	2.68	0.47
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.78	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:A:36:HIS:HD2	1:A:38:GLY:H	1.61	0.47
1:B:149:VAL:O	1:B:149:VAL:CG1	2.63	0.47
1:A:288:ASP:CA	1:A:291:VAL:HG12	2.42	0.47
1:A:241:TYR:O	1:A:259:PRO:CD	2.60	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: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:B:71:ASP:OD1	1:B:72:ARG:CD	2.63	0.47
1:A:98:THR:HG23	1:A:330:ARG:HD2	1.96	0.46
1:A:234:ALA:HA	1:A:296:ILE:HG22	1.95	0.46
1:B:241:TYR:O	1:B:259:PRO:HG2	2.14	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: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:A:56:LEU:HD13	1:A:97:THR:HG23	1.98	0.46
1:B:274:VAL:C	1:B:276:ALA:N	2.69	0.46
1:C:258:ASN:HD22	1:C:258:ASN:C	2.18	0.46
1:A:32:THR:HG22	1:A:32:THR:O	2.15	0.46
1:C:310:ARG:O	1:C:314:GLU:HG3	2.15	0.46
1:A:99:CYS:HB2	1:A:323:PHE:CZ	2.50	0.46
1:A:33:GLY:HA2	1:A:79:ASN:ND2	2.31	0.46
1:A:242:THR:HB	1:A:258:ASN:ND2	2.30	0.46
1:A:277:LEU:HD13	1:A:280:GLN:NE2	2.31	0.46
1:A:32:THR:HG23	1:A:69:HIS:CE1	2.51	0.46
1:B:22:ARG:CD	1:B:23:PRO:HD3	2.46	0.46
1:A:36:HIS:O	1:A:38:GLY:N	2.49	0.46
1:A:255:VAL:HG21	1:A:278:LYS:HD3	1.98	0.46
1:A:290:LYS:N	1:A:290:LYS:HE2	2.30	0.46
1:A:46:ASN:ND2	1:A:50:LEU:HG	2.30	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:333:GLU:O	1:B:337:GLN:HG3	2.16	0.46
1:B:263:PHE:CB	1:B:295:LEU:HD11	2.46	0.46
1:C:311:ALA:CA	1:C:314:GLU:HG3	2.43	0.46
1:B:344:ARG:NH1	1:B:344:ARG:HG3	2.30	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:C:187:ASN:CG	1:C:192:PRO:HA	2.36	0.45
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: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: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: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:255:VAL:HG13	1:A:261:PHE:HB3	1.99	0.45
1:B:51:GLN:NE2	1:B:97:THR:CG2	2.71	0.45
1:C:210:LEU:HD21	1:C:224:ILE:HG13	1.97	0.45
1:C:30:ARG:HD2	1:C:64:GLN:HE21	1.81	0.45
1:B:184:ARG:CG	1:B:184:ARG:NH2	2.76	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:A:303:LEU:HB3	1:A:307:ARG:NH2	2.31	0.45
1:B:264:LEU:O	1:B:268:ASP:HB3	2.17	0.45
1:B:278:LYS:HB2	1:B:278:LYS:HE3	1.76	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:187:ASN:OD1	1:A:192:PRO:HA	2.16	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:B:219:SER:HA	3:B:1401:HOH:O	2.16	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:A:249:ALA:CB	1:A:287:GLY:HA3	2.47	0.45
1:A:211:ASP:C	1:A:213:GLN:N	2.70	0.45
1:B:74:GLU:OE2	1:C:347:ARG:NH1	2.50	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:C:51:GLN:NE2	1:C:97:THR:CG2	2.79	0.44
1:B:169:GLY:O	1:B:170:ASP:C	2.55	0.44
1:B:74:GLU:CD	1:C:347:ARG:NH1	2.70	0.44
1:C:271:PRO:HG2	3:C:1373:HOH:O	2.17	0.44
1:B:175:MET:C	1:B:175:MET:SD	2.95	0.44
1:A:130:VAL:CG1	1:A:131:LYS:N	2.79	0.44
1:B:122:SER:HG	1:C:141:GLU:HB3	1.83	0.44
1:A:105:VAL:HA	1:A:106:PRO:HD2	1.80	0.44
1:A:68:ASP:OD2	1:A:137:LYS:NZ	2.45	0.44
