



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SVA
Title : SIMIAN VIRUS 40
Authors : Stehle, T.; Gamblin, S.J.; Harrison, S.C.
Deposited on : 1995-11-27
Resolution : 3.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

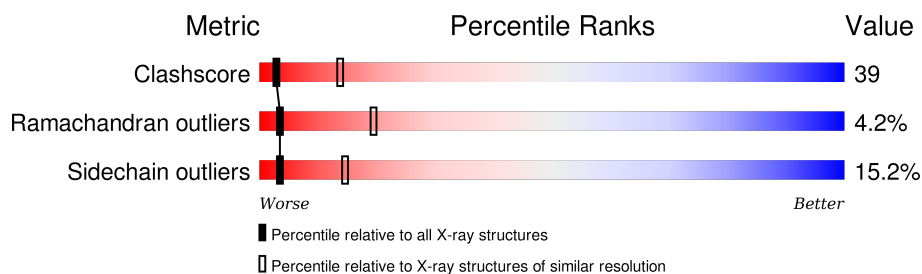
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	361	
1	2	361	
1	3	361	
1	4	361	
1	5	361	
1	6	361	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15983 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 SIMIAN VIRUS 40.

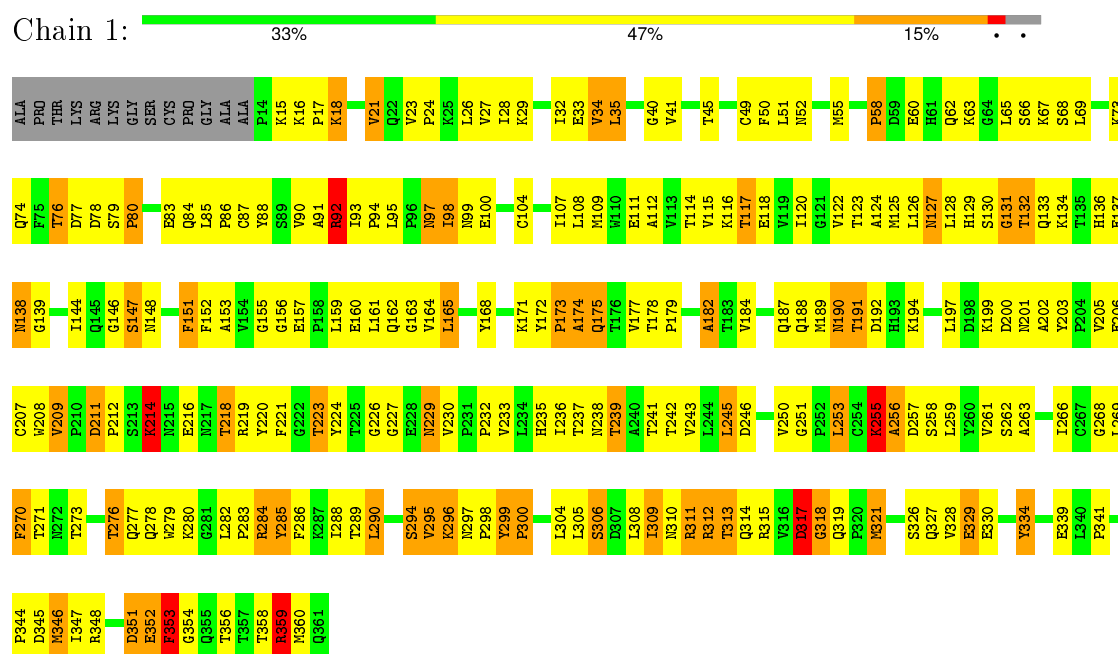
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	348	Total	C	N	O	S	0	0	0
			2707	1703	460	530	14			
1	2	348	Total	C	N	O	S	0	0	0
			2707	1703	460	530	14			
1	3	342	Total	C	N	O	S	0	0	0
			2658	1675	450	520	13			
1	4	331	Total	C	N	O	S	0	0	0
			2560	1612	435	501	12			
1	5	347	Total	C	N	O	S	0	0	0
			2700	1698	459	529	14			
1	6	341	Total	C	N	O	S	0	0	0
			2651	1670	449	519	13			

3 Residue-property plots

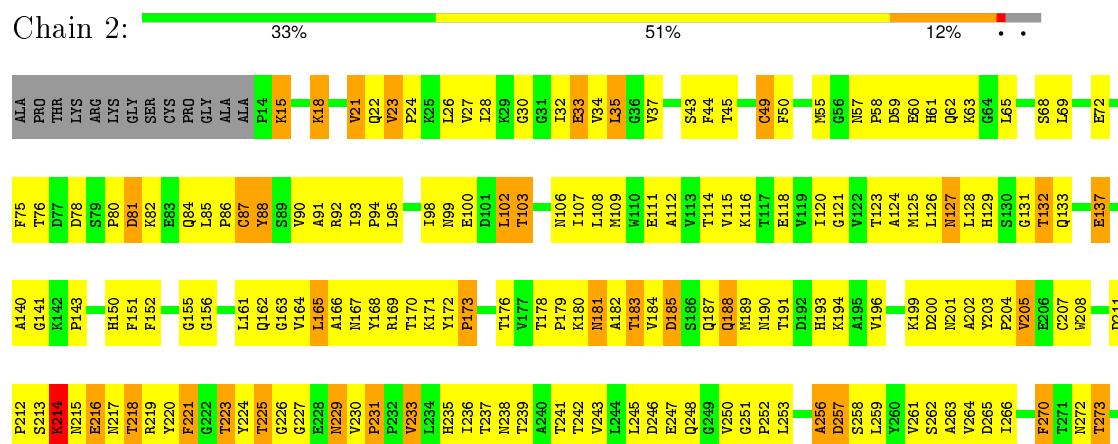
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: SIMIAN VIRUS 40

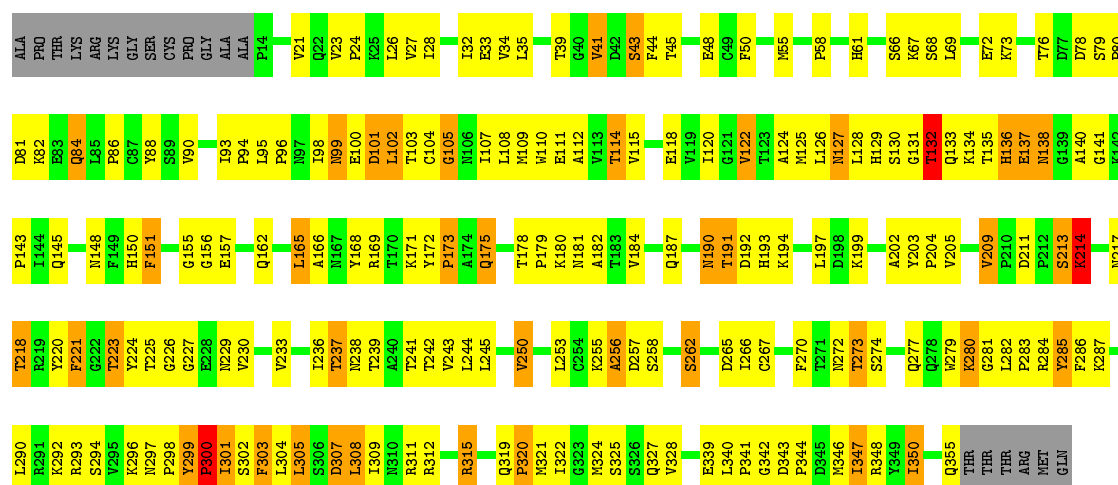


• Molecule 1: SIMIAN VIRUS 40



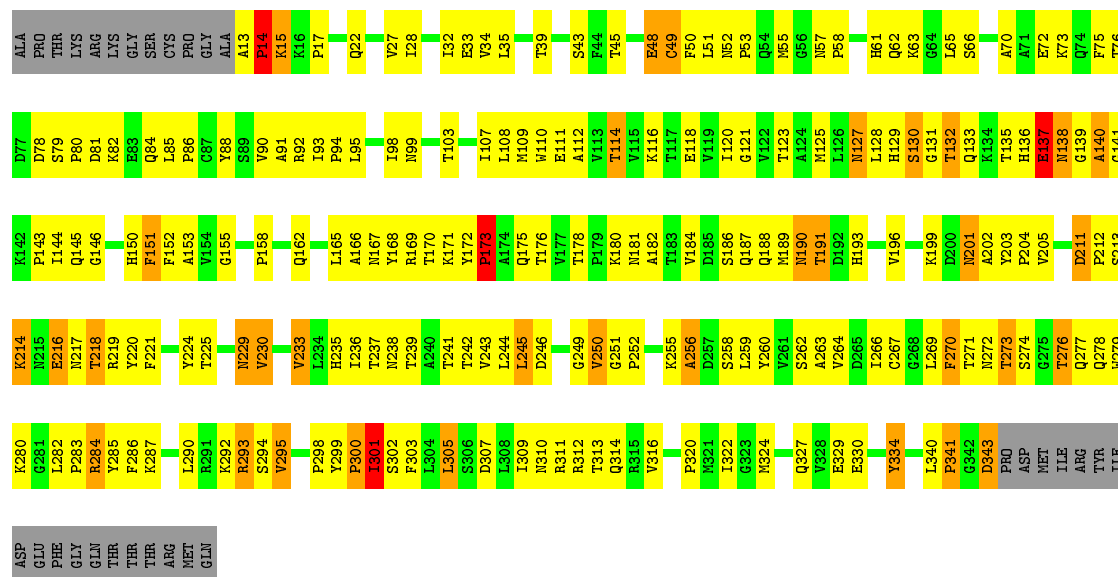
- Molecule 1: SIMIAN VIRUS 40

Chain 3: 40% 43% 11% • 5%



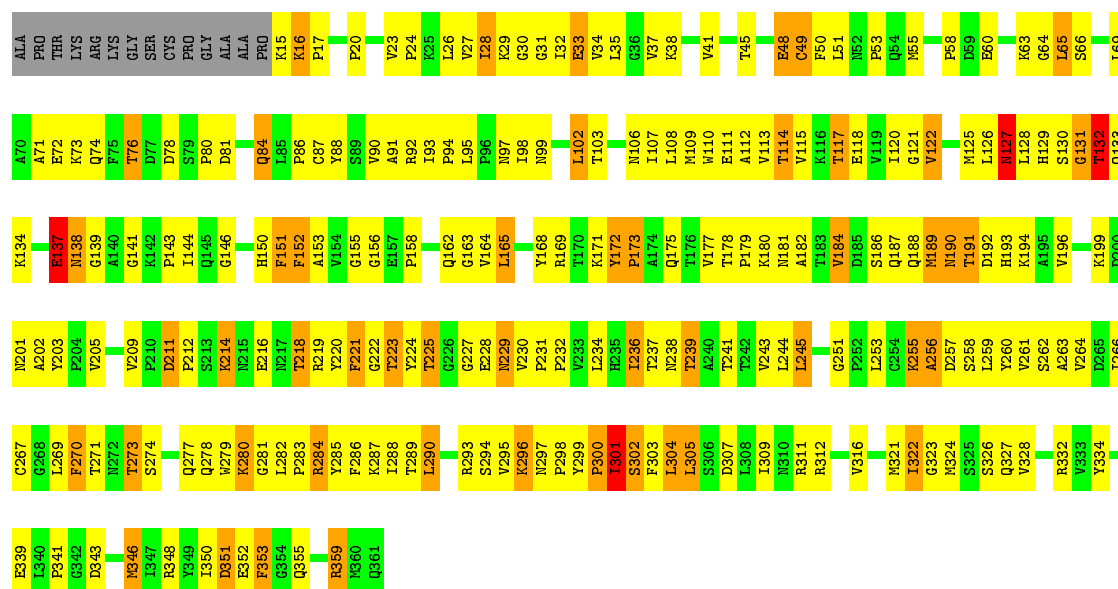
- Molecule 1: SIMIAN VIRUS 40

Chain 4: 35% 47% 9% 1% 8%



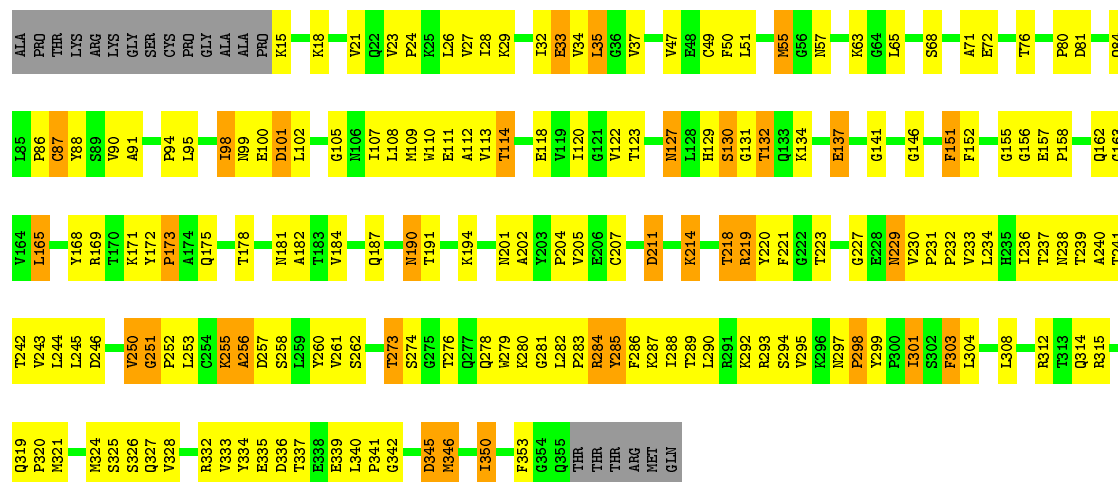
- Molecule 1: SIMIAN VIRUS 40

Chain 5:  34% 48% 14% . .