1:A:293:LYS:HD2	1:A:296:ILE:HD11	1.99	0.44
1:B:140:GLY:O	1:B:143:VAL:CG2	2.66	0.44
1:C:185:ARG:O	1:C:189:LEU:HB2	2.16	0.44
1:B:165:LEU:HD23	1:B:198:GLN:O	2.18	0.44
1:C:36:HIS:CG	1:C:216:MET:HE2	2.52	0.44
1:A:136:GLN:CG	1:A:136:GLN:O	2.66	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:201:LEU:HD22	1:C:202:SER:HB3	2.00	0.44
1:C:62:ASP:OD2	1:C:103:SER:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:149:VAL:O	1:A:152:VAL:HG13	2.17	0.44
1:A:119:VAL:HG22	1:A:120:THR:N	2.32	0.44
1:A:76:VAL:CG1	1:A:77:ARG:N	2.81	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:B:123:HIS:HE1	3:B:1334:HOH:O	2.01	0.43
1:C:154:GLN:O	1:C:158:ILE:HG12	2.18	0.43
1:C:154:GLN:NE2	2:C:3000:TRP:CD2	2.86	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: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:A:237:VAL:HA	1:A:240:MET:HG3	2.00	0.43
1:B:346:MET:CE	1:B:348:LEU:HD11	2.49	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:C:203:ARG:C	1:C:204:VAL:O	2.57	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:204:VAL:HG12	1:C:205:PRO:CD	2.36	0.43
1:A:293:LYS:O	1:A:296:ILE:CG1	2.66	0.43
1:A:250:SER:O	1:A:284:GLY:CA	2.66	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:334:VAL:HA	1:A:337:GLN:HG3	2.01	0.42
1:A:254:ARG:CD	1:A:256:GLU:HB2	2.47	0.42
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.87	0.42
1:A:173:LEU:HD13	3:A:2045:HOH:O	2.18	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:208:PRO:HG3	1:A:262:THR:CG2	2.48	0.42
1:B:58:VAL:HG23	1:B:99:CYS:HA	2.00	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:C:52:ASP:OD2	1:C:96:LYS:NZ	2.49	0.42
1:A:62:ASP:H	1:A:102:GLN:HB3	1.84	0.42
1:A:105:VAL:O	1:A:105:VAL:HG13	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:A:241:TYR:CD1	1:A:241:TYR:O	2.73	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: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:B:30:ARG:HH22	1:B:68:ASP:CB	2.33	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:C:231:ASP:OD1	1:C:235:ARG:CZ	2.68	0.42
1:B:346:MET:HE3	1:B:348:LEU:HD11	2.02	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:211:ASP:CB	1:B:213:GLN:HG3	2.50	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: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: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:A:216:MET:CG	1:A:223:ALA:HA	2.47	0.41
1:A:22:ARG:N	1:A:23:PRO:HD2	2.34	0.41
1:C:248:ARG:O	1:C:251:ASP:HB2	2.20	0.41
1:A:305:PRO:HG2	1:A:306:ILE:N	2.31	0.41
1:B:273:ARG:O	1:B:277:LEU:HD22	2.20	0.41
1:C:64:GLN:H	1:C:102:GLN:NE2	2.15	0.41
1:B:278:LYS:HG2	1:B:282:ARG:NH2	2.34	0.41
1:A:203:ARG:HD2	3:A:1508:HOH:O	2.20	0.41
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.51	0.41
1:B:344:ARG:NH1	1:B:344:ARG:CG	2.80	0.41
1:C:32:THR:O	1:C:32:THR:HG22	2.19	0.41
1:A:273:ARG:HD3	3:A:1187:HOH:O	2.20	0.41
1:B:142:ARG:HA	1:C:120:THR:OG1	2.20	0.41
1:A:110:GLU:HG2	1:A:114:TYR:CE1	2.54	0.41