• Molecule 1: SIMIAN VIRUS 40

Chain 6: 45% 40% 9% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	558.00 Å 558.00 Å 558.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10	Depositor
% Data completeness (in resolution range)	80.2 (12.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.257 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15983	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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	1	0.85	1/2766 (0.0%)	1.10	9/3761 (0.2%)
1	2	0.92	5/2766 (0.2%)	1.08	5/3761 (0.1%)
1	3	0.90	0/2717	1.11	7/3695 (0.2%)
1	4	0.96	5/2616 (0.2%)	1.09	8/3560 (0.2%)
1	5	0.91	2/2758 (0.1%)	1.09	11/3750 (0.3%)
1	6	0.99	5/2709 (0.2%)	1.10	8/3684 (0.2%)
All	All	0.92	18/16332 (0.1%)	1.10	48/22211 (0.2%)

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	2	0	1
1	6	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	49	CYS	CB-SG	-8.52	1.67	1.82
1	6	49	CYS	CB-SG	-8.00	1.68	1.82
1	2	49	CYS	CB-SG	-7.44	1.69	1.82
1	4	216	GLU	CB-CG	7.32	1.66	1.52
1	5	216	GLU	CB-CG	6.77	1.65	1.52
1	5	216	GLU	CG-CD	6.59	1.61	1.51
1	4	138	ASN	N-CA	6.17	1.58	1.46
1	4	216	GLU	CG-CD	6.05	1.61	1.51
1	2	216	GLU	CB-CG	6.04	1.63	1.52
1	2	247	GLU	CB-CG	5.58	1.62	1.52
1	1	353	PHE	CB-CG	5.53	1.60	1.51
1	6	240	ALA	CA-CB	-5.51	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	48	GLU	CG-CD	5.51	1.60	1.51
1	2	216	GLU	CG-CD	5.39	1.60	1.51
1	6	113	VAL	CB-CG1	-5.31	1.41	1.52
1	6	87	CYS	CB-SG	-5.24	1.73	1.81
1	2	87	CYS	CB-SG	-5.15	1.73	1.81
1	6	33	GLU	CD-OE1	-5.01	1.20	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	105	GLY	N-CA-C	9.12	135.91	113.10
1	1	256	ALA	N-CA-C	-7.80	89.94	111.00
1	3	256	ALA	N-CA-C	-7.65	90.34	111.00
1	4	256	ALA	N-CA-C	-7.37	91.11	111.00
1	6	256	ALA	N-CA-C	-6.94	92.27	111.00
1	6	244	LEU	CA-CB-CG	-6.75	99.77	115.30
1	4	15	LYS	N-CA-C	-6.72	92.86	111.00
1	1	359	ARG	N-CA-C	6.66	128.97	111.00
1	5	256	ALA	N-CA-C	-6.40	93.72	111.00
1	1	35	LEU	CA-CB-CG	-6.34	100.73	115.30
1	5	304	LEU	CA-CB-CG	-6.17	101.10	115.30
1	1	92	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	1	290	LEU	CA-CB-CG	-6.14	101.17	115.30
1	4	214	LYS	N-CA-C	6.13	127.56	111.00
1	3	300	PRO	N-CA-C	6.13	128.04	112.10
1	5	102	LEU	N-CA-C	6.12	127.53	111.00
1	1	253	LEU	CA-CB-CG	-6.11	101.25	115.30
1	2	214	LYS	N-CA-C	6.01	127.23	111.00
1	5	290	LEU	CA-CB-CG	-5.99	101.52	115.30
1	6	211	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	6	71	ALA	N-CA-C	5.96	127.11	111.00
1	6	219	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	3	214	LYS	N-CA-C	5.92	126.98	111.00
1	2	256	ALA	N-CA-C	-5.91	95.05	111.00
1	2	103	THR	N-CA-C	5.82	126.72	111.00
1	3	237	THR	CB-CA-C	-5.71	96.17	111.60
1	2	343	ASP	CB-CG-OD2	5.70	123.43	118.30
1	1	209	VAL	N-CA-C	-5.62	95.83	111.00
1	5	137	GLU	O-C-N	-5.60	113.73	122.70
1	4	211	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	5	211	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	5	214	LYS	N-CA-C	5.49	125.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	137	GLU	C-N-CA	-5.47	108.03	121.70
1	4	49	CYS	CA-CB-SG	-5.41	104.25	114.00
1	4	343	ASP	N-CA-C	5.41	125.62	111.00
1	6	251	GLY	N-CA-C	-5.40	99.61	113.10
1	6	214	LYS	N-CA-C	5.37	125.49	111.00
1	3	299	TYR	N-CA-C	5.34	125.42	111.00
1	6	105	GLY	N-CA-C	5.34	126.45	113.10
1	5	71	ALA	N-CA-C	5.28	125.24	111.00
1	1	174	ALA	N-CA-C	5.26	125.22	111.00
1	3	166	ALA	N-CA-C	-5.23	96.88	111.00
1	5	219	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	1	214	LYS	N-CA-C	5.08	124.72	111.00
1	5	296	LYS	CD-CE-NZ	5.07	123.36	111.70
1	2	21	VAL	CB-CA-C	-5.03	101.84	111.40
1	4	166	ALA	N-CA-C	-5.00	97.49	111.00
1	5	172	TYR	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	88	TYR	Sidechain
1	6	285	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	1	2707	0	2676	258	0
1	2	2707	0	2676	245	0
1	3	2658	0	2625	224	0
1	4	2560	0	2535	234	0
1	5	2700	0	2668	266	0
1	6	2651	0	2617	179	0
All	All	15983	0	15797	1254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1254) 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)
1:2:121:GLY:HA2	1:3:209:VAL:HG11	1.28	1.12
1:4:27:VAL:HG12	1:4:28:ILE:HG22	1.31	1.12
1:1:27:VAL:HG12	1:1:28:ILE:HG22	1.26	1.10
1:6:237:THR:HG22	1:6:239:THR:H	1.14	1.09
1:5:165:LEU:HD11	1:5:168:TYR:HA	1.39	1.05
1:1:79:SER:HB2	1:1:171:LYS:HB2	1.37	1.01
1:2:22:GLN:HG3	1:6:337:THR:HB	1.43	1.01
1:3:243:VAL:HG12	1:3:245:LEU:H	1.21	1.00
1:2:237:THR:HG22	1:2:239:THR:H	1.24	0.99
1:2:15:LYS:HD3	1:3:41:VAL:HB	1.45	0.98
1:4:132:THR:HG21	1:4:141:GLY:HA3	1.44	0.98
1:1:237:THR:HG22	1:1:239:THR:H	1.30	0.96
1:3:237:THR:HG22	1:3:239:THR:H	1.28	0.96
1:6:168:TYR:HB2	1:6:182:ALA:HB1	1.45	0.95
1:5:199:LYS:HG3	1:5:202:ALA:HB2	1.48	0.94
1:3:132:THR:HG21	1:3:141:GLY:HA3	1.49	0.94
1:5:69:LEU:HD12	1:5:278:GLN:HA	1.49	0.94
1:1:73:LYS:HD3	1:1:78:ASP:HA	1.48	0.93
1:4:233:VAL:HG13	1:5:225:THR:HG23	1.48	0.93
1:3:140:ALA:H	1:4:277:GLN:HE21	1.17	0.91
1:4:120:ILE:HB	1:4:283:PRO:HG2	1.52	0.91
1:4:121:GLY:HA2	1:5:209:VAL:HG11	1.48	0.91
1:1:162:GLN:HB2	1:1:211:ASP:HB2	1.50	0.90
1:2:155:GLY:HA3	1:2:218:THR:HB	1.50	0.90
1:1:298:PRO:HG2	1:1:299:TYR:CE1	2.06	0.90
1:4:127:ASN:ND2	1:4:130:SER:H	1.70	0.89
1:2:45:THR:HG22	1:6:333:VAL:HG22	1.54	0.89
1:1:155:GLY:HA3	1:1:218:THR:HB	1.56	0.88
1:6:127:ASN:HD21	1:6:130:SER:H	1.22	0.88
1:3:99:ASN:ND2	1:3:108:LEU:H	1.72	0.88
1:3:99:ASN:HD22	1:3:108:LEU:H	1.22	0.87
1:5:237:THR:HG22	1:5:239:THR:H	1.40	0.85
1:6:237:THR:HG22	1:6:239:THR:N	1.92	0.84
1:3:125:MET:HE1	1:4:224:TYR:HE2	1.39	0.84
1:4:155:GLY:HA3	1:4:218:THR:HB	1.60	0.84
1:4:165:LEU:HD11	1:4:168:TYR:HA	1.57	0.84
1:1:92:ARG:HG3	1:1:258:SER:HB3	1.59	0.84
1:4:132:THR:CG2	1:4:141:GLY:HA3	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:347:ILE:HB	1:1:358:THR:HG23	1.60	0.83
1:3:155:GLY:HA3	1:3:218:THR:HB	1.60	0.83
1:6:27:VAL:HG12	1:6:28:ILE:HG22	1.58	0.82
1:3:175:GLN:HA	1:3:175:GLN:HE21	1.43	0.82
1:2:120:ILE:HB	1:2:283:PRO:HG2	1.60	0.82
1:4:98:ILE:HD13	1:4:292:LYS:HG2	1.62	0.82
1:5:155:GLY:HA3	1:5:218:THR:HB	1.62	0.81
1:4:127:ASN:HD21	1:4:130:SER:H	1.26	0.81
1:5:270:PHE:HD1	1:5:271:THR:N	1.78	0.81
1:1:88:TYR:HE1	1:1:205:VAL:HA	1.46	0.81
1:2:243:VAL:HG12	1:2:245:LEU:H	1.46	0.81
1:2:168:TYR:HB2	1:2:182:ALA:HB1	1.61	0.81
1:2:61:HIS:HD2	1:3:168:TYR:OH	1.64	0.80
1:1:108:LEU:HD23	1:1:294:SER:HA	1.62	0.79
1:5:243:VAL:HG12	1:5:245:LEU:H	1.43	0.79
1:5:23:VAL:HB	1:5:24:PRO:HD2	1.63	0.79
1:2:99:ASN:HD22	1:2:102:LEU:HD23	1.47	0.79
1:5:120:ILE:HB	1:5:283:PRO:HG2	1.64	0.79
1:2:165:LEU:O	1:2:187:GLN:HA	1.83	0.79
1:1:151:PHE:HE2	1:1:220:TYR:HB2	1.48	0.79
1:5:98:ILE:HD11	1:5:110:TRP:CE2	2.18	0.79
1:5:165:LEU:O	1:5:187:GLN:HA	1.82	0.79
1:2:28:ILE:HG21	1:2:37:VAL:HG21	1.65	0.79
1:5:88:TYR:HE1	1:5:205:VAL:HA	1.48	0.79
1:3:98:ILE:HD11	1:3:110:TRP:CE2	2.19	0.78
1:1:284:ARG:HD3	1:1:286:PHE:CZ	2.17	0.78
1:4:298:PRO:HG2	1:4:299:TYR:CD2	2.18	0.78
1:2:321:MET:HE2	1:2:328:VAL:HG23	1.65	0.78
1:6:28:ILE:HG21	1:6:37:VAL:HG21	1.65	0.78
1:2:237:THR:HG22	1:2:239:THR:N	1.98	0.78
1:5:31:GLY:O	1:5:34:VAL:HG23	1.84	0.77
1:1:163:GLY:O	1:1:164:VAL:HG23	1.84	0.77
1:1:112:ALA:HA	1:1:290:LEU:HD23	1.67	0.77
1:3:227:GLY:HA3	1:3:230:VAL:HG13	1.66	0.77
1:4:132:THR:O	1:4:273:THR:HG23	1.85	0.76
1:1:98:ILE:HD11	1:1:108:LEU:HD12	1.67	0.76
1:1:172:TYR:CG	1:1:178:THR:HG21	2.19	0.76
1:4:168:TYR:HB2	1:4:182:ALA:HB1	1.68	0.76
1:3:55:MET:HE1	1:3:266:ILE:HA	1.66	0.76
1:2:322:ILE:HG22	1:2:323:GLY:H	1.51	0.76
1:5:28:ILE:HG13	1:5:29:LYS:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:132:THR:CG2	1:3:141:GLY:HA3	2.16	0.76
1:1:88:TYR:CE1	1:1:205:VAL:HA	2.20	0.76
1:1:235:HIS:CD2	1:2:223:THR:HB	2.21	0.76
1:4:165:LEU:O	1:4:187:GLN:HA	1.84	0.76
1:5:80:PRO:O	1:5:173:PRO:HG3	1.86	0.76
1:5:88:TYR:CE1	1:5:205:VAL:HA	2.21	0.75
1:1:227:GLY:HA3	1:1:230:VAL:CG1	2.17	0.75
1:5:350:ILE:HG12	1:5:355:GLN:HG3	1.68	0.75
1:2:68:SER:HB3	1:2:276:THR:HG21	1.69	0.74
1:3:237:THR:HG23	1:4:220:TYR:O	1.87	0.74
1:6:32:ILE:CD1	1:6:35:LEU:HD12	2.18	0.74
1:1:162:GLN:CB	1:1:211:ASP:HB2	2.18	0.74
1:1:256:ALA:O	1:1:258:SER:N	2.21	0.74
1:5:51:LEU:HD11	1:5:261:VAL:HG12	1.68	0.73
1:5:359:ARG:HB3	1:5:359:ARG:CZ	2.16	0.73
1:6:112:ALA:HA	1:6:290:LEU:HD23	1.70	0.73
1:6:127:ASN:ND2	1:6:130:SER:H	1.86	0.73