1:C:129:THR:O	1:C:133:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:O	1:A:51:GLN:N	2.51	0.41
1:C:170:ASP:N	1:C:170:ASP:OD1	2.53	0.41
1:B:244:PRO:C	1:B:246:HIS:H	2.24	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:C:255:VAL:O	1:C:258:ASN:HB3	2.20	0.41
1:A:201:LEU:HD22	1:A:202:SER:N	2.35	0.41
1:A:72:ARG:N	1:A:73:PRO:CD	2.83	0.41
1:C:293:LYS:HA	1:C:293:LYS:HD2	1.93	0.41
1:C:25:VAL:HG11	1:C:50:LEU:HD13	2.02	0.41
1:A:51:GLN:OE1	1:A:93:ASP:N	2.43	0.41
1:A:32:THR:CG2	1:A:69:HIS:HE1	2.33	0.41
1:A:125:ARG:NH2	1:A:125:ARG:HG3	2.35	0.41
1:A:89:ALA:O	1:A:306:ILE:HB	2.20	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: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: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:137:LYS:HE3	3:B:1218:HOH:O	2.19	0.41
1:A:36:HIS:O	1:A:39:HIS:N	2.51	0.41
1:B:210:LEU:HD21	1:B:224:ILE:HG13	2.03	0.41
1:B:184:ARG:HE	1:B:196:GLU:CD	2.23	0.40
1:B:67:THR:HG22	1:C:117:ASN:HD21	1.85	0.40
1:B:295:LEU:C	1:B:298:VAL:HG12	2.39	0.40
1:B:61:ALA:HB1	1:B:64:GLN:HB3	2.04	0.40
1:A:36:HIS:CE1	1:A:39:HIS:NE2	2.89	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:B:93:ASP:O	1:B:97:THR:CG2	2.69	0.40
1:C:270:ASP:OD2	1:C:273:ARG:NH1	2.54	0.40
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.57	0.40
1:B:33:GLY:HA2	1:B:79:ASN:OD1	2.21	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:B:260:VAL:HG23	1:B:261:PHE:N	2.37	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: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: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:C:58:VAL:HG23	1:C:58:VAL:O	2.21	0.40
1:B:322:ARG:HG2	1:B:322:ARG:NH2	2.32	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

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:A:235:ARG:CG	3:C:2021:HOH:O[1_554]	2.12	0.08
1:B:170:ASP:OD1	3:A:1031:HOH:O[2_655]	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%)	3	1
1	B	329/351 (94%)	294 (89%)	28 (8%)	7 (2%)	9	3
1	C	329/351 (94%)	312 (95%)	13 (4%)	4 (1%)	16	10
All	All	987/1053 (94%)	884 (90%)	78 (8%)	25 (2%)	7	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 ⓘ

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%)	6	3
1	B	264/282 (94%)	230 (87%)	34 (13%)	5	2
1	C	262/282 (93%)	232 (88%)	30 (12%)	7	3
All	All	782/846 (92%)	686 (88%)	96 (12%)	6	3

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	12,16,16	1.09	0	7,22,22	0.88	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	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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, 95th 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	331/351 (94%)	5.67	301 (90%)  	37, 72, 96, 99	0
1	B	331/351 (94%)	3.87	276 (83%)  	24, 46, 82, 88	1 (0%)
1	C	331/351 (94%)	3.64	277 (83%)  	16, 31, 56, 65	0
All	All	993/1053 (94%)	4.39	854 (86%)  	16, 46, 91, 99	1 (0%)

All (854) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	GLY	29.1
1	A	219	SER	26.9
1	A	205	PRO	21.7
1	A	252	PRO	21.2
1	A	249	ALA	19.6
1	A	130	VAL	19.3
1	A	267	PHE	18.1
1	B	266	ALA	16.9
1	A	281	TYR	16.3
1	A	286	LEU	16.3
1	A	220	LEU	15.8
1	A	204	VAL	15.2
1	A	269	PRO	14.8
1	A	289	VAL	14.7
1	A	245	GLY	14.7
1	A	272	ALA	14.1
1	A	307	ARG	13.9
1	A	135	ALA	13.9
1	A	44	LEU	13.3
1	A	225	ALA	13.2
1	A	247	LEU	13.2
1	C	321	LEU	13.0
1	B	277	LEU	13.0

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Mol	Chain	Res	Type	RSRZ
1	C	244	PRO	12.7
1	B	257	GLY	12.7
1	A	275	GLN	12.6
1	A	313	TYR	12.2
1	A	71	ASP	12.1
1	A	50	LEU	12.1
1	A	296	ILE	12.0
1	C	273	ARG	11.9
1	B	338	THR	11.6
1	A	274	VAL	11.6
1	A	311	ALA	11.6
1	A	131	LYS	11.5
1	A	264	LEU	11.4
1	C	253	GLY	11.4
1	A	287	GLY	11.2
1	A	273	ARG	11.2
1	A	276	ALA	11.2
1	A	199	ALA	11.1
1	C	34	ALA	11.1
1	B	76	VAL	11.0
1	B	204	VAL	11.0
1	B	279	ASP	11.0
1	B	281	TYR	10.9
1	A	263	PHE	10.8
1	A	69	HIS	10.8
1	B	32	THR	10.8
1	B	320	VAL	10.7
1	A	85	LEU	10.7
1	C	271	PRO	10.3
1	A	63	VAL	10.3
1	A	94	PRO	10.2
1	A	254	ARG	10.2
1	A	161	PHE	10.2
1	A	280	GLN	10.1
1	B	233	VAL	10.1
1	A	97	THR	9.7
1	B	224	ILE	9.7
1	A	285	GLY	9.7
1	C	139	TYR	9.6
1	A	48	VAL	9.6
1	A	40	LEU	9.5
1	A	126	GLN	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	211	ASP	9.4
1	A	261	PHE	9.3
1	C	160	ALA	9.2
1	A	210	LEU	9.2
1	A	221	GLY	9.2
1	C	324	VAL	9.2
1	A	324	VAL	9.1
1	A	218	LYS	9.0
1	A	260	VAL	9.0
1	A	239	GLY	9.0
1	C	88	LEU	9.0
1	A	268	ASP	9.0
1	B	267	PHE	8.9
1	A	128	PRO	8.9
1	A	255	VAL	8.8
1	C	299	LEU	8.8
1	A	262	THR	8.7
1	A	92	LEU	8.7
1	C	202	SER	8.5
1	B	293	LYS	8.5
1	B	66	LEU	8.5
1	A	175	MET	8.5
1	A	233	VAL	8.4
1	A	299	LEU	8.4
1	B	89	ALA	8.4
1	A	73	PRO	8.4
1	A	277	LEU	8.4
1	C	277	LEU	8.4
1	A	215	LYS	8.3
1	A	208	PRO	8.3
1	A	243	ASP	8.3
1	C	159	ALA	8.3
1	A	271	PRO	8.2
1	B	261	PHE	8.2
1	A	227	GLY	8.2
1	B	241	TYR	8.1
1	A	155	ALA	8.1
1	A	256	GLU	8.1
1	A	238	MET	8.0
1	C	336	ALA	8.0
1	C	320	VAL	7.9
1	C	303	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	7.9
1	B	97	THR	7.8
1	B	150	TYR	7.8
1	C	293	LYS	7.8
1	B	134	ILE	7.7
1	C	239	GLY	7.7
1	B	203	ARG	7.7
1	B	42	GLY	7.7
1	A	54	ALA	7.7
1	A	207	LEU	7.6
1	B	152	VAL	7.6
1	A	165	LEU	7.5
1	C	165	LEU	7.5
1	A	80	VAL	7.5
1	A	226	LEU	7.4
1	C	306	ILE	7.3
1	C	245	GLY	7.3
1	C	286	LEU	7.3
1	A	37	LEU	7.3
1	A	266	ALA	7.2
1	A	93	ASP	7.2
1	B	315	ARG	7.2
1	C	315	ARG	7.2
1	C	186	PHE	7.2
1	B	247	LEU	7.1
1	B	248	ARG	7.1
1	B	296	ILE	7.0
1	A	194	LEU	7.0
1	A	26	LEU	6.9
1	B	162	GLY	6.9
1	A	284	GLY	6.9
1	A	89	ALA	6.9
1	B	73	PRO	6.9
1	B	105	VAL	6.9
1	C	50	LEU	6.9
1	C	94	PRO	6.9
1	A	36	HIS	6.8
1	B	141	GLU	6.8
1	A	195	ALA	6.8
1	A	123	HIS	6.8
1	A	242	THR	6.6
1	B	264	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	115	PHE	6.6
1	A	134	ILE	6.6
1	A	43	SER	6.5
1	A	224	ILE	6.5
1	C	323	PHE	6.5
1	B	342	VAL	6.5
1	B	40	LEU	6.5
1	A	310	ARG	6.5
1	A	320	VAL	6.5
1	B	322	ARG	6.4
1	A	139	TYR	6.4
1	C	255	VAL	6.4
1	C	282	ARG	6.4
1	B	189	LEU	6.4
1	A	116	LEU	6.4
1	B	300	ASN	6.4
1	B	173	LEU	6.4
1	C	281	TYR	6.4
1	A	248	ARG	6.4
1	A	303	LEU	6.4
1	A	107	GLU	6.3
1	B	158	ILE	6.3