1:1:243:VAL:HG12	1:1:245:LEU:H	1.51	0.73
1:4:237:THR:HG22	1:4:239:THR:H	1.53	0.73
1:1:298:PRO:HG2	1:1:299:TYR:CD1	2.23	0.73
1:3:27:VAL:HG12	1:3:28:ILE:HG22	1.68	0.73
1:4:139:GLY:HA3	1:5:277:GLN:HE21	1.54	0.73
1:2:321:MET:CE	1:2:328:VAL:HG23	2.18	0.73
1:1:299:TYR:CD1	1:1:299:TYR:N	2.54	0.73
1:1:209:VAL:HG11	1:5:121:GLY:HA2	1.71	0.73
1:1:32:ILE:HD12	1:1:35:LEU:HD12	1.70	0.73
1:3:88:TYR:CE1	1:3:205:VAL:HA	2.23	0.73
1:1:165:LEU:O	1:1:187:GLN:HA	1.87	0.73
1:3:73:LYS:HD2	1:3:78:ASP:HA	1.70	0.73
1:6:80:PRO:HG2	1:6:173:PRO:HD3	1.71	0.72
1:6:321:MET:HE3	1:6:328:VAL:HG23	1.71	0.72
1:2:322:ILE:HG22	1:2:323:GLY:N	2.04	0.72
1:4:88:TYR:CE1	1:4:205:VAL:HA	2.24	0.72
1:2:109:MET:CE	1:2:295:VAL:HG21	2.20	0.72
1:2:121:GLY:CA	1:3:209:VAL:HG11	2.16	0.72
1:2:123:THR:OG1	1:3:209:VAL:HG12	1.89	0.72
1:5:165:LEU:CD1	1:5:168:TYR:HA	2.19	0.72
1:3:168:TYR:HD1	1:3:187:GLN:HE21	1.37	0.72
1:2:55:MET:HE1	1:2:266:ILE:HA	1.71	0.72
1:2:342:GLY:O	1:2:344:PRO:HD3	1.90	0.72
1:2:33:GLU:H	1:2:33:GLU:CD	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:132:THR:O	1:3:273:THR:HG23	1.89	0.71
1:1:80:PRO:O	1:1:173:PRO:HG3	1.90	0.71
1:4:121:GLY:HA2	1:5:209:VAL:CG1	2.20	0.71
1:5:351:ASP:CG	1:5:352:GLU:H	1.93	0.71
1:6:32:ILE:HD11	1:6:35:LEU:HD12	1.71	0.71
1:5:128:LEU:HD13	1:5:141:GLY:O	1.91	0.71
1:5:99:ASN:HD21	1:5:108:LEU:N	1.87	0.71
1:4:137:GLU:CD	1:4:137:GLU:H	1.94	0.71
1:2:34:VAL:O	1:2:37:VAL:HG23	1.90	0.71
1:4:13:ALA:HB1	1:4:14:PRO:HD2	1.72	0.71
1:3:172:TYR:CG	1:3:178:THR:HG21	2.26	0.71
1:1:227:GLY:HA3	1:1:230:VAL:HG13	1.72	0.70
1:2:112:ALA:HA	1:2:290:LEU:HD23	1.73	0.70
1:5:112:ALA:HA	1:5:290:LEU:HD23	1.73	0.70
1:3:237:THR:HG22	1:3:239:THR:N	2.06	0.70
1:1:99:ASN:HD21	1:1:108:LEU:H	1.39	0.70
1:4:127:ASN:HD21	1:4:130:SER:N	1.89	0.70
1:6:80:PRO:O	1:6:173:PRO:HG3	1.91	0.70
1:3:120:ILE:HD11	1:3:285:TYR:HB2	1.72	0.70
1:1:299:TYR:H	1:1:299:TYR:HD1	1.40	0.70
1:6:98:ILE:HD13	1:6:292:LYS:HG2	1.74	0.70
1:5:26:LEU:HD12	1:5:27:VAL:H	1.54	0.70
1:3:168:TYR:HB2	1:3:182:ALA:HB1	1.74	0.70
1:6:99:ASN:HD21	1:6:107:ILE:HG23	1.55	0.70
1:2:43:SER:HB3	1:6:335:GLU:HG3	1.73	0.70
1:3:118:GLU:CD	1:3:236:ILE:HG13	2.13	0.69
1:1:97:ASN:ND2	1:1:99:ASN:H	1.90	0.69
1:3:347:ILE:HB	1:6:299:TYR:OH	1.92	0.69
1:2:49:CYS:HB2	1:6:321:MET:HE1	1.75	0.69
1:5:120:ILE:O	1:5:282:LEU:HD22	1.92	0.69
1:4:55:MET:HE1	1:4:266:ILE:HA	1.73	0.69
1:5:298:PRO:HG2	1:5:299:TYR:CD2	2.28	0.69
1:2:233:VAL:HG13	1:3:225:THR:HG23	1.74	0.69
1:3:140:ALA:H	1:4:277:GLN:NE2	1.88	0.69
1:4:99:ASN:HD22	1:4:108:LEU:H	1.41	0.69
1:6:227:GLY:HA3	1:6:230:VAL:HG13	1.75	0.68
1:3:237:THR:HG21	1:3:239:THR:OG1	1.92	0.68
1:3:281:GLY:O	1:3:282:LEU:HD23	1.93	0.68
1:4:17:PRO:HB3	1:5:108:LEU:HD21	1.76	0.68
1:3:233:VAL:HG22	1:4:225:THR:HG23	1.74	0.68
1:6:32:ILE:O	1:6:35:LEU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:121:GLY:HA2	1:3:209:VAL:CG1	2.15	0.68
1:6:81:ASP:HB2	1:6:84:GLN:HG3	1.76	0.67
1:1:178:THR:HB	1:1:179:PRO:HD2	1.75	0.67
1:3:284:ARG:HD3	1:3:286:PHE:CZ	2.29	0.67
1:4:99:ASN:ND2	1:4:107:ILE:HA	2.09	0.67
1:1:233:VAL:HG13	1:2:225:THR:HG23	1.75	0.67
1:6:120:ILE:HB	1:6:283:PRO:HG2	1.76	0.67
1:3:88:TYR:HE1	1:3:205:VAL:HA	1.60	0.67
1:1:41:VAL:H	1:5:15:LYS:HD2	1.59	0.67
1:6:162:GLN:NE2	1:6:194:LYS:HD3	2.10	0.67
1:5:16:LYS:HG2	1:5:17:PRO:O	1.95	0.67
1:1:86:PRO:O	1:1:205:VAL:HG22	1.95	0.67
1:1:125:MET:HE3	1:1:144:ILE:HB	1.75	0.66
1:6:155:GLY:HA3	1:6:218:THR:HB	1.75	0.66
1:1:172:TYR:CB	1:1:178:THR:HG21	2.25	0.66
1:4:237:THR:HG23	1:5:220:TYR:O	1.95	0.66
1:2:60:GLU:O	1:3:184:VAL:HG21	1.95	0.66
1:4:273:THR:CG2	1:5:72:GLU:HB3	2.26	0.66
1:6:243:VAL:HG12	1:6:245:LEU:H	1.60	0.66
1:4:118:GLU:OE2	1:4:236:ILE:HG13	1.96	0.66
1:5:95:LEU:HD12	1:5:110:TRP:CG	2.31	0.66
1:1:90:VAL:HG22	1:1:91:ALA:N	2.11	0.66
1:1:184:VAL:HG12	1:5:63:LYS:HB2	1.76	0.66
1:6:109:MET:CE	1:6:295:VAL:HG21	2.26	0.66
1:4:93:ILE:HD12	1:4:93:ILE:N	2.10	0.66
1:6:28:ILE:HD13	1:6:34:VAL:HG13	1.76	0.65
1:1:28:ILE:HG12	1:1:34:VAL:HG13	1.77	0.65
1:2:21:VAL:HG21	1:3:293:ARG:HH21	1.62	0.65
1:1:120:ILE:HD11	1:1:285:TYR:HB2	1.78	0.65
1:6:175:GLN:HA	1:6:175:GLN:HE21	1.60	0.65
1:6:237:THR:HG21	1:6:239:THR:OG1	1.96	0.65
1:2:109:MET:HE2	1:2:295:VAL:HG21	1.77	0.65
1:5:32:ILE:HD12	1:5:35:LEU:HD12	1.79	0.65
1:3:112:ALA:HA	1:3:290:LEU:HD23	1.78	0.65
1:2:359:ARG:HB3	1:2:359:ARG:CZ	2.27	0.65
1:4:98:ILE:CD1	1:4:292:LYS:HG2	2.26	0.65
1:6:127:ASN:HD21	1:6:130:SER:N	1.92	0.65
1:2:129:HIS:O	1:2:129:HIS:CD2	2.51	0.65
1:2:132:THR:O	1:3:72:GLU:HG2	1.97	0.64
1:5:284:ARG:HG2	1:5:285:TYR:N	2.11	0.64
1:6:256:ALA:O	1:6:258:SER:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:132:THR:HG23	1:6:141:GLY:CA	2.26	0.64
1:3:344:PRO:HD2	1:6:255:LYS:HD2	1.78	0.64
1:1:156:GLY:HA3	1:1:253:LEU:O	1.98	0.64
1:2:99:ASN:ND2	1:2:108:LEU:H	1.95	0.64
1:5:73:LYS:HD3	1:5:78:ASP:HA	1.80	0.64
1:3:80:PRO:O	1:3:173:PRO:HG3	1.97	0.64
1:2:49:CYS:HA	1:6:328:VAL:HA	1.78	0.64
1:2:359:ARG:HB3	1:2:359:ARG:NH1	2.13	0.64
1:3:131:GLY:HA3	1:4:75:PHE:HE1	1.63	0.64
1:5:125:MET:CE	1:5:144:ILE:HB	2.28	0.64
1:6:99:ASN:ND2	1:6:107:ILE:HA	2.13	0.64
1:3:340:LEU:HD12	1:3:341:PRO:HD2	1.79	0.64
1:2:199:LYS:HG3	1:2:202:ALA:HB2	1.78	0.64
1:3:157:GLU:HG2	1:3:255:LYS:HD2	1.79	0.64
1:5:99:ASN:HD21	1:5:108:LEU:H	1.45	0.64
1:1:284:ARG:HG2	1:1:286:PHE:CE1	2.33	0.64
1:3:98:ILE:HD13	1:3:292:LYS:HG2	1.79	0.63
1:2:49:CYS:HB2	1:6:321:MET:CE	2.28	0.63
1:1:118:GLU:OE2	1:1:236:ILE:HG13	1.99	0.63
1:4:235:HIS:CD2	1:5:223:THR:HB	2.33	0.63
1:2:32:ILE:HD11	1:2:35:LEU:HD12	1.81	0.63
1:6:98:ILE:CD1	1:6:292:LYS:HG2	2.29	0.63
1:1:18:LYS:H	1:1:18:LYS:HD2	1.63	0.63
1:3:120:ILE:HB	1:3:283:PRO:HG2	1.81	0.63
1:1:184:VAL:HG21	1:5:60:GLU:O	1.98	0.63
1:4:243:VAL:HG12	1:4:245:LEU:H	1.63	0.62
1:2:308:LEU:O	1:2:312:ARG:HB2	1.98	0.62
1:3:256:ALA:O	1:3:258:SER:N	2.31	0.62
1:1:309:ILE:HD11	1:5:30:GLY:HA2	1.80	0.62
1:2:86:PRO:O	1:2:205:VAL:HG22	2.00	0.62
1:4:94:PRO:C	1:4:95:LEU:HD23	2.19	0.62
1:2:127:ASN:HD22	1:2:129:HIS:H	1.46	0.62
1:4:82:LYS:HD2	1:4:176:THR:HG22	1.82	0.62
1:1:73:LYS:HB2	1:5:129:HIS:O	1.98	0.62
1:3:35:LEU:HD13	1:3:96:PRO:HD3	1.80	0.62
1:4:90:VAL:HG22	1:4:91:ALA:N	2.15	0.62
1:4:130:SER:O	1:4:132:THR:N	2.32	0.62
1:3:32:ILE:HD11	1:3:35:LEU:HD12	1.82	0.62
1:5:150:HIS:HA	1:5:264:VAL:O	2.00	0.62
1:2:256:ALA:O	1:2:258:SER:N	2.32	0.62
1:6:127:ASN:ND2	1:6:129:HIS:H	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:151:PHE:CE2	1:1:220:TYR:HB2	2.32	0.62
1:3:342:GLY:O	1:3:344:PRO:HD3	2.00	0.62
1:4:93:ILE:HB	1:4:259:LEU:HB3	1.82	0.62
1:6:127:ASN:C	1:6:127:ASN:HD22	2.03	0.61
1:1:63:LYS:HB2	1:2:184:VAL:HG12	1.81	0.61
1:1:189:MET:HG2	1:5:50:PHE:CE2	2.35	0.61
1:1:288:ILE:N	1:1:288:ILE:HD12	2.15	0.61
1:5:301:ILE:N	1:5:301:ILE:HD12	2.15	0.61
1:4:125:MET:HB3	1:4:144:ILE:HD12	1.80	0.61
1:6:127:ASN:HD22	1:6:129:HIS:H	1.46	0.61
1:5:227:GLY:HA3	1:5:230:VAL:HG13	1.81	0.61
1:4:94:PRO:O	1:4:95:LEU:HD23	2.01	0.61
1:2:43:SER:HB2	1:6:334:TYR:O	1.99	0.61
1:3:237:THR:HG22	1:3:238:ASN:N	2.15	0.61
1:5:95:LEU:HD12	1:5:110:TRP:CD1	2.35	0.61
1:6:107:ILE:HG22	1:6:108:LEU:N	2.15	0.61
1:4:172:TYR:CG	1:4:178:THR:HG21	2.35	0.61
1:6:114:THR:HG23	1:6:241:THR:HG23	1.83	0.61
1:2:305:LEU:HD23	1:2:305:LEU:N	2.15	0.61
1:1:157:GLU:HG2	1:1:255:LYS:HD3	1.82	0.61
1:2:300:PRO:O	1:2:304:LEU:HG	2.01	0.61
1:3:168:TYR:CE1	1:3:169:ARG:HD2	2.35	0.60
1:4:58:PRO:HG2	1:4:62:GLN:HB2	1.82	0.60
1:6:165:LEU:O	1:6:187:GLN:HA	2.01	0.60
1:5:237:THR:CG2	1:5:239:THR:OG1	2.49	0.60
1:1:188:GLN:HG3	1:1:189:MET:N	2.16	0.60
1:4:99:ASN:ND2	1:4:108:LEU:N	2.49	0.60
1:4:112:ALA:HA	1:4:290:LEU:HD23	1.82	0.60
1:3:125:MET:HE1	1:4:224:TYR:CE2	2.30	0.60
1:1:172:TYR:HB3	1:1:178:THR:HG21	1.83	0.60
1:5:178:THR:HB	1:5:179:PRO:HD2	1.83	0.60
1:5:168:TYR:HB2	1:5:182:ALA:HB1	1.83	0.60
1:3:133:GLN:HA	1:3:273:THR:HA	1.83	0.60
1:6:99:ASN:HD21	1:6:107:ILE:CG2	2.14	0.60
1:2:214:LYS:O	1:2:216:GLU:N	2.35	0.60
1:2:99:ASN:HA	1:2:102:LEU:HB2	1.82	0.60
1:2:28:ILE:HD13	1:2:34:VAL:HG13	1.82	0.60
1:6:98:ILE:CG2	1:6:108:LEU:HB3	2.31	0.60
1:4:118:GLU:CD	1:4:236:ILE:HG13	2.21	0.60
1:2:94:PRO:O	1:2:95:LEU:HD23	2.02	0.60
1:1:132:THR:O	1:2:72:GLU:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:152:PHE:HA	1:4:263:ALA:HA	1.83	0.60
1:2:237:THR:HG23	1:3:220:TYR:O	2.01	0.60
1:1:131:GLY:HA3	1:2:75:PHE:CE1	2.37	0.60
1:3:237:THR:CG2	1:3:239:THR:H	2.11	0.60
1:2:205:VAL:HG11	1:2:264:VAL:HG11	1.84	0.60
1:5:300:PRO:HD2	1:5:303:PHE:HB3	1.83	0.60
1:4:334:TYR:CD1	1:4:334:TYR:N	2.69	0.60
1:5:177:VAL:HG11	1:5:203:TYR:CE2	2.36	0.60
1:4:237:THR:HG21	1:4:239:THR:OG1	2.01	0.59
1:4:32:ILE:O	1:4:35:LEU:HB2	2.02	0.59
1:5:55:MET:CE	1:5:279:TRP:HB3	2.31	0.59
1:4:199:LYS:HG3	1:4:202:ALA:HB2	1.84	0.59
1:3:61:HIS:HD2	1:4:168:TYR:OH	1.85	0.59
1:5:32:ILE:CD1	1:5:35:LEU:HD12	2.31	0.59
1:4:28:ILE:HG12	1:4:34:VAL:CG1	2.32	0.59
1:5:165:LEU:CD2	1:5:179:PRO:HG3	2.33	0.59
1:6:33:GLU:HG2	1:6:34:VAL:N	2.17	0.59
1:1:298:PRO:CG	1:1:299:TYR:CE1	2.83	0.59
1:6:132:THR:HG23	1:6:141:GLY:HA3	1.84	0.59
1:3:82:LYS:HD3	1:3:175:GLN:HB2	1.84	0.59
1:4:82:LYS:HD3	1:4:175:GLN:HB2	1.84	0.59
1:1:125:MET:HE2	1:2:224:TYR:CE2	2.38	0.59
1:1:28:ILE:HG12	1:1:34:VAL:CG1	2.33	0.59
1:5:288:ILE:N	1:5:288:ILE:HD12	2.17	0.59
1:5:111:GLU:OE1	1:5:293:ARG:NH1	2.35	0.59
1:6:112:ALA:HB3	1:6:252:PRO:HD2	1.83	0.59
1:2:123:THR:HB	1:3:205:VAL:O	2.03	0.59
1:1:65:LEU:HD22	1:1:278:GLN:HG3	1.84	0.59
1:2:80:PRO:HD2	1:2:171:LYS:O	2.03	0.58
1:2:44:PHE:HB2	1:2:290:LEU:O	2.03	0.58
1:1:32:ILE:O	1:1:35:LEU:HB2	2.03	0.58
1:5:163:GLY:O	1:5:164:VAL:HG23	2.03	0.58
1:1:326:SER:OG	1:1:328:VAL:HG13	2.03	0.58
1:1:243:VAL:HG12	1:1:245:LEU:N	2.18	0.58
1:3:342:GLY:CA	1:6:109:MET:HE1	2.34	0.58
1:2:111:GLU:OE2	1:2:250:VAL:HA	2.03	0.58
1:3:165:LEU:O	1:3:187:GLN:HA	2.04	0.58
1:2:227:GLY:HA3	1:2:230:VAL:HG13	1.84	0.58
1:6:28:ILE:CD1	1:6:34:VAL:HG13	2.33	0.58
1:1:162:GLN:HE21	1:1:194:LYS:NZ	2.01	0.58
1:4:237:THR:HG22	1:4:239:THR:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:301:ILE:H	1:3:301:ILE:HD13	1.69	0.58
1:1:99:ASN:ND2	1:1:107:ILE:HG23	2.18	0.58
1:4:125:MET:HE2	1:5:224:TYR:CE2	2.38	0.58
1:1:285:TYR:HE2	1:2:213:SER:HA	1.69	0.58
1:3:284:ARG:HG2	1:3:286:PHE:CE1	2.39	0.58
1:3:285:TYR:CE2	1:4:212:PRO:HB2	2.39	0.58
1:5:286:PHE:HB3	1:5:288:ILE:HD11	1.85	0.57
1:4:107:ILE:HG22	1:4:108:LEU:H	1.68	0.57
1:5:113:VAL:HG13	1:5:245:LEU:HD21	1.85	0.57
1:5:221:PHE:N	1:5:221:PHE:CD1	2.70	0.57
1:1:93:ILE:HG22	1:1:95:LEU:HD21	1.85	0.57
1:1:76:THR:O	1:1:171:LYS:HE3	2.03	0.57
1:5:245:LEU:N	1:5:245:LEU:CD2	2.67	0.57
1:5:65:LEU:HB3	1:5:278:GLN:HE21	1.68	0.57
1:4:298:PRO:HG2	1:4:299:TYR:H	1.68	0.57
1:6:301:ILE:O	1:6:304:LEU:HB3	2.04	0.57
1:1:270:PHE:O	1:1:277:GLN:HA	2.05	0.57
1:4:120:ILE:HD11	1:4:285:TYR:HB2	1.85	0.57
1:5:270:PHE:CD1	1:5:271:THR:N	2.68	0.57
1:5:343:ASP:O	1:5:346:MET:HB3	2.05	0.57
1:2:27:VAL:HG12	1:2:28:ILE:HG22	1.86	0.57
1:1:21:VAL:HG21	1:2:293:ARG:HH21	1.70	0.57
1:4:109:MET:SD	1:4:255:LYS:HA	2.45	0.57
1:3:221:PHE:CD1	1:3:221:PHE:N	2.73	0.57
1:5:95:LEU:HD23	1:5:95:LEU:N	2.20	0.57
1:1:94:PRO:C	1:1:95:LEU:HD23	2.25	0.57
1:4:320:PRO:O	1:4:327:GLN:HG3	2.05	0.57
1:6:112:ALA:O	1:6:251:GLY:HA3	2.05	0.56
1:4:259:LEU:HD12	1:4:260:TYR:H	1.70	0.56
1:2:32:ILE:O	1:2:35:LEU:HB2	2.05	0.56
1:5:303:PHE:CE1	1:5:307:ASP:HB2	2.40	0.56
1:3:304:LEU:HA	1:3:307:ASP:HB3	1.86	0.56
1:2:231:PRO:HB2	1:3:226:GLY:O	2.05	0.56
1:5:106:ASN:O	1:5:107:ILE:HD13	2.05	0.56
1:5:133:GLN:O	1:5:141:GLY:HA2	2.05	0.56
1:1:277:GLN:HE21	1:5:139:GLY:CA	2.18	0.56
1:2:50:PHE:CD1	1:2:50:PHE:C	2.78	0.56
1:2:45:THR:CG2	1:6:333:VAL:HG22	2.30	0.56
1:1:273:THR:HG23	1:2:72:GLU:CG	2.36	0.56
1:1:93:ILE:HG22	1:1:95:LEU:CD2	2.36	0.56
1:1:270:PHE:HD1	1:1:271:THR:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:339:GLU:O	1:5:341:PRO:HD3	2.05	0.56
1:1:190:ASN:O	1:1:192:ASP:N	2.39	0.56
1:2:26:LEU:HD12	1:6:333:VAL:O	2.04	0.56
1:1:79:SER:CB	1:1:171:LYS:HB2	2.23	0.56
1:4:107:ILE:HG22	1:4:108:LEU:N	2.21	0.56
1:1:269:LEU:HD21	1:1:279:TRP:CE3	2.40	0.56
1:1:60:GLU:O	1:2:184:VAL:HG11	2.06	0.56
1:1:86:PRO:HG2	1:1:279:TRP:CD1	2.41	0.56
1:5:130:SER:O	1:5:132:THR:N	2.38	0.56
1:1:190:ASN:C	1:1:190:ASN:HD22	2.09	0.56
1:1:285:TYR:CD1	1:1:286:PHE:N	2.74	0.56
1:6:55:MET:CE	1:6:86:PRO:HB3	2.36	0.56
1:2:307:ASP:O	1:2:311:ARG:HB3	2.06	0.56
1:2:55:MET:HE3	1:2:266:ILE:HG13	1.87	0.56
1:6:108:LEU:HD23	1:6:294:SER:HA	1.88	0.56
1:4:259:LEU:HD12	1:4:260:TYR:N	2.21	0.56
1:3:131:GLY:HA3	1:4:75:PHE:CE1	2.41	0.56
1:5:301:ILE:CD1	1:5:302:SER:H	2.19	0.56
1:2:163:GLY:O	1:2:164:VAL:HG23	2.05	0.56
1:4:99:ASN:HD22	1:4:108:LEU:N	2.03	0.55
1:4:150:HIS:CE1	1:4:267:CYS:HA	2.41	0.55
1:3:143:PRO:HG2	1:3:145:GLN:NE2	2.21	0.55
1:5:133:GLN:HG3	1:5:134:LYS:H	1.71	0.55
1:3:111:GLU:OE2	1:3:250:VAL:HA	2.07	0.55
1:6:202:ALA:O	1:6:204:PRO:HD3	2.05	0.55
1:4:129:HIS:HD2	1:5:78:ASP:OD2	1.88	0.55
1:1:118:GLU:CD	1:1:236:ILE:HG13	2.26	0.55
1:5:211:ASP:OD2	1:5:214:LYS:HG2	2.07	0.55
1:5:172:TYR:CG	1:5:178:THR:HG21	2.41	0.55
1:5:286:PHE:HB3	1:5:288:ILE:CD1	2.35	0.55
1:1:120:ILE:N	1:1:120:ILE:HD12	2.21	0.55
1:4:137:GLU:CD	1:4:137:GLU:N	2.56	0.55
1:3:285:TYR:CD2	1:4:212:PRO:HB2	2.42	0.55
1:6:55:MET:HE2	1:6:86:PRO:HB3	1.88	0.55
1:2:99:ASN:HD21	1:2:108:LEU:H	1.53	0.55
1:2:231:PRO:O	1:2:231:PRO:HG2	2.06	0.55
1:1:203:TYR:HD1	1:1:203:TYR:H	1.51	0.55
1:2:257:ASP:OD2	1:3:350:ILE:HD11	2.07	0.55
1:1:243:VAL:CG1	1:1:245:LEU:H	2.19	0.55
1:6:99:ASN:HD21	1:6:107:ILE:HA	1.70	0.55
1:3:140:ALA:N	1:4:277:GLN:HE21	1.98	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:168:TYR:HB2	1:1:182:ALA:HB1	1.88	0.55
1:2:32:ILE:O	1:2:32:ILE:HD12	2.07	0.55
1:4:186:SER:HA	1:4:190:ASN:HB2	1.89	0.55
1:1:139:GLY:HA2	1:2:277:GLN:HE21	1.71	0.55
1:5:321:MET:CE	1:5:327:GLN:HB2	2.37	0.55
1:1:238:ASN:HB3	1:2:220:TYR:CE2	2.42	0.55
1:2:102:LEU:HD21	1:2:108:LEU:HD12	1.88	0.55
1:2:90:VAL:HG22	1:2:91:ALA:N	2.21	0.55
1:2:109:MET:HE3	1:2:295:VAL:HG21	1.88	0.55
1:2:98:ILE:HD11	1:2:108:LEU:C	2.27	0.55
1:5:94:PRO:C	1:5:95:LEU:HD23	2.28	0.55
1:6:321:MET:CE	1:6:328:VAL:HG23	2.36	0.55
1:3:270:PHE:O	1:3:277:GLN:HA	2.07	0.55
1:4:70:ALA:HB2	1:4:84:GLN:HE22	1.70	0.55
1:3:162:GLN:NE2	1:3:194:LYS:HD3	2.22	0.54
1:5:190:ASN:C	1:5:190:ASN:HD22	2.09	0.54
1:3:303:PHE:CE2	1:6:350:ILE:HG12	2.42	0.54
1:6:350:ILE:HD13	1:6:350:ILE:O	2.07	0.54
1:5:284:ARG:HD3	1:5:286:PHE:CZ	2.43	0.54
1:1:282:LEU:HD23	1:1:283:PRO:HD2	1.89	0.54
1:2:284:ARG:HG2	1:2:286:PHE:CE1	2.42	0.54
1:5:118:GLU:OE2	1:5:236:ILE:HG13	2.07	0.54
1:4:340:LEU:HD12	1:4:341:PRO:N	2.23	0.54
1:3:299:TYR:N	1:3:300:PRO:HD2	2.22	0.54
1:6:243:VAL:HG12	1:6:245:LEU:N	2.23	0.54
1:3:199:LYS:HG3	1:3:202:ALA:HB2	1.89	0.54
1:4:73:LYS:HD3	1:4:78:ASP:HA	1.90	0.54
1:5:28:ILE:HG12	1:5:34:VAL:CG1	2.37	0.54
1:4:136:HIS:O	1:4:136:HIS:CD2	2.61	0.54
1:1:32:ILE:CD1	1:1:35:LEU:HD12	2.38	0.54
1:2:188:GLN:HG3	1:2:189:MET:N	2.23	0.54
1:1:73:LYS:HE2	1:1:79:SER:H	1.72	0.54
1:1:203:TYR:N	1:1:203:TYR:CD1	2.75	0.54
1:3:297:ASN:OD1	1:3:300:PRO:HD3	2.07	0.54
1:6:90:VAL:HG22	1:6:91:ALA:N	2.22	0.54
1:4:61:HIS:CD2	1:5:168:TYR:OH	2.60	0.53
1:1:73:LYS:CD	1:1:78:ASP:HA	2.29	0.53
1:4:111:GLU:OE1	1:4:293:ARG:NH1	2.41	0.53
1:3:285:TYR:CD1	1:3:285:TYR:C	2.81	0.53
1:1:212:PRO:HB2	1:5:285:TYR:CE2	2.43	0.53
1:2:132:THR:HG21	1:2:141:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:107:ILE:HG22	1:6:108:LEU:H	1.73	0.53
1:5:164:VAL:HG22	1:5:188:GLN:O	2.08	0.53
1:1:277:GLN:HE21	1:5:139:GLY:HA3	1.74	0.53
1:1:123:THR:O	1:1:126:LEU:HB2	2.09	0.53
1:6:100:GLU:O	1:6:101:ASP:HB3	2.08	0.53
1:4:22:GLN:OE1	1:4:22:GLN:HA	2.08	0.53
1:6:132:THR:HG23	1:6:141:GLY:HA2	1.88	0.53
1:4:98:ILE:HD11	1:4:110:TRP:CE2	2.44	0.53
1:6:229:ASN:N	1:6:229:ASN:ND2	2.55	0.53
1:6:120:ILE:HD11	1:6:285:TYR:HB2	1.90	0.53
1:2:359:ARG:CB	1:2:359:ARG:CZ	2.86	0.53
1:6:111:GLU:OE1	1:6:293:ARG:NH1	2.40	0.53
1:5:156:GLY:HA3	1:5:253:LEU:O	2.09	0.53
1:1:339:GLU:O	1:1:341:PRO:HD3	2.07	0.53
1:6:172:TYR:CG	1:6:178:THR:HG21	2.43	0.53
1:6:122:VAL:HG23	1:6:123:THR:N	2.23	0.53
1:5:168:TYR:CE1	1:5:169:ARG:HD2	2.43	0.53
1:6:114:THR:HG23	1:6:241:THR:CG2	2.38	0.53
1:1:23:VAL:HG23	1:1:24:PRO:HG2	1.91	0.53
1:1:139:GLY:CA	1:2:277:GLN:HE21	2.22	0.53
1:3:211:ASP:OD2	1:3:214:LYS:HG2	2.09	0.53
1:3:32:ILE:CD1	1:3:35:LEU:HD12	2.39	0.53
1:5:301:ILE:CD1	1:5:301:ILE:N	2.72	0.53
1:6:219:ARG:NH2	1:6:246:ASP:HB3	2.24	0.53
1:4:28:ILE:CD1	1:4:34:VAL:HG13	2.38	0.53
1:4:128:LEU:HD13	1:4:141:GLY:O	2.09	0.53
1:5:26:LEU:HD12	1:5:27:VAL:N	2.23	0.53
1:1:162:GLN:NE2	1:1:194:LYS:HD3	2.23	0.53
1:5:125:MET:HE3	1:5:144:ILE:HB	1.91	0.53
1:4:90:VAL:HG22	1:4:91:ALA:H	1.72	0.53