1	B	118	LEU	6.3
1	B	289	VAL	6.3
1	C	274	VAL	6.3
1	A	99	CYS	6.3
1	A	294	HIS	6.3
1	A	119	VAL	6.2
1	A	232	GLU	6.2
1	A	35	LEU	6.2
1	A	88	LEU	6.1
1	A	34	ALA	6.1
1	C	280	GLN	6.1
1	C	57	PHE	6.1
1	C	147	PHE	6.1
1	A	228	ASP	6.1
1	A	244	PRO	6.0
1	A	237	VAL	6.0
1	B	272	ALA	6.0
1	A	171	ASP	6.0
1	A	121	VAL	6.0
1	B	218	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	259	PRO	6.0
1	C	272	ALA	6.0
1	A	246	HIS	5.9
1	C	308	THR	5.9
1	B	37	LEU	5.9
1	C	108	LEU	5.9
1	B	262	THR	5.9
1	A	182	ILE	5.8
1	B	98	THR	5.8
1	B	212	GLY	5.8
1	B	44	LEU	5.8
1	A	231	ASP	5.8
1	A	283	ALA	5.8
1	C	95	GLN	5.8
1	B	306	ILE	5.8
1	C	238	MET	5.8
1	A	234	ALA	5.7
1	C	199	ALA	5.7
1	A	222	ASN	5.7
1	B	278	LYS	5.6
1	A	67	THR	5.6
1	A	41	ALA	5.6
1	A	302	VAL	5.6
1	B	291	VAL	5.6
1	B	301	GLY	5.6
1	C	203	ARG	5.5
1	A	68	ASP	5.5
1	A	153	SER	5.5
1	C	211	ASP	5.4
1	A	278	LYS	5.4
1	A	158	ILE	5.4
1	B	263	PHE	5.4
1	A	60	LEU	5.4
1	A	95	GLN	5.4
1	C	234	ALA	5.4
1	B	285	GLY	5.4
1	A	168	VAL	5.4
1	C	105	VAL	5.4
1	B	256	GLU	5.4
1	A	136	GLN	5.4
1	A	156	ALA	5.4
1	A	108	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	344	ARG	5.4
1	B	275	GLN	5.4
1	C	71	ASP	5.3
1	B	276	ALA	5.3
1	B	182	ILE	5.3
1	B	295	LEU	5.3
1	B	54	ALA	5.3
1	A	39	HIS	5.3
1	B	274	VAL	5.3
1	A	57	PHE	5.3
1	B	83	VAL	5.3
1	C	140	GLY	5.3
1	B	321	LEU	5.2
1	C	58	VAL	5.2
1	C	28	GLY	5.2
1	B	132	ALA	5.2
1	A	315	ARG	5.2
1	B	238	MET	5.2
1	A	250	SER	5.2
1	C	229	SER	5.2
1	A	223	ALA	5.2
1	A	251	ASP	5.2
1	A	193	VAL	5.1
1	B	56	LEU	5.1
1	B	124	LEU	5.1
1	B	136	GLN	5.1
1	A	347	ARG	5.1
1	C	267	PHE	5.1
1	B	25	VAL	5.1
1	B	175	MET	5.1
1	C	346	MET	5.1
1	C	51	GLN	5.1
1	A	53	GLU	5.1
1	C	197	PRO	5.1
1	A	104	ALA	5.0
1	A	306	ILE	5.0
1	A	333	GLU	5.0
1	A	143	VAL	5.0
1	A	59	LEU	5.0
1	A	66	LEU	5.0
1	A	117	ASN	5.0
1	A	295	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	294	HIS	5.0
1	B	298	VAL	5.0
1	C	285	GLY	5.0
1	A	82	ALA	5.0
1	C	175	MET	5.0
1	B	280	GLN	5.0
1	B	341	GLN	5.0
1	C	177	GLU	5.0
1	B	115	PHE	5.0
1	A	185	ARG	4.9
1	A	91	GLY	4.9
1	A	235	ARG	4.9
1	B	270	ASP	4.9
1	B	95	GLN	4.9
1	C	349	PHE	4.9
1	B	75	GLN	4.9
1	B	313	TYR	4.9
1	A	293	LYS	4.8
1	A	58	VAL	4.8
1	B	92	LEU	4.8
1	B	209	GLY	4.8
1	A	25	VAL	4.8
1	C	270	ASP	4.8
1	B	286	LEU	4.8
1	C	252	PRO	4.8
1	A	164	THR	4.8
1	B	50	LEU	4.8
1	C	313	TYR	4.8
1	C	77	ARG	4.7
1	B	210	LEU	4.7
1	C	302	VAL	4.7
1	B	334	VAL	4.7
1	A	298	VAL	4.7
1	B	87	TYR	4.7
1	B	323	PHE	4.7
1	C	166	VAL	4.7
1	A	98	THR	4.7
1	B	309	ARG	4.7
1	A	142	ARG	4.7
1	C	125	ARG	4.7
1	A	229	SER	4.6
1	C	117	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	4.6
1	B	168	VAL	4.6
1	A	55	GLU	4.6
1	B	254	ARG	4.6
1	B	223	ALA	4.6
1	C	307	ARG	4.6
1	C	46	ASN	4.6
1	A	339	LEU	4.6
1	B	67	THR	4.6
1	A	125	ARG	4.6
1	A	145	ALA	4.6
1	B	299	LEU	4.6
1	C	291	VAL	4.6
1	B	186	PHE	4.5
1	B	244	PRO	4.5
1	A	167	PRO	4.5
1	B	273	ARG	4.5
1	C	251	ASP	4.5
1	B	319	ALA	4.5
1	B	245	GLY	4.5
1	C	170	ASP	4.5
1	A	214	ALA	4.5
1	A	290	LYS	4.5
1	B	47	ARG	4.5
1	A	42	GLY	4.5
1	A	148	PHE	4.4
1	A	203	ARG	4.4