1:4:151:PHE:CD1	1:4:151:PHE:C	2.81	0.53
1:1:147:SER:O	1:1:268:GLY:HA2	2.09	0.53
1:5:237:THR:HG22	1:5:238:ASN:N	2.24	0.52
1:5:99:ASN:ND2	1:5:107:ILE:HA	2.24	0.52
1:6:229:ASN:N	1:6:229:ASN:HD22	2.07	0.52
1:4:214:LYS:O	1:4:216:GLU:N	2.42	0.52
1:1:88:TYR:HB3	1:1:197:LEU:HD21	1.91	0.52
1:1:98:ILE:O	1:1:98:ILE:HD12	2.10	0.52
1:6:297:ASN:OD1	1:6:298:PRO:HD2	2.08	0.52
1:3:111:GLU:OE1	1:3:293:ARG:NH1	2.42	0.52
1:2:298:PRO:HG2	1:2:299:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:130:SER:C	1:1:132:THR:H	2.13	0.52
1:5:266:ILE:N	1:5:266:ILE:HD12	2.24	0.52
1:2:112:ALA:HA	1:2:290:LEU:CD2	2.38	0.52
1:4:112:ALA:O	1:4:251:GLY:HA3	2.09	0.52
1:2:350:ILE:HG23	1:2:354:GLY:O	2.08	0.52
1:4:139:GLY:HA2	1:5:277:GLN:HG3	1.92	0.52
1:4:270:PHE:O	1:4:277:GLN:HA	2.10	0.52
1:3:285:TYR:CD1	1:3:286:PHE:N	2.78	0.52
1:3:32:ILE:O	1:3:35:LEU:HB2	2.09	0.52
1:5:321:MET:SD	1:5:328:VAL:HG23	2.50	0.52
1:1:115:VAL:HG22	1:1:117:THR:HG22	1.90	0.52
1:5:137:GLU:H	1:5:137:GLU:CD	2.13	0.52
1:2:284:ARG:HD3	1:2:286:PHE:CZ	2.45	0.52
1:5:125:MET:HE1	1:5:144:ILE:HB	1.92	0.52
1:1:237:THR:HG23	1:2:220:TYR:O	2.10	0.52
1:3:130:SER:O	1:3:132:THR:N	2.43	0.52
1:3:98:ILE:HD11	1:3:110:TRP:CD2	2.44	0.52
1:2:162:GLN:NE2	1:2:194:LYS:HD3	2.24	0.52
1:1:160:GLU:O	1:1:161:LEU:HD23	2.09	0.52
1:3:122:VAL:HG23	1:4:224:TYR:HB2	1.91	0.52
1:4:98:ILE:HG21	1:4:108:LEU:HB3	1.91	0.52
1:1:55:MET:HE3	1:1:279:TRP:HB3	1.91	0.52
1:5:99:ASN:ND2	1:5:108:LEU:H	2.08	0.52
1:3:48:GLU:OE2	1:4:213:SER:O	2.28	0.52
1:1:321:MET:SD	1:1:327:GLN:HB2	2.50	0.52
1:4:66:SER:O	1:4:278:GLN:NE2	2.42	0.52
1:1:237:THR:HG22	1:1:238:ASN:N	2.25	0.52
1:2:168:TYR:HD1	1:2:187:GLN:HE21	1.58	0.52
1:1:286:PHE:HB3	1:1:288:ILE:HD11	1.92	0.52
1:1:163:GLY:HA2	1:1:207:CYS:O	2.10	0.52
1:2:49:CYS:SG	1:2:286:PHE:HB2	2.50	0.52
1:2:111:GLU:OE1	1:2:293:ARG:NH1	2.43	0.52
1:3:151:PHE:CE2	1:3:220:TYR:HB2	2.45	0.52
1:5:237:THR:CG2	1:5:238:ASN:N	2.73	0.52
1:1:207:CYS:HB2	1:1:208:TRP:CD1	2.45	0.52
1:5:122:VAL:O	1:5:125:MET:HG3	2.10	0.52
1:5:326:SER:OG	1:5:328:VAL:HB	2.10	0.52
1:1:160:GLU:C	1:1:161:LEU:HD23	2.31	0.52
1:6:94:PRO:O	1:6:95:LEU:HD23	2.09	0.52
1:4:284:ARG:HG2	1:4:286:PHE:CE1	2.45	0.51
1:1:285:TYR:CE2	1:2:212:PRO:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:118:GLU:CD	1:5:236:ILE:HG13	2.31	0.51
1:5:158:PRO:HB2	1:5:196:VAL:CG2	2.39	0.51
1:1:153:ALA:HA	1:1:219:ARG:O	2.10	0.51
1:3:150:HIS:CE1	1:3:267:CYS:HA	2.45	0.51
1:4:301:ILE:H	1:4:301:ILE:CD1	2.23	0.51
1:2:360:MET:HG3	1:2:361:GLN:H	1.74	0.51
1:3:61:HIS:HB3	1:4:169:ARG:NH1	2.24	0.51
1:4:293:ARG:HD2	1:4:294:SER:H	1.76	0.51
1:5:114:THR:N	1:5:244:LEU:HD12	2.25	0.51
1:1:310:ASN:OD1	1:1:311:ARG:HB2	2.10	0.51
1:2:162:GLN:HE21	1:2:194:LYS:NZ	2.09	0.51
1:1:241:THR:HG22	1:1:242:THR:N	2.26	0.51
1:3:320:PRO:HD2	1:3:327:GLN:NE2	2.26	0.51
1:4:298:PRO:HG2	1:4:299:TYR:N	2.25	0.51
1:6:57:ASN:OD1	1:6:63:LYS:HA	2.11	0.51
1:4:99:ASN:ND2	1:4:108:LEU:H	2.06	0.51
1:2:188:GLN:HG3	1:2:189:MET:H	1.76	0.51
1:4:48:GLU:HA	1:4:286:PHE:O	2.11	0.51
1:5:288:ILE:HG22	1:5:289:THR:N	2.25	0.51
1:5:133:GLN:HG3	1:5:134:LYS:N	2.26	0.51
1:3:347:ILE:HB	1:6:299:TYR:CZ	2.45	0.51
1:2:314:GLN:HA	1:2:314:GLN:OE1	2.10	0.51
1:4:145:GLN:HE22	1:5:228:GLU:HB2	1.76	0.51
1:5:115:VAL:HG22	1:5:117:THR:HG22	1.92	0.51
1:3:107:ILE:O	1:3:108:LEU:HD23	2.11	0.51
1:5:108:LEU:HD23	1:5:294:SER:HA	1.92	0.51
1:5:311:ARG:HH11	1:5:311:ARG:HG2	1.74	0.51
1:6:237:THR:HG22	1:6:238:ASN:N	2.24	0.51
1:1:237:THR:CG2	1:1:239:THR:OG1	2.58	0.51
1:3:55:MET:CE	1:3:266:ILE:HG13	2.40	0.51
1:4:301:ILE:H	1:4:301:ILE:HD13	1.75	0.51
1:2:87:CYS:HA	1:2:204:PRO:HA	1.91	0.51
1:6:284:ARG:HD3	1:6:286:PHE:CZ	2.45	0.51
1:2:237:THR:HG21	1:2:239:THR:OG1	2.11	0.51
1:6:165:LEU:N	1:6:165:LEU:CD2	2.72	0.51
1:4:98:ILE:HD11	1:4:110:TRP:CD2	2.46	0.51
1:1:136:HIS:CE1	1:2:277:GLN:NE2	2.79	0.51
1:2:281:GLY:O	1:2:282:LEU:HD23	2.11	0.51
1:5:53:PRO:HD3	1:5:283:PRO:HA	1.92	0.51
1:1:90:VAL:HG22	1:1:91:ALA:H	1.74	0.51
1:4:245:LEU:HD23	1:4:245:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:140:ALA:H	1:3:277:GLN:NE2	2.09	0.51
1:2:185:ASP:O	1:2:190:ASN:HB2	2.09	0.51
1:1:66:SER:HB3	1:1:279:TRP:HB2	1.93	0.51
1:1:310:ASN:CG	1:1:311:ARG:N	2.64	0.51
1:1:209:VAL:CG1	1:5:121:GLY:HA2	2.38	0.51
1:3:48:GLU:HG2	1:3:285:TYR:OH	2.11	0.51
1:4:266:ILE:N	1:4:266:ILE:HD12	2.25	0.51
1:6:23:VAL:HB	1:6:24:PRO:HD2	1.92	0.51
1:1:351:ASP:OD1	1:1:354:GLY:N	2.44	0.51
1:1:107:ILE:HG22	1:1:108:LEU:N	2.26	0.50
1:4:205:VAL:HG11	1:4:264:VAL:HG11	1.92	0.50
1:1:223:THR:HA	1:5:234:LEU:O	2.11	0.50
1:3:90:VAL:HG23	1:3:262:SER:HB3	1.91	0.50
1:3:243:VAL:HG12	1:3:244:LEU:N	2.26	0.50
1:4:121:GLY:CA	1:5:209:VAL:HG11	2.33	0.50
1:5:133:GLN:CG	1:5:134:LYS:N	2.75	0.50
1:4:55:MET:CE	1:4:266:ILE:HA	2.42	0.50
1:1:130:SER:O	1:1:132:THR:N	2.45	0.50
1:3:94:PRO:C	1:3:95:LEU:HD23	2.32	0.50
1:5:64:GLY:O	1:5:65:LEU:HG	2.12	0.50
1:5:117:THR:HB	1:5:285:TYR:O	2.12	0.50
1:3:293:ARG:HD2	1:3:294:SER:H	1.76	0.50
1:4:188:GLN:HG3	1:4:189:MET:N	2.26	0.50
1:1:229:ASN:ND2	1:1:229:ASN:N	2.60	0.50
1:4:27:VAL:HG12	1:4:28:ILE:CG2	2.22	0.50
1:5:184:VAL:O	1:5:187:GLN:HB2	2.12	0.50
1:2:221:PHE:CD1	1:2:221:PHE:N	2.79	0.50
1:3:128:LEU:O	1:3:132:THR:HG21	2.11	0.50
1:3:340:LEU:HD12	1:3:341:PRO:CD	2.40	0.50
1:3:69:LEU:HD11	1:3:279:TRP:CD1	2.46	0.50
1:3:190:ASN:O	1:3:192:ASP:N	2.45	0.50
1:3:115:VAL:HA	1:3:287:LYS:O	2.11	0.50
1:3:81:ASP:O	1:3:84:GLN:HG3	2.12	0.50
1:4:28:ILE:HG12	1:4:34:VAL:HG11	1.93	0.50
1:1:229:ASN:HD22	1:1:229:ASN:N	2.09	0.50
1:4:63:LYS:HD2	1:5:184:VAL:HB	1.94	0.50
1:5:49:CYS:SG	1:5:50:PHE:N	2.85	0.50
1:2:55:MET:CE	1:2:266:ILE:HA	2.40	0.50
1:6:175:GLN:HA	1:6:175:GLN:NE2	2.24	0.50
1:4:79:SER:HB2	1:4:171:LYS:HB2	1.93	0.50
1:3:220:TYR:C	1:3:221:PHE:CG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:66:SER:O	1:1:278:GLN:NE2	2.45	0.49
1:1:120:ILE:HD11	1:1:285:TYR:CB	2.40	0.49
1:2:69:LEU:HG	1:2:278:GLN:HA	1.93	0.49
1:2:167:ASN:ND2	1:2:170:THR:OG1	2.45	0.49
1:2:272:ASN:HD22	1:2:276:THR:HB	1.77	0.49
1:3:178:THR:HB	1:3:179:PRO:HD2	1.94	0.49
1:3:296:LYS:HD3	1:6:339:GLU:HB2	1.93	0.49
1:3:156:GLY:HA3	1:3:253:LEU:O	2.12	0.49
1:3:138:ASN:O	1:4:276:THR:HA	2.12	0.49
1:2:351:ASP:N	1:2:351:ASP:OD1	2.45	0.49
1:2:180:LYS:O	1:2:181:ASN:HB2	2.12	0.49
1:6:285:TYR:CD1	1:6:285:TYR:C	2.86	0.49
1:4:93:ILE:HG22	1:4:95:LEU:CD2	2.42	0.49
1:4:128:LEU:O	1:4:132:THR:HG21	2.12	0.49
1:4:139:GLY:CA	1:5:277:GLN:HE21	2.25	0.49
1:2:229:ASN:N	1:2:229:ASN:ND2	2.59	0.49
1:2:237:THR:HG22	1:2:238:ASN:N	2.26	0.49
1:5:88:TYR:CD1	1:5:205:VAL:HG12	2.47	0.49
1:5:133:GLN:HA	1:5:273:THR:HA	1.95	0.49
1:6:332:ARG:HD3	1:6:334:TYR:OH	2.13	0.49
1:2:57:ASN:OD1	1:2:63:LYS:HA	2.12	0.49
1:6:151:PHE:CD1	1:6:151:PHE:C	2.84	0.49
1:2:82:LYS:HD2	1:2:176:THR:HG22	1.94	0.49
1:2:137:GLU:CD	1:2:137:GLU:H	2.16	0.49
1:3:220:TYR:C	1:3:221:PHE:CD1	2.85	0.49
1:2:304:LEU:HA	1:6:308:LEU:HD11	1.94	0.49
1:5:162:GLN:NE2	1:5:194:LYS:HD3	2.28	0.49
1:3:23:VAL:HG13	1:3:24:PRO:HD2	1.94	0.49
1:1:237:THR:HG22	1:1:239:THR:N	2.13	0.49
1:1:60:GLU:O	1:2:184:VAL:CG1	2.61	0.49
1:4:28:ILE:HG12	1:4:34:VAL:HG13	1.95	0.49
1:1:125:MET:HE2	1:2:224:TYR:HE2	1.75	0.49
1:2:248:GLN:HB2	1:2:250:VAL:HG13	1.95	0.49
1:5:199:LYS:CG	1:5:202:ALA:HB2	2.34	0.49
1:6:28:ILE:CG1	1:6:29:LYS:N	2.75	0.49
1:4:305:LEU:O	1:4:309:ILE:HG13	2.13	0.49
1:2:203:TYR:N	1:2:203:TYR:CD1	2.81	0.49
1:2:98:ILE:HD11	1:2:109:MET:N	2.27	0.49
1:1:120:ILE:H	1:1:120:ILE:HD12	1.78	0.49
1:5:86:PRO:CG	1:5:279:TRP:CD1	2.96	0.49
1:1:68:SER:HB3	1:1:276:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:98:ILE:HD11	1:5:110:TRP:CZ2	2.48	0.48
1:3:115:VAL:HG13	1:3:242:THR:HB	1.94	0.48
1:1:348:ARG:HA	1:1:356:THR:O	2.13	0.48
1:2:339:GLU:O	1:2:341:PRO:HD3	2.13	0.48
1:6:237:THR:CG2	1:6:239:THR:OG1	2.60	0.48
1:3:237:THR:CG2	1:3:239:THR:OG1	2.61	0.48
1:5:151:PHE:CG	1:5:152:PHE:N	2.80	0.48
1:2:353:PHE:N	1:2:353:PHE:CD1	2.80	0.48
1:5:113:VAL:C	1:5:244:LEU:HD12	2.33	0.48
1:2:80:PRO:O	1:2:173:PRO:HD3	2.13	0.48
1:6:55:MET:SD	1:6:281:GLY:HA3	2.53	0.48
1:4:84:GLN:O	1:4:86:PRO:HD3	2.13	0.48
1:1:23:VAL:HG23	1:1:24:PRO:CD	2.43	0.48
1:6:151:PHE:CG	1:6:152:PHE:N	2.80	0.48
1:2:352:GLU:C	1:2:353:PHE:CG	2.86	0.48
1:3:321:MET:SD	1:3:328:VAL:HG23	2.53	0.48
1:1:109:MET:CE	1:1:295:VAL:HG21	2.43	0.48
1:3:88:TYR:HB3	1:3:197:LEU:HD21	1.95	0.48