1	B	45	GLN	4.4
1	A	51	GLN	4.4
1	B	94	PRO	4.4
1	B	269	PRO	4.4
1	B	290	LYS	4.4
1	C	220	LEU	4.4
1	B	138	GLY	4.4
1	B	24	ARG	4.4
1	A	101	VAL	4.4
1	A	133	GLU	4.4
1	C	334	VAL	4.4
1	A	230	ALA	4.3
1	A	118	LEU	4.3
1	C	48	VAL	4.3
1	B	198	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	51	GLN	4.3
1	C	350	GLY	4.3
1	A	216	MET	4.3
1	C	44	LEU	4.3
1	B	252	PRO	4.3
1	B	57	PHE	4.3
1	C	269	PRO	4.3
1	B	246	HIS	4.3
1	B	63	VAL	4.2
1	A	137	LYS	4.2
1	A	162	GLY	4.2
1	C	319	ALA	4.2
1	B	28	GLY	4.2
1	B	153	SER	4.2
1	C	268	ASP	4.2
1	B	139	TYR	4.2
1	B	125	ARG	4.2
1	A	279	ASP	4.2
1	B	85	LEU	4.2
1	C	26	LEU	4.2
1	C	22	ARG	4.2
1	C	101	VAL	4.2
1	C	143	VAL	4.2
1	C	182	ILE	4.2
1	B	41	ALA	4.2
1	A	90	ALA	4.1
1	B	26	LEU	4.1
1	C	176	LEU	4.1
1	A	291	VAL	4.1
1	A	61	ALA	4.1
1	C	335	ALA	4.1
1	C	97	THR	4.1
1	B	58	VAL	4.1
1	A	288	ASP	4.1
1	A	84	ALA	4.1
1	A	56	LEU	4.1
1	A	114	TYR	4.1
1	C	333	GLU	4.1
1	C	230	ALA	4.1
1	B	165	LEU	4.1
1	A	201	LEU	4.1
1	C	314	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	130	VAL	4.0
1	B	237	VAL	4.0
1	C	112	THR	4.0
1	C	263	PHE	4.0
1	B	201	LEU	4.0
1	B	265	ASP	4.0
1	B	23	PRO	4.0
1	A	323	PHE	4.0
1	B	60	LEU	4.0
1	A	76	VAL	4.0
1	A	105	VAL	4.0
1	A	240	MET	4.0
1	A	342	VAL	4.0
1	C	82	ALA	4.0
1	C	138	GLY	4.0
1	C	332	ARG	4.0
1	B	337	GLN	4.0
1	A	200	GLN	4.0
1	B	240	MET	4.0
1	C	21	ALA	4.0
1	B	282	ARG	4.0
1	C	309	ARG	4.0
1	C	257	GLY	3.9
1	B	147	PHE	3.9
1	B	183	VAL	3.9
1	C	130	VAL	3.9
1	B	347	ARG	3.9
1	A	150	TYR	3.9
1	A	190	TYR	3.9
1	A	241	TYR	3.9
1	C	114	TYR	3.9
1	C	37	LEU	3.9
1	B	192	PRO	3.9
1	A	202	SER	3.9
1	B	220	LEU	3.9
1	A	173	LEU	3.9
1	B	317	PRO	3.9
1	B	302	VAL	3.9
1	C	61	ALA	3.9
1	B	27	THR	3.9
1	C	78	GLU	3.9
1	B	108	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	3.8
1	A	322	ARG	3.8
1	A	330	ARG	3.8
1	C	72	ARG	3.8
1	C	300	ASN	3.8
1	B	90	ALA	3.8
1	C	276	ALA	3.8
1	B	52	ASP	3.8
1	B	65	ALA	3.8
1	C	98	THR	3.8
1	C	134	ILE	3.8
1	A	217	SER	3.8
1	C	116	LEU	3.8
1	C	185	ARG	3.8
1	C	66	LEU	3.8
1	A	70	PHE	3.8
1	A	27	THR	3.8
1	C	104	ALA	3.8
1	C	237	VAL	3.8
1	B	318	ASP	3.8
1	C	90	ALA	3.7
1	A	113	VAL	3.7
1	C	119	VAL	3.7
1	C	144	PRO	3.7
1	C	227	GLY	3.7
1	B	161	PHE	3.7
1	C	106	PRO	3.7
1	C	59	LEU	3.7
1	C	250	SER	3.7
1	B	188	ALA	3.7
1	B	339	LEU	3.7
1	C	63	VAL	3.7
1	B	111	LEU	3.7
1	B	330	ARG	3.7
1	A	176	LEU	3.7
1	C	40	LEU	3.7
1	C	184	ARG	3.7
1	C	207	LEU	3.7
1	C	262	THR	3.7
1	C	84	ALA	3.7
1	C	183	VAL	3.6
1	A	29	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	172	GLN	3.6
1	B	21	ALA	3.6
1	A	326	GLU	3.6
1	A	152	VAL	3.6
1	C	113	VAL	3.6
1	C	254	ARG	3.6
1	C	283	ALA	3.6
1	A	196	GLU	3.6
1	C	289	VAL	3.6
1	B	234	ALA	3.6
1	A	138	GLY	3.6
1	B	151	PRO	3.6
1	A	174	PRO	3.6
1	B	53	GLU	3.6
1	A	292	LYS	3.6
1	C	225	ALA	3.6
1	A	87	TYR	3.6
1	C	301	GLY	3.6
1	B	157	ASP	3.6
1	C	60	LEU	3.5
1	B	345	ALA	3.5
1	C	193	VAL	3.5
1	A	81	LEU	3.5
1	C	150	TYR	3.5
1	C	310	ARG	3.5
1	B	219	SER	3.5
1	B	195	ALA	3.5
1	B	100	VAL	3.5
1	B	167	PRO	3.5
1	A	350	GLY	3.5
1	A	314	GLU	3.5
1	C	85	LEU	3.5
1	C	226	LEU	3.5
1	B	229	SER	3.5
1	B	114	TYR	3.5
1	B	129	THR	3.5
1	A	129	THR	3.5
1	A	47	ARG	3.5
1	A	183	VAL	3.5
1	B	31	PRO	3.5
1	A	197	PRO	3.5
1	A	160	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	331	GLY	3.5
1	B	48	VAL	3.4
1	B	43	SER	3.4
1	B	74	GLU	3.4
1	A	144	PRO	3.4
1	B	176	LEU	3.4
1	A	321	LEU	3.4
1	C	35	LEU	3.4
1	C	214	ALA	3.4
1	C	73	PRO	3.4
1	B	255	VAL	3.4
1	B	59	LEU	3.4
1	C	210	LEU	3.4
1	B	72	ARG	3.4
1	B	213	GLN	3.4
1	A	180	ARG	3.4
1	C	216	MET	3.4
1	B	39	HIS	3.4
1	B	159	ALA	3.4
1	C	124	LEU	3.4
1	B	205	PRO	3.4
1	A	189	LEU	3.4
1	C	43	SER	3.4
1	A	181	GLU	3.4
1	C	27	THR	3.3
1	C	80	VAL	3.3
1	C	92	LEU	3.3
1	B	140	GLY	3.3
1	A	186	PHE	3.3
1	C	141	GLU	3.3
1	C	56	LEU	3.3
1	A	309	ARG	3.3
1	C	67	THR	3.3
1	C	31	PRO	3.3
1	C	341	GLN	3.3
1	A	28	GLY	3.3
1	A	109	ALA	3.3
1	C	288	ASP	3.3
1	B	216	MET	3.3
1	C	328	THR	3.3
1	C	259	PRO	3.3
1	C	146	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	318	ASP	3.3
1	C	318	ASP	3.3
1	B	196	GLU	3.3
1	C	317	PRO	3.3
1	B	160	ALA	3.2
1	A	319	ALA	3.2
1	B	250	SER	3.2
1	B	35	LEU	3.2
1	B	242	THR	3.2
1	C	243	ASP	3.2
1	C	198	GLN	3.2
1	C	329	ALA	3.2
1	B	236	LYS	3.2
1	A	112	THR	3.2
1	A	308	THR	3.2
1	A	316	ASP	3.2
1	A	282	ARG	3.2
1	C	62	ASP	3.2
1	B	164	THR	3.2
1	A	127	ASN	3.2
1	C	164	THR	3.2
1	B	131	LYS	3.2
1	B	137	LYS	3.2
1	C	111	LEU	3.2
1	B	30	ARG	3.2
1	C	223	ALA	3.2
1	A	258	ASN	3.2
1	C	136	GLN	3.2
1	B	303	LEU	3.2
1	C	275	GLN	3.2
1	C	103	SER	3.1
1	C	70	PHE	3.1
1	C	304	ALA	3.1
1	A	120	THR	3.1
1	B	206	ARG	3.1
1	A	83	VAL	3.1
1	B	348	LEU	3.1
1	C	295	LEU	3.1
1	C	132	ALA	3.1
1	B	123	HIS	3.1
1	A	111	LEU	3.1
1	C	171	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	322	ARG	3.1
1	A	74	GLU	3.1
1	B	91	GLY	3.1
1	B	260	VAL	3.1
1	C	249	ALA	3.1
1	C	129	THR	3.1
1	C	326	GLU	3.1
1	B	171	ASP	3.1
1	B	148	PHE	3.0
1	B	349	PHE	3.0
1	B	144	PRO	3.0
1	C	173	LEU	3.0
1	C	128	PRO	3.0
1	B	96	LYS	3.0
1	C	65	ALA	3.0
1	C	260	VAL	3.0
1	C	339	LEU	3.0
1	B	222	ASN	3.0
1	C	148	PHE	3.0
1	C	305	PRO	3.0
1	C	311	ALA	3.0
1	C	296	ILE	3.0
1	C	294	HIS	3.0
1	A	178	GLN	3.0
1	C	204	VAL	3.0
1	C	292	LYS	3.0
1	C	298	VAL	3.0
1	B	133	GLU	3.0
1	A	30	ARG	3.0
1	A	110	GLU	3.0
1	C	25	VAL	3.0
1	C	152	VAL	3.0
1	C	247	LEU	3.0
1	A	132	ALA	3.0
1	A	177	GLU	2.9
1	C	241	TYR	2.9
1	C	142	ARG	2.9
1	A	33	GLY	2.9
1	C	192	PRO	2.9
1	B	253	GLY	2.9
1	C	174	PRO	2.9
1	B	49	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	2.9
1	A	32	THR	2.9
1	B	62	ASP	2.9
1	A	257	GLY	2.9
1	C	201	LEU	2.9
1	C	83	VAL	2.9
1	B	230	ALA	2.9
1	B	329	ALA	2.9
1	C	127	ASN	2.9
1	C	135	ALA	2.9
1	C	32	THR	2.9
1	A	147	PHE	2.8
1	C	215	LYS	2.8
1	C	265	ASP	2.8
1	A	338	THR	2.8
1	C	87	TYR	2.8
1	B	61	ALA	2.8
1	C	145	ALA	2.8
1	C	266	ALA	2.8
1	C	330	ARG	2.8
1	B	288	ASP	2.8
1	B	310	ARG	2.8
1	C	246	HIS	2.8
1	C	248	ARG	2.8
1	A	21	ALA	2.8
1	C	163	ALA	2.8
1	B	331	GLY	2.8
1	A	270	ASP	2.8
1	A	78	GLU	2.8
1	A	103	SER	2.8
1	C	188	ALA	2.8
1	B	86	ASP	2.8
1	B	193	VAL	2.8
1	C	151	PRO	2.8
1	C	340	GLY	2.8
1	B	112	THR	2.8
1	C	342	VAL	2.8