1:5:109:MET:SD	1:5:255:LYS:HA	2.54	0.48
1:1:87:CYS:HB3	1:1:203:TYR:O	2.13	0.48
1:6:152:PHE:CD1	1:6:152:PHE:C	2.87	0.48
1:5:92:ARG:O	1:5:94:PRO:HD3	2.13	0.48
1:2:93:ILE:HB	1:2:259:LEU:HB3	1.95	0.48
1:4:211:ASP:HA	1:4:212:PRO:HD2	1.58	0.48
1:1:51:LEU:HD11	1:1:261:VAL:HG12	1.96	0.48
1:1:214:LYS:HB3	1:1:214:LYS:HE2	1.72	0.48
1:3:98:ILE:HD11	1:3:110:TRP:CZ2	2.49	0.48
1:4:109:MET:CE	1:4:295:VAL:HG21	2.42	0.48
1:2:85:LEU:HD23	1:2:85:LEU:N	2.26	0.48
1:2:133:GLN:HA	1:2:273:THR:HA	1.95	0.48
1:1:35:LEU:HD23	1:1:35:LEU:HA	1.57	0.48
1:2:93:ILE:HG12	1:6:321:MET:HG3	1.96	0.48
1:3:297:ASN:CG	1:3:300:PRO:HD3	2.34	0.48
1:2:204:PRO:HG2	1:2:207:CYS:SG	2.54	0.48
1:5:280:LYS:HG3	1:5:281:GLY:N	2.28	0.48
1:2:172:TYR:CB	1:2:178:THR:HG21	2.43	0.48
1:1:69:LEU:HD11	1:1:279:TRP:CD1	2.48	0.48
1:6:98:ILE:HD11	1:6:110:TRP:CE2	2.49	0.48
1:1:40:GLY:HA3	1:5:15:LYS:HE2	1.95	0.48
1:5:256:ALA:O	1:5:258:SER:N	2.47	0.48
1:2:118:GLU:CD	1:2:236:ILE:HG13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:137:GLU:H	1:6:137:GLU:CD	2.17	0.48
1:6:190:ASN:C	1:6:190:ASN:HD22	2.16	0.48
1:2:322:ILE:CG2	1:2:323:GLY:N	2.75	0.48
1:3:302:SER:HA	1:3:305:LEU:HB2	1.95	0.48
1:5:28:ILE:HG12	1:5:34:VAL:HG13	1.96	0.48
1:5:300:PRO:C	1:5:301:ILE:HD12	2.33	0.48
1:4:80:PRO:O	1:4:173:PRO:HG3	2.14	0.48
1:3:241:THR:HG22	1:3:242:THR:N	2.28	0.48
1:5:90:VAL:HG22	1:5:91:ALA:H	1.78	0.48
1:6:130:SER:O	1:6:132:THR:N	2.48	0.47
1:1:358:THR:OG1	1:1:359:ARG:N	2.46	0.47
1:1:229:ASN:HD22	1:1:229:ASN:H	1.61	0.47
1:4:15:LYS:HA	1:5:41:VAL:HB	1.96	0.47
1:6:237:THR:CG2	1:6:238:ASN:N	2.76	0.47
1:5:128:LEU:HD21	1:5:143:PRO:HB3	1.94	0.47
1:3:35:LEU:HD23	1:3:35:LEU:HA	1.67	0.47
1:5:162:GLN:HA	1:5:193:HIS:O	2.14	0.47
1:1:295:VAL:C	1:5:20:PRO:HG3	2.34	0.47
1:4:52:ASN:OD1	1:5:189:MET:HB2	2.14	0.47
1:4:300:PRO:O	1:4:303:PHE:HB3	2.14	0.47
1:1:288:ILE:HG22	1:1:289:THR:N	2.28	0.47
1:3:298:PRO:C	1:3:300:PRO:HD2	2.35	0.47
1:6:158:PRO:HG3	1:6:260:TYR:CE2	2.49	0.47
1:1:334:TYR:N	1:1:334:TYR:CD1	2.81	0.47
1:1:15:LYS:HA	1:1:15:LYS:HD3	1.77	0.47
1:6:118:GLU:OE2	1:6:236:ILE:HG13	2.14	0.47
1:4:107:ILE:O	1:4:108:LEU:HD23	2.14	0.47
1:1:151:PHE:CG	1:1:152:PHE:N	2.83	0.47
1:1:90:VAL:CG2	1:1:91:ALA:N	2.76	0.47
1:3:308:LEU:HG	1:3:309:ILE:N	2.30	0.47
1:6:86:PRO:O	1:6:205:VAL:HG22	2.15	0.47
1:1:127:ASN:HD22	1:1:129:HIS:H	1.61	0.47
1:1:17:PRO:HG3	1:2:106:ASN:HB3	1.96	0.47
1:4:165:LEU:CD1	1:4:168:TYR:HA	2.36	0.47
1:5:93:ILE:HA	1:5:94:PRO:HD3	1.43	0.47
1:5:162:GLN:HE21	1:5:194:LYS:NZ	2.11	0.47
1:2:90:VAL:HG22	1:2:91:ALA:H	1.79	0.47
1:3:180:LYS:O	1:3:181:ASN:HB2	2.13	0.47
1:3:133:GLN:CG	1:3:134:LYS:N	2.77	0.47
1:1:211:ASP:HA	1:1:212:PRO:HD2	1.43	0.47
1:2:98:ILE:CD1	1:2:108:LEU:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:237:THR:CG2	1:4:239:THR:OG1	2.61	0.47
1:1:165:LEU:HD11	1:1:168:TYR:HA	1.96	0.47
1:2:162:GLN:HB2	1:2:211:ASP:HB2	1.97	0.47
1:2:348:ARG:HA	1:2:356:THR:O	2.14	0.47
1:1:86:PRO:CG	1:1:279:TRP:CD1	2.98	0.47
1:5:95:LEU:CB	1:5:110:TRP:CD1	2.97	0.47
1:1:282:LEU:CD2	1:1:283:PRO:HD2	2.43	0.47
1:5:30:GLY:HA3	1:5:34:VAL:HG21	1.97	0.47
1:3:55:MET:HE3	1:3:266:ILE:HG13	1.95	0.47
1:3:148:ASN:HB2	1:3:266:ILE:O	2.14	0.47
1:1:138:ASN:O	1:2:276:THR:HA	2.14	0.47
1:5:351:ASP:CG	1:5:352:GLU:N	2.66	0.47
1:6:107:ILE:CD1	1:6:298:PRO:HD2	2.45	0.47
1:4:55:MET:HE3	1:4:266:ILE:HG13	1.96	0.47
1:1:199:LYS:O	1:1:202:ALA:HB3	2.15	0.47
1:5:90:VAL:HG22	1:5:91:ALA:N	2.30	0.47
1:4:201:ASN:C	1:4:201:ASN:HD22	2.18	0.47
1:5:74:GLN:OE1	1:5:74:GLN:HA	2.14	0.47
1:1:168:TYR:HD2	1:1:182:ALA:O	1.98	0.47
1:4:129:HIS:CD2	1:5:78:ASP:OD2	2.67	0.47
1:5:285:TYR:CE1	1:5:287:LYS:HB2	2.50	0.47
1:1:311:ARG:C	1:1:313:THR:H	2.16	0.47
1:5:220:TYR:C	1:5:221:PHE:CD1	2.89	0.47
1:2:129:HIS:O	1:2:129:HIS:CG	2.65	0.47
1:5:55:MET:HE1	1:5:266:ILE:HG13	1.97	0.47
1:6:90:VAL:HG22	1:6:91:ALA:H	1.79	0.47
1:1:28:ILE:CG1	1:1:29:LYS:N	2.78	0.47
1:6:26:LEU:HD11	1:6:28:ILE:O	2.15	0.47
1:1:286:PHE:HB3	1:1:288:ILE:CD1	2.45	0.47
1:6:241:THR:HG22	1:6:242:THR:N	2.28	0.47
1:5:211:ASP:HA	1:5:212:PRO:HD2	1.72	0.47
1:1:295:VAL:O	1:5:20:PRO:HG3	2.15	0.47
1:3:33:GLU:CD	1:3:33:GLU:H	2.18	0.47
1:3:126:LEU:HD21	1:4:224:TYR:HE1	1.80	0.46
1:4:108:LEU:HA	1:4:293:ARG:O	2.15	0.46
1:1:94:PRO:O	1:1:95:LEU:HD23	2.14	0.46
1:1:202:ALA:HB3	1:1:203:TYR:CD1	2.50	0.46
1:1:352:GLU:C	1:1:353:PHE:CG	2.88	0.46
1:1:305:LEU:HD22	1:1:305:LEU:H	1.80	0.46
1:2:15:LYS:HB2	1:3:41:VAL:HB	1.97	0.46
1:3:61:HIS:CD2	1:4:168:TYR:OH	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:151:PHE:CD1	1:5:151:PHE:C	2.88	0.46
1:4:112:ALA:HB3	1:4:252:PRO:HD2	1.97	0.46
1:2:84:GLN:C	1:2:85:LEU:HD23	2.36	0.46
1:4:128:LEU:HD21	1:4:143:PRO:HB3	1.97	0.46
1:5:48:GLU:HG2	1:5:285:TYR:OH	2.15	0.46
1:1:285:TYR:CD1	1:1:285:TYR:C	2.89	0.46
1:3:28:ILE:HG12	1:3:34:VAL:CG1	2.45	0.46
1:2:265:ASP:OD1	1:2:284:ARG:NH1	2.49	0.46
1:6:98:ILE:HG21	1:6:108:LEU:HB3	1.97	0.46
1:3:94:PRO:O	1:3:95:LEU:HD23	2.15	0.46
1:4:39:THR:HB	1:4:43:SER:HB3	1.97	0.46
1:5:138:ASN:OD1	1:5:138:ASN:N	2.49	0.46
1:5:269:LEU:HA	1:5:269:LEU:HD23	1.66	0.46
1:4:158:PRO:HB2	1:4:196:VAL:CG2	2.45	0.46
1:2:245:LEU:HD23	1:2:245:LEU:HA	1.67	0.46
1:5:132:THR:CG2	1:5:141:GLY:HA3	2.45	0.46
1:4:73:LYS:NZ	1:4:80:PRO:HA	2.30	0.46
1:3:319:GLN:HA	1:3:320:PRO:HD3	1.60	0.46
1:4:39:THR:HB	1:4:43:SER:CB	2.45	0.46
1:5:270:PHE:C	1:5:270:PHE:CD1	2.87	0.46
1:5:23:VAL:HB	1:5:24:PRO:CD	2.38	0.46
1:1:120:ILE:HB	1:1:283:PRO:HG2	1.98	0.46
1:3:227:GLY:HA3	1:3:230:VAL:CG1	2.41	0.46
1:1:273:THR:HG23	1:2:72:GLU:HG2	1.98	0.46
1:4:341:PRO:HA	1:4:343:ASP:OD1	2.15	0.46
1:4:180:LYS:HA	1:4:180:LYS:HD3	1.71	0.46
1:1:211:ASP:OD2	1:1:214:LYS:HG2	2.15	0.46
1:3:122:VAL:CG2	1:4:224:TYR:HB2	2.46	0.46
1:2:68:SER:HB3	1:2:276:THR:CG2	2.42	0.46
1:6:94:PRO:C	1:6:95:LEU:HD23	2.36	0.46
1:4:92:ARG:HD2	1:4:258:SER:HB3	1.97	0.46
1:2:125:MET:HE2	1:3:224:TYR:CE1	2.50	0.46
1:6:107:ILE:HD12	1:6:298:PRO:CD	2.45	0.46
1:3:339:GLU:O	1:3:341:PRO:HD3	2.16	0.46
1:2:35:LEU:HA	1:2:35:LEU:HD23	1.68	0.46
1:4:125:MET:HB3	1:4:125:MET:HE3	1.70	0.46
1:5:55:MET:O	1:5:66:SER:HA	2.16	0.46
1:3:308:LEU:HA	1:3:311:ARG:HD3	1.97	0.46
1:6:190:ASN:C	1:6:190:ASN:ND2	2.69	0.46
1:5:259:LEU:HD12	1:5:260:TYR:N	2.29	0.46
1:3:101:ASP:C	1:3:103:THR:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:116:LYS:HB2	1:4:287:LYS:HB3	1.97	0.46
1:3:135:THR:HG22	1:3:136:HIS:ND1	2.30	0.46
1:5:284:ARG:HB2	1:5:284:ARG:HH11	1.81	0.46
1:6:80:PRO:HD2	1:6:171:LYS:O	2.15	0.46
1:1:139:GLY:CA	1:2:277:GLN:NE2	2.79	0.46
1:2:115:VAL:HG22	1:2:116:LYS:N	2.31	0.46
1:2:23:VAL:O	1:6:337:THR:HA	2.16	0.46
1:2:15:LYS:HD3	1:3:41:VAL:CB	2.31	0.46
1:2:152:PHE:HA	1:2:263:ALA:HA	1.97	0.46
1:5:229:ASN:ND2	1:5:229:ASN:N	2.63	0.46
1:3:50:PHE:C	1:3:50:PHE:CD1	2.89	0.46
1:4:146:GLY:C	1:4:230:VAL:HG23	2.36	0.46
1:2:123:THR:HG1	1:3:209:VAL:HG12	1.80	0.46
1:1:84:GLN:C	1:1:85:LEU:HD23	2.36	0.46
1:6:163:GLY:HA2	1:6:207:CYS:O	2.15	0.46
1:1:285:TYR:HE2	1:2:213:SER:CA	2.29	0.45
1:2:211:ASP:OD2	1:2:214:LYS:HG2	2.16	0.45
1:5:55:MET:HE2	1:5:279:TRP:HB3	1.97	0.45
1:1:49:CYS:SG	1:1:50:PHE:N	2.88	0.45
1:3:151:PHE:CD1	1:3:151:PHE:C	2.90	0.45
1:3:26:LEU:HD12	1:3:27:VAL:N	2.31	0.45
1:6:55:MET:HA	1:6:55:MET:CE	2.45	0.45
1:2:313:THR:HG22	1:2:314:GLN:H	1.81	0.45
1:5:175:GLN:HA	1:5:175:GLN:HE21	1.81	0.45
1:4:270:PHE:C	1:4:270:PHE:CD1	2.90	0.45
1:1:69:LEU:HD11	1:1:279:TRP:NE1	2.32	0.45
1:4:152:PHE:CD1	1:4:153:ALA:N	2.84	0.45
1:6:233:VAL:O	1:6:234:LEU:HD23	2.16	0.45
1:3:203:TYR:HA	1:3:204:PRO:HD2	1.74	0.45
1:4:219:ARG:NH2	1:4:246:ASP:HB3	2.31	0.45
1:5:127:ASN:C	1:5:127:ASN:HD22	2.20	0.45
1:6:168:TYR:CE1	1:6:169:ARG:HD2	2.51	0.45
1:4:270:PHE:HD1	1:4:271:THR:N	2.14	0.45
1:5:30:GLY:HA3	1:5:34:VAL:CG2	2.47	0.45
1:5:304:LEU:HA	1:5:304:LEU:HD23	1.71	0.45
1:5:55:MET:HE2	1:5:279:TRP:CB	2.46	0.45
1:6:132:THR:O	1:6:273:THR:HG23	2.16	0.45
1:3:265:ASP:OD2	1:3:284:ARG:NH1	2.49	0.45
1:6:334:TYR:N	1:6:334:TYR:CD1	2.84	0.45
1:4:175:GLN:HA	1:4:175:GLN:HE21	1.82	0.45
1:6:122:VAL:CG2	1:6:123:THR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:17:PRO:CB	1:5:108:LEU:HD21	2.43	0.45
1:6:109:MET:HE1	1:6:295:VAL:HG21	1.99	0.45
1:5:284:ARG:CG	1:5:285:TYR:N	2.79	0.45
1:1:269:LEU:CD2	1:1:279:TRP:CE3	3.00	0.45
1:5:95:LEU:HB2	1:5:110:TRP:CD1	2.52	0.45
1:2:63:LYS:HB2	1:3:184:VAL:HG12	1.97	0.45
1:2:88:TYR:CE1	1:2:205:VAL:HA	2.51	0.45
1:5:300:PRO:O	1:5:303:PHE:N	2.49	0.45
1:2:340:LEU:HA	1:2:341:PRO:HD2	1.82	0.45
1:4:167:ASN:ND2	1:4:170:THR:OG1	2.50	0.45
1:2:219:ARG:NH2	1:2:246:ASP:HB3	2.31	0.45
1:2:156:GLY:HA3	1:2:253:LEU:O	2.15	0.45
1:5:270:PHE:C	1:5:270:PHE:HD1	2.19	0.45
1:6:28:ILE:HG12	1:6:34:VAL:HG11	1.97	0.45
1:1:310:ASN:HB3	1:5:28:ILE:HD11	1.99	0.45
1:5:30:GLY:CA	1:5:34:VAL:HG21	2.46	0.45
1:2:127:ASN:C	1:2:127:ASN:HD22	2.20	0.45
1:2:168:TYR:CE2	1:2:169:ARG:HG3	2.51	0.45
1:5:109:MET:HG3	1:5:295:VAL:HG21	1.99	0.45
1:1:285:TYR:CD2	1:2:212:PRO:HB2	2.52	0.45
1:3:293:ARG:HD2	1:3:294:SER:N	2.32	0.45
1:4:151:PHE:CG	1:4:152:PHE:N	2.84	0.45
1:2:151:PHE:CD1	1:2:151:PHE:C	2.90	0.45
1:4:17:PRO:HG3	1:5:106:ASN:HB3	1.99	0.45
1:1:33:GLU:O	1:1:35:LEU:N	2.50	0.45
1:6:107:ILE:HD12	1:6:298:PRO:HD2	1.98	0.45
1:6:108:LEU:HD23	1:6:108:LEU:HA	1.57	0.45
1:3:304:LEU:CA	1:3:307:ASP:HB3	2.47	0.45
1:4:81:ASP:HB2	1:4:84:GLN:HG3	1.99	0.45
1:5:190:ASN:O	1:5:192:ASP:N	2.50	0.45
1:2:179:PRO:HB3	1:2:193:HIS:CG	2.52	0.45
1:2:59:ASP:OD1	1:2:62:GLN:N	2.50	0.45
1:1:266:ILE:HD12	1:1:266:ILE:N	2.32	0.45
1:1:28:ILE:CD1	1:1:34:VAL:HG13	2.47	0.44
1:1:312:ARG:O	1:1:314:GLN:N	2.49	0.44
1:5:151:PHE:CD1	1:5:152:PHE:N	2.84	0.44
1:5:152:PHE:C	1:5:152:PHE:CD1	2.89	0.44
1:5:153:ALA:HB2	1:5:220:TYR:CB	2.47	0.44
1:3:172:TYR:CD2	1:3:178:THR:HG21	2.51	0.44
1:6:301:ILE:H	1:6:301:ILE:HD12	1.82	0.44
1:2:214:LYS:HB3	1:2:214:LYS:HE2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:140:ALA:H	1:3:277:GLN:HE21	1.64	0.44
1:3:114:THR:HG23	1:3:115:VAL:N	2.31	0.44
1:2:172:TYR:CG	1:2:178:THR:HG21	2.52	0.44
1:5:76:THR:O	1:5:171:LYS:HE3	2.17	0.44
1:1:73:LYS:HD3	1:1:77:ASP:O	2.17	0.44
1:2:23:VAL:HB	1:2:24:PRO:HD2	1.99	0.44
1:1:309:ILE:HG12	1:1:310:ASN:HD22	1.81	0.44
1:2:93:ILE:CG1	1:6:321:MET:HG3	2.48	0.44
1:4:35:LEU:HD23	1:4:35:LEU:HA	1.55	0.44
1:3:297:ASN:HA	1:3:298:PRO:HD2	1.83	0.44
1:3:127:ASN:ND2	1:3:129:HIS:CD2	2.85	0.44
1:4:65:LEU:HA	1:4:279:TRP:O	2.15	0.44
1:3:151:PHE:HE2	1:3:220:TYR:HB2	1.82	0.44
1:3:98:ILE:CG2	1:3:108:LEU:HB2	2.46	0.44
1:3:61:HIS:O	1:4:187:GLN:NE2	2.50	0.44
1:6:194:LYS:HD2	1:6:211:ASP:OD2	2.16	0.44
1:1:144:ILE:HD13	1:1:280:LYS:HB3	1.99	0.44
1:1:133:GLN:HA	1:1:273:THR:HA	1.99	0.44
1:3:319:GLN:NE2	1:3:327:GLN:OE1	2.50	0.44
1:4:180:LYS:O	1:4:181:ASN:HB2	2.17	0.44
1:3:203:TYR:CD1	1:3:203:TYR:N	2.85	0.44
1:1:148:ASN:HB2	1:1:266:ILE:O	2.17	0.44
1:5:305:LEU:HD12	1:5:309:ILE:HG13	1.99	0.44
1:1:79:SER:HA	1:1:171:LYS:O	2.17	0.44
1:4:162:GLN:HB2	1:4:211:ASP:HB2	1.98	0.44
1:3:80:PRO:O	1:3:173:PRO:CG	2.65	0.44
1:2:32:ILE:CD1	1:2:35:LEU:HD12	2.46	0.44
1:4:175:GLN:HA	1:4:175:GLN:NE2	2.32	0.44
1:5:321:MET:HE1	1:5:327:GLN:HB2	1.99	0.44
1:2:172:TYR:HB3	1:2:178:THR:HG21	1.99	0.44
1:5:322:ILE:HG23	1:5:323:GLY:N	2.33	0.44
1:5:165:LEU:HD23	1:5:179:PRO:HG3	2.00	0.44
1:4:133:GLN:HB2	1:4:272:ASN:O	2.17	0.44
1:1:309:ILE:HG22	1:1:312:ARG:HB2	2.00	0.44
1:6:157:GLU:OE2	1:6:255:LYS:HE3	2.17	0.44
1:2:220:TYR:C	1:2:221:PHE:CG	2.90	0.44
1:5:270:PHE:O	1:5:277:GLN:HA	2.18	0.44
1:5:131:GLY:O	1:5:273:THR:OG1	2.33	0.44
1:4:282:LEU:HA	1:4:282:LEU:HD23	1.73	0.44
1:4:238:ASN:HB3	1:5:220:TYR:CE2	2.53	0.44
1:3:120:ILE:H	1:3:120:ILE:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:227:GLY:HA3	1:6:230:VAL:CG1	2.46	0.44
1:3:194:LYS:HZ2	1:3:211:ASP:CG	2.21	0.44
1:6:288:ILE:HD12	1:6:288:ILE:N	2.32	0.44
1:6:50:PHE:C	1:6:50:PHE:CD1	2.91	0.44
1:1:28:ILE:HG13	1:1:29:LYS:N	2.31	0.44
1:5:120:ILE:N	1:5:120:ILE:HD12	2.32	0.44
1:5:162:GLN:OE1	1:5:163:GLY:O	2.35	0.44
1:1:219:ARG:NH2	1:1:246:ASP:HB3	2.32	0.44
1:2:18:LYS:HG3	1:2:18:LYS:H	1.53	0.44
1:4:329:GLU:O	1:4:330:GLU:HB2	2.18	0.44
1:1:26:LEU:HG	1:1:27:VAL:N	2.32	0.44
1:2:24:PRO:HA	1:6:336:ASP:O	2.18	0.44
1:1:146:GLY:C	1:1:230:VAL:HG22	2.38	0.44
1:6:321:MET:SD	1:6:327:GLN:HB2	2.58	0.44
1:3:342:GLY:HA3	1:6:109:MET:HE1	1.99	0.44
1:5:35:LEU:HD23	1:5:35:LEU:HA	1.70	0.44
1:2:127:ASN:ND2	1:2:129:HIS:H	2.15	0.44
1:6:88:TYR:CE1	1:6:205:VAL:HA	2.53	0.44
1:5:214:LYS:HB3	1:5:214:LYS:HE2	1.79	0.44
1:2:207:CYS:HB2	1:2:208:TRP:CD1	2.52	0.44
1:1:351:ASP:OD1	1:1:351:ASP:N	2.50	0.44
1:3:67:LYS:HG2	1:3:68:SER:N	2.33	0.44
1:6:168:TYR:HD1	1:6:187:GLN:HE21	1.65	0.43
1:6:99:ASN:HD21	1:6:107:ILE:CA	2.30	0.43
1:3:282:LEU:HA	1:3:282:LEU:HD23	1.73	0.43
1:2:132:THR:CG2	1:2:141:GLY:HA3	2.48	0.43
1:1:253:LEU:HD23	1:1:253:LEU:HA	1.41	0.43
1:5:146:GLY:O	1:5:230:VAL:HG22	2.18	0.43
1:4:305:LEU:HD11	1:4:309:ILE:HD11	2.00	0.43
1:6:231:PRO:HA	1:6:232:PRO:HD2	1.84	0.43
1:5:37:VAL:HG12	1:5:38:LYS:O	2.18	0.43
1:3:118:GLU:OE2	1:3:236:ILE:HG13	2.17	0.43
1:4:120:ILE:O	1:4:282:LEU:HD13	2.18	0.43
1:5:285:TYR:CD1	1:5:286:PHE:N	2.87	0.43
1:1:60:GLU:C	1:1:62:GLN:H	2.22	0.43
1:1:108:LEU:HA	1:1:108:LEU:HD23	1.82	0.43
1:1:288:ILE:N	1:1:288:ILE:CD1	2.81	0.43
1:4:237:THR:HG22	1:4:238:ASN:N	2.32	0.43
1:4:33:GLU:O	1:4:35:LEU:N	2.51	0.43
1:3:135:THR:O	1:3:136:HIS:HB3	2.18	0.43
1:4:50:PHE:O	1:4:51:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:57:ASN:OD1	1:4:63:LYS:HA	2.17	0.43
1:2:22:GLN:CG	1:6:337:THR:HB	2.30	0.43
1:5:199:LYS:HG3	1:5:202:ALA:CB	2.34	0.43
1:5:277:GLN:O	1:5:278:GLN:HB3	2.18	0.43
1:5:267:CYS:SG	1:5:282:LEU:HD12	2.58	0.43
1:5:237:THR:CG2	1:5:239:THR:H	2.23	0.43
1:5:227:GLY:HA3	1:5:230:VAL:CG1	2.47	0.43
1:2:338:GLU:CD	1:2:348:ARG:HH12	2.22	0.43
1:1:28:ILE:CG1	1:1:34:VAL:HG13	2.44	0.43
1:3:243:VAL:HG12	1:3:245:LEU:N	2.06	0.43
1:3:98:ILE:HG22	1:3:108:LEU:HB2	2.01	0.43
1:3:125:MET:CE	1:4:224:TYR:HE2	2.22	0.43
1:1:55:MET:CE	1:1:279:TRP:HB3	2.47	0.43
1:6:87:CYS:HA	1:6:204:PRO:HA	2.00	0.43
1:4:84:GLN:O	1:4:85:LEU:HD23	2.19	0.43
1:3:129:HIS:HD2	1:4:78:ASP:OD2	2.00	0.43
1:6:286:PHE:CD1	1:6:286:PHE:N	2.85	0.43
1:2:343:ASP:O	1:2:346:MET:HB3	2.18	0.43
1:2:270:PHE:CD1	1:2:270:PHE:C	2.91	0.43
1:4:284:ARG:HD3	1:4:286:PHE:CZ	2.53	0.43
1:6:33:GLU:CG	1:6:34:VAL:N	2.81	0.43
1:4:293:ARG:HD2	1:4:294:SER:N	2.33	0.43
1:3:343:ASP:HA	1:3:344:PRO:HD3	1.74	0.43
1:5:301:ILE:HD13	1:5:302:SER:H	1.83	0.43
1:1:200:ASP:C	1:1:202:ALA:N	2.71	0.43
1:5:137:GLU:N	1:5:137:GLU:CD	2.70	0.43
1:1:297:ASN:HB3	1:1:300:PRO:CG	2.49	0.43
1:4:168:TYR:CE1	1:4:169:ARG:HD2	2.53	0.43
1:6:99:ASN:ND2	1:6:108:LEU:H	2.16	0.43
1:4:125:MET:HE2	1:5:224:TYR:HE2	1.83	0.43
1:2:304:LEU:N	1:2:304:LEU:HD23	2.32	0.43
1:3:307:ASP:O	1:3:311:ARG:HD3	2.19	0.43
1:4:241:THR:HG22	1:4:242:THR:N	2.33	0.43
1:2:347:ILE:O	1:2:357:THR:HA	2.19	0.43
1:2:285:TYR:HE2	1:3:213:SER:HA	1.83	0.43
1:5:288:ILE:N	1:5:288:ILE:CD1	2.82	0.43
1:6:33:GLU:HG2	1:6:34:VAL:H	1.80	0.43
1:5:95:LEU:HD12	1:5:110:TRP:CB	2.49	0.43
1:5:27:VAL:C	1:5:28:ILE:HG22	2.39	0.43
1:1:112:ALA:O	1:1:251:GLY:HA3	2.18	0.43
1:5:50:PHE:O	1:5:51:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:162:GLN:HA	1:4:193:HIS:O	2.18	0.43
1:4:290:LEU:HA	1:4:290:LEU:HD23	1.79	0.43
1:4:162:GLN:CB	1:4:211:ASP:HB2	2.49	0.43
1:2:300:PRO:HG2	1:2:303:PHE:HB2	2.00	0.43
1:5:285:TYR:C	1:5:286:PHE:CD1	2.92	0.43
1:5:284:ARG:CD	1:5:286:PHE:CZ	3.02	0.43
1:2:168:TYR:CG	1:2:183:THR:O	2.71	0.43
1:5:114:THR:HG23	1:5:241:THR:CG2	2.48	0.43
1:4:93:ILE:HA	1:4:94:PRO:HD3	1.80	0.43
1:3:127:ASN:HD22	1:3:129:HIS:H	1.66	0.43
1:3:93:ILE:HA	1:3:94:PRO:HD3	1.63	0.43
1:1:232:PRO:HD2	1:2:226:GLY:O	2.18	0.43
1:5:120:ILE:HD11	1:5:285:TYR:HB2	2.01	0.43
1:2:162:GLN:HE21	1:2:194:LYS:HZ3	1.67	0.43
1:5:87:CYS:HB3	1:5:203:TYR:O	2.19	0.43
1:1:69:LEU:HD11	1:1:279:TRP:CE2	2.54	0.42
1:1:172:TYR:CD2	1:1:178:THR:HG21	2.54	0.42
1:4:79:SER:HA	1:4:171:LYS:O	2.18	0.42
1:2:196:VAL:HG13	1:2:196:VAL:O	2.18	0.42
1:3:315:ARG:HG2	1:3:315:ARG:NH1	2.34	0.42
1:5:288:ILE:CG2	1:5:289:THR:N	2.82	0.42
1:5:146:GLY:C	1:5:230:VAL:HG22	2.40	0.42
1:4:152:PHE:CD1	1:4:152:PHE:C	2.92	0.42
1:5:321:MET:HE2	1:5:327:GLN:HB2	2.01	0.42
1:5:180:LYS:O	1:5:181:ASN:HB2	2.18	0.42
1:4:220:TYR:C	1:4:221:PHE:CD1	2.92	0.42
1:3:130:SER:C	1:3:132:THR:H	2.22	0.42
1:4:136:HIS:CE1	1:5:277:GLN:NE2	2.87	0.42
1:3:342:GLY:HA2	1:6:109:MET:HE1	2.00	0.42
1:2:280:LYS:HG3	1:2:281:GLY:N	2.35	0.42
1:1:352:GLU:O	1:1:353:PHE:CG	2.72	0.42
1:6:288:ILE:HG22	1:6:289:THR:N	2.33	0.42
1:4:50:PHE:C	1:4:50:PHE:CD1	2.93	0.42
1:3:243:VAL:CG1	1:3:244:LEU:N	2.83	0.42
1:1:107:ILE:HD13	1:1:107:ILE:N	2.34	0.42