1	B	69	HIS	2.7
1	C	172	GLN	2.7
1	C	232	GLU	2.7
1	B	191	ALA	2.7
1	C	149	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	64	GLN	2.7
1	B	127	ASN	2.7
1	B	351	HIS	2.7
1	B	116	LEU	2.7
1	A	64	GLN	2.7
1	A	106	PRO	2.7
1	C	224	ILE	2.7
1	B	149	VAL	2.7
1	B	239	GLY	2.7
1	C	41	ALA	2.7
1	C	191	ALA	2.7
1	C	102	GLN	2.7
1	A	38	GLY	2.7
1	A	328	THR	2.7
1	C	200	GLN	2.7
1	C	49	ARG	2.7
1	C	123	HIS	2.7
1	A	236	LYS	2.7
1	C	167	PRO	2.7
1	B	340	GLY	2.7
1	A	140	GLY	2.7
1	B	101	VAL	2.7
1	B	81	LEU	2.6
1	A	124	LEU	2.6
1	A	151	PRO	2.6
1	C	115	PHE	2.6
1	C	158	ILE	2.6
1	A	100	VAL	2.6
1	B	311	ALA	2.6
1	C	325	THR	2.6
1	B	217	SER	2.6
1	B	292	LYS	2.6
1	B	190	TYR	2.6
1	B	102	GLN	2.6
1	B	312	GLU	2.6
1	C	181	GLU	2.6
1	C	190	TYR	2.6
1	A	343	ARG	2.6
1	B	316	ASP	2.6
1	B	199	ALA	2.6
1	A	192	PRO	2.6
1	C	118	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	2.6
1	A	188	ALA	2.6
1	C	24	ARG	2.6
1	B	33	GLY	2.5
1	C	179	THR	2.5
1	B	194	LEU	2.5
1	A	154	GLN	2.5
1	C	337	GLN	2.5
1	B	346	MET	2.5
1	B	166	VAL	2.5
1	C	196	GLU	2.5
1	B	305	PRO	2.5
1	C	338	THR	2.5
1	C	195	ALA	2.5
1	C	233	VAL	2.5
1	C	236	LYS	2.5
1	C	81	LEU	2.5
1	B	80	VAL	2.5
1	A	141	GLU	2.5
1	A	335	ALA	2.5
1	B	200	GLN	2.5
1	B	259	PRO	2.5
1	C	121	VAL	2.5
1	C	69	HIS	2.5
1	C	47	ARG	2.5
1	C	316	ASP	2.4
1	A	305	PRO	2.4
1	B	184	ARG	2.4
1	B	333	GLU	2.4
1	C	76	VAL	2.4
1	C	242	THR	2.4
1	A	317	PRO	2.4
1	C	261	PHE	2.4
1	A	300	ASN	2.4
1	B	29	ASP	2.4
1	C	29	ASP	2.4
1	B	156	ALA	2.4
1	A	301	GLY	2.4
1	A	52	ASP	2.4
1	C	345	ALA	2.4
1	A	79	ASN	2.4
1	B	142	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	30	ARG	2.4
1	B	284	GLY	2.4
1	A	31	PRO	2.4
1	A	184	ARG	2.4
1	A	209	GLY	2.4
1	A	349	PHE	2.4
1	C	153	SER	2.4
1	C	348	LEU	2.4
1	B	225	ALA	2.3
1	A	65	ALA	2.3
1	C	208	PRO	2.3
1	B	119	VAL	2.3
1	B	77	ARG	2.3
1	A	337	GLN	2.3
1	B	179	THR	2.3
1	A	149	VAL	2.3
1	C	52	ASP	2.3
1	B	235	ARG	2.3
1	B	106	PRO	2.3
1	C	162	GLY	2.3
1	B	344	ARG	2.3
1	A	45	GLN	2.3
1	B	215	LYS	2.3
1	B	325	THR	2.3
1	A	179	THR	2.3
1	C	89	ALA	2.3
1	B	350	GLY	2.3
1	A	169	GLY	2.3
1	B	324	VAL	2.3
1	B	172	GLN	2.3
1	B	251	ASP	2.3
1	C	218	LYS	2.3
1	C	168	VAL	2.2
1	B	328	THR	2.2
1	B	185	ARG	2.2
1	C	343	ARG	2.2
1	A	157	ASP	2.2
1	B	258	ASN	2.2
1	C	209	GLY	2.2
1	C	221	GLY	2.2
1	A	23	PRO	2.2
1	A	334	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	2.2
1	B	38	GLY	2.2
1	C	327	GLY	2.2
1	A	346	MET	2.2
1	B	22	ARG	2.2
1	B	36	HIS	2.2
1	C	256	GLU	2.2
1	B	283	ALA	2.2
1	C	155	ALA	2.2
1	B	154	GLN	2.1
1	A	49	ARG	2.1
1	C	39	HIS	2.1
1	B	46	ASN	2.1
1	A	332	ARG	2.1
1	C	347	ARG	2.1
1	B	145	ALA	2.1
1	B	211	ASP	2.1
1	B	297	ASP	2.1
1	C	86	ASP	2.1
1	C	38	GLY	2.1
1	C	75	GLN	2.1
1	B	163	ALA	2.1
1	A	351	HIS	2.1
1	A	331	GLY	2.1
1	C	55	GLU	2.1
1	A	102	GLN	2.1
1	B	126	GLN	2.1
1	B	70	PHE	2.1
1	B	113	VAL	2.1
1	C	42	GLY	2.0
1	B	197	PRO	2.0
1	C	240	MET	2.0
1	A	46	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	TRP	C	3000	15/15	0.47	0.50	3.61	52,54,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.