1:2:112:ALA:O	1:2:251:GLY:HA3	2.19	0.42
1:6:146:GLY:HA2	1:6:229:ASN:HA	2.01	0.42
1:4:93:ILE:CD1	1:4:93:ILE:N	2.79	0.42
1:2:150:HIS:HA	1:2:264:VAL:O	2.19	0.42
1:4:33:GLU:CD	1:4:33:GLU:H	2.22	0.42
1:1:159:LEU:HG	1:1:161:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:78:ASP:O	1:2:170:THR:HG23	2.20	0.42
1:1:134:LYS:HE3	1:1:134:LYS:HB2	1.71	0.42
1:6:353:PHE:HA	1:6:353:PHE:HD1	1.73	0.42
1:6:250:VAL:HG23	1:6:251:GLY:O	2.20	0.42
1:1:93:ILE:HB	1:1:259:LEU:HB3	2.01	0.42
1:1:16:LYS:HG2	1:1:17:PRO:HD2	2.01	0.42
1:6:47:VAL:O	1:6:287:LYS:HA	2.19	0.42
1:1:175:GLN:HG2	1:1:175:GLN:H	1.51	0.42
1:4:132:THR:HG22	1:4:133:GLN:N	2.35	0.42
1:1:220:TYR:C	1:1:221:PHE:CD1	2.93	0.42
1:3:266:ILE:HD12	1:3:266:ILE:N	2.35	0.42
1:1:224:TYR:CB	1:5:122:VAL:CG2	2.97	0.42
1:1:131:GLY:HA3	1:2:75:PHE:HE1	1.81	0.42
1:6:280:LYS:CG	1:6:281:GLY:N	2.82	0.42
1:3:190:ASN:C	1:3:190:ASN:HD22	2.22	0.42
1:2:180:LYS:HD3	1:2:180:LYS:HA	1.81	0.42
1:1:317:ASP:O	1:1:318:GLY:O	2.37	0.42
1:2:333:VAL:HG12	1:2:334:TYR:N	2.35	0.42
1:2:168:TYR:CD1	1:2:184:VAL:HA	2.55	0.42
1:4:123:THR:HB	1:5:205:VAL:O	2.20	0.42
1:1:311:ARG:HH21	1:5:33:GLU:HG2	1.85	0.42
1:1:90:VAL:CG2	1:1:91:ALA:H	2.33	0.42
1:4:95:LEU:HD23	1:4:95:LEU:N	2.35	0.42
1:2:126:LEU:HD21	1:3:224:TYR:HE2	1.84	0.42
1:6:319:GLN:HA	1:6:320:PRO:HD3	1.48	0.42
1:4:220:TYR:C	1:4:221:PHE:CG	2.93	0.42
1:1:65:LEU:HD23	1:1:65:LEU:HA	1.83	0.42
1:2:98:ILE:HG13	1:2:108:LEU:HB2	2.01	0.42
1:5:152:PHE:CD1	1:5:153:ALA:N	2.88	0.42
1:3:28:ILE:HG12	1:3:34:VAL:HG13	2.01	0.42
1:3:127:ASN:HD22	1:3:127:ASN:C	2.23	0.42
1:2:340:LEU:HD12	1:2:341:PRO:N	2.35	0.42
1:5:322:ILE:CG2	1:5:323:GLY:N	2.83	0.42
1:4:63:LYS:HB2	1:5:184:VAL:HG12	2.02	0.42
1:3:99:ASN:ND2	1:3:108:LEU:O	2.52	0.42
1:3:125:MET:HE2	1:3:125:MET:HB3	1.79	0.42
1:1:84:GLN:O	1:1:86:PRO:HD3	2.19	0.42
1:1:209:VAL:HG11	1:5:121:GLY:CA	2.45	0.42
1:4:84:GLN:C	1:4:85:LEU:HD23	2.40	0.42
1:2:115:VAL:HG13	1:2:242:THR:HB	2.00	0.42
1:4:49:CYS:SG	1:4:50:PHE:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:67:LYS:HB2	1:1:83:GLU:HB3	2.01	0.42
1:6:221:PHE:N	1:6:221:PHE:CD1	2.88	0.42
1:6:51:LEU:HD11	1:6:261:VAL:HG12	2.01	0.42
1:5:334:TYR:N	1:5:334:TYR:CD1	2.88	0.42
1:1:88:TYR:CE1	1:1:205:VAL:HG12	2.55	0.42
1:1:152:PHE:HA	1:1:263:ALA:HA	2.02	0.42
1:2:30:GLY:HA3	1:2:34:VAL:HG21	2.02	0.42
1:1:18:LYS:H	1:1:18:LYS:CD	2.27	0.42
1:2:304:LEU:HB2	1:6:304:LEU:HD21	2.02	0.42
1:4:151:PHE:CD1	1:4:152:PHE:N	2.87	0.42
1:2:227:GLY:HA3	1:2:230:VAL:CG1	2.50	0.42
1:3:86:PRO:HG2	1:3:279:TRP:CD1	2.55	0.42
1:3:79:SER:HB2	1:3:171:LYS:HB2	2.02	0.42
1:4:130:SER:C	1:4:132:THR:H	2.24	0.41
1:3:99:ASN:ND2	1:3:108:LEU:N	2.53	0.41
1:6:55:MET:HA	1:6:55:MET:HE3	2.02	0.41
1:4:85:LEU:HA	1:4:86:PRO:HD3	1.93	0.41
1:3:137:GLU:HB3	1:3:138:ASN:OD1	2.19	0.41
1:4:303:PHE:CE1	1:4:307:ASP:HB2	2.55	0.41
1:2:161:LEU:HA	1:2:161:LEU:HD23	1.72	0.41
1:4:111:GLU:OE2	1:4:250:VAL:HA	2.20	0.41
1:5:352:GLU:HB2	1:5:353:PHE:CD1	2.56	0.41
1:3:343:ASP:OD1	1:6:255:LYS:HE2	2.20	0.41
1:3:157:GLU:HG3	1:3:217:ASN:HD22	1.84	0.41
1:5:230:VAL:HA	1:5:231:PRO:HD2	1.76	0.41
1:4:158:PRO:HB2	1:4:196:VAL:HG21	2.00	0.41
1:3:102:LEU:C	1:3:104:CYS:N	2.72	0.41
1:2:217:ASN:OD1	1:2:252:PRO:HA	2.19	0.41
1:6:282:LEU:HD23	1:6:282:LEU:HA	1.83	0.41
1:4:270:PHE:C	1:4:270:PHE:HD1	2.24	0.41
1:1:214:LYS:HA	1:1:216:GLU:OE2	2.19	0.41
1:6:132:THR:CG2	1:6:141:GLY:CA	2.96	0.41
1:6:28:ILE:HG12	1:6:29:LYS:N	2.36	0.41
1:3:347:ILE:HG22	1:6:303:PHE:CZ	2.55	0.41
1:1:259:LEU:HD12	1:1:259:LEU:HA	1.77	0.41
1:4:114:THR:HG23	1:4:241:THR:CG2	2.50	0.41
1:4:313:THR:CG2	1:4:314:GLN:N	2.83	0.41
1:4:203:TYR:HA	1:4:204:PRO:HD2	1.86	0.41
1:4:244:LEU:HA	1:4:244:LEU:HD23	1.77	0.41
1:4:269:LEU:HD23	1:4:269:LEU:HA	1.88	0.41
1:1:311:ARG:C	1:1:313:THR:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:177:VAL:HG11	1:1:203:TYR:CE2	2.55	0.41
1:3:129:HIS:HD2	1:4:78:ASP:OD1	2.03	0.41
1:1:124:ALA:C	1:1:126:LEU:H	2.24	0.41
1:3:114:THR:CG2	1:3:115:VAL:N	2.81	0.41
1:2:166:ALA:O	1:2:167:ASN:HB3	2.20	0.41
1:6:325:SER:O	1:6:326:SER:C	2.57	0.41
1:2:128:LEU:HD23	1:2:128:LEU:HA	1.71	0.41
1:3:128:LEU:HA	1:3:128:LEU:HD23	1.73	0.41
1:5:107:ILE:HB	1:5:295:VAL:HG23	2.01	0.41
1:2:28:ILE:CD1	1:2:34:VAL:HG13	2.49	0.41
1:4:266:ILE:N	1:4:266:ILE:CD1	2.84	0.41
1:5:55:MET:CE	1:5:279:TRP:CB	2.98	0.41
1:1:115:VAL:HG22	1:1:116:LYS:N	2.35	0.41
1:3:253:LEU:HA	1:3:253:LEU:HD23	1.60	0.41
1:4:305:LEU:CD1	1:4:309:ILE:HD11	2.51	0.41
1:6:345:ASP:O	1:6:346:MET:C	2.59	0.41
1:1:74:GLN:OE1	1:1:74:GLN:HA	2.21	0.41
1:6:127:ASN:ND2	1:6:127:ASN:C	2.73	0.41
1:1:107:ILE:CG2	1:1:108:LEU:N	2.83	0.41
1:5:245:LEU:N	1:5:245:LEU:HD23	2.33	0.41
1:5:151:PHE:HA	1:5:222:GLY:HA2	2.01	0.41
1:6:98:ILE:HD11	1:6:110:TRP:CZ2	2.55	0.41
1:4:245:LEU:HB3	1:4:249:GLY:HA2	2.01	0.41
1:1:23:VAL:HG23	1:1:24:PRO:CG	2.49	0.41
1:2:126:LEU:CD2	1:3:224:TYR:HE2	2.34	0.41
1:2:116:LYS:HB2	1:2:287:LYS:HB3	2.02	0.41
1:2:241:THR:HG22	1:2:242:THR:N	2.35	0.41
1:1:329:GLU:O	1:1:330:GLU:HB2	2.21	0.41
1:5:81:ASP:O	1:5:84:GLN:HG3	2.21	0.41
1:2:220:TYR:C	1:2:221:PHE:CD1	2.94	0.41
1:3:118:GLU:OE1	1:3:237:THR:N	2.52	0.41
1:5:98:ILE:HG22	1:5:108:LEU:HB2	2.03	0.41
1:1:33:GLU:C	1:1:35:LEU:N	2.74	0.41
1:2:266:ILE:HD12	1:2:266:ILE:N	2.36	0.41
1:5:132:THR:HB	1:5:141:GLY:HA3	2.02	0.41
1:6:243:VAL:CG1	1:6:245:LEU:H	2.31	0.41
1:5:186:SER:HA	1:5:190:ASN:HB2	2.02	0.41
1:3:127:ASN:HD21	1:3:129:HIS:CD2	2.39	0.41
1:1:226:GLY:HA3	1:5:232:PRO:HG2	2.01	0.41
1:1:206:GLU:OE2	1:5:129:HIS:HE1	2.03	0.41
1:1:245:LEU:HD22	1:1:251:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:153:ALA:HB2	1:5:220:TYR:HB2	2.02	0.41
1:2:199:LYS:HD2	1:2:200:ASP:N	2.35	0.41
1:2:211:ASP:CG	1:2:214:LYS:HG2	2.40	0.41
1:6:220:TYR:C	1:6:221:PHE:CG	2.93	0.41
1:6:340:LEU:HD12	1:6:341:PRO:HD2	2.02	0.41
1:2:65:LEU:HD23	1:2:65:LEU:HA	1.89	0.41
1:4:285:TYR:C	1:4:286:PHE:CD1	2.95	0.41
1:1:58:PRO:HG2	1:1:62:GLN:HB2	2.03	0.41
1:3:347:ILE:CG2	1:6:303:PHE:CZ	3.04	0.41
1:4:245:LEU:HD13	1:4:249:GLY:C	2.41	0.41
1:5:303:PHE:O	1:5:304:LEU:C	2.59	0.41
1:4:217:ASN:O	1:4:252:PRO:HB3	2.20	0.41
1:3:298:PRO:HD3	1:6:342:GLY:HA3	2.03	0.41
1:1:52:ASN:OD1	1:2:188:GLN:HG3	2.21	0.41
1:2:178:THR:HB	1:2:179:PRO:CD	2.51	0.41
1:1:17:PRO:CG	1:2:106:ASN:HB3	2.51	0.41
1:1:297:ASN:HB3	1:1:300:PRO:HB3	2.02	0.41
1:2:128:LEU:HD21	1:2:143:PRO:HB3	2.02	0.41
1:5:112:ALA:O	1:5:251:GLY:HA3	2.21	0.41
1:3:347:ILE:O	1:3:347:ILE:HG22	2.22	0.41
1:2:92:ARG:CG	1:2:258:SER:HB3	2.51	0.41
1:4:66:SER:OG	1:4:279:TRP:N	2.53	0.41
1:4:145:GLN:OE1	1:4:229:ASN:HB3	2.21	0.41
1:6:156:GLY:HA3	1:6:253:LEU:O	2.21	0.41
1:2:235:HIS:CD2	1:3:223:THR:HB	2.56	0.41
1:2:81:ASP:N	1:2:81:ASP:OD1	2.54	0.41
1:3:245:LEU:HD23	1:3:245:LEU:N	2.36	0.40
1:5:53:PRO:HD3	1:5:283:PRO:CA	2.51	0.40
1:1:359:ARG:HG2	1:1:359:ARG:NH1	2.36	0.40
1:4:98:ILE:CG2	1:4:108:LEU:HB3	2.50	0.40
1:6:298:PRO:HG2	1:6:299:TYR:N	2.36	0.40
1:5:16:LYS:CG	1:5:17:PRO:O	2.68	0.40
1:1:296:LYS:HA	1:1:296:LYS:HD2	1.67	0.40
1:3:44:PHE:CD1	1:3:44:PHE:C	2.94	0.40
1:3:133:GLN:HB2	1:3:272:ASN:O	2.21	0.40
1:5:126:LEU:O	1:5:128:LEU:N	2.55	0.40
1:3:280:LYS:CG	1:3:281:GLY:N	2.84	0.40
1:4:125:MET:CB	1:4:144:ILE:HD12	2.50	0.40
1:3:109:MET:HE3	1:6:342:GLY:CA	2.52	0.40
1:3:66:SER:HB3	1:3:279:TRP:HB2	2.03	0.40
1:5:127:ASN:HD22	1:5:129:HIS:H	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:126:LEU:HA	1:3:126:LEU:HD23	1.80	0.40
1:5:114:THR:HG23	1:5:241:THR:HG23	2.03	0.40
1:5:97:ASN:OD1	1:5:99:ASN:N	2.54	0.40
1:2:326:SER:OG	1:2:328:VAL:HB	2.20	0.40
1:3:93:ILE:HG22	1:3:95:LEU:HD21	2.03	0.40
1:4:53:PRO:HD3	1:4:283:PRO:CA	2.52	0.40
1:6:26:LEU:HD21	1:6:29:LYS:HB3	2.03	0.40
1:2:168:TYR:CE1	1:2:184:VAL:HA	2.56	0.40
1:6:146:GLY:C	1:6:230:VAL:HG22	2.41	0.40
1:4:93:ILE:O	1:4:259:LEU:N	2.51	0.40
1:1:93:ILE:HA	1:1:94:PRO:HD3	1.62	0.40
1:4:301:ILE:O	1:4:302:SER:C	2.59	0.40
1:2:253:LEU:HA	1:2:253:LEU:HD23	1.84	0.40
1:5:81:ASP:HB2	1:5:84:GLN:HG3	2.03	0.40
1:3:39:THR:HB	1:3:43:SER:CB	2.51	0.40
1:6:65:LEU:HA	1:6:279:TRP:O	2.20	0.40
1:4:139:GLY:O	1:4:140:ALA:O	2.39	0.40
1:1:162:GLN:HE21	1:1:194:LYS:HZ2	1.69	0.40
1:5:152:PHE:HA	1:5:263:ALA:HA	2.03	0.40
1:2:259:LEU:HD12	1:2:259:LEU:HA	1.61	0.40
1:5:352:GLU:HB2	1:5:353:PHE:CE1	2.56	0.40
1:5:298:PRO:HG2	1:5:299:TYR:H	1.86	0.40
1:5:298:PRO:HG2	1:5:299:TYR:N	2.36	0.40
1:4:256:ALA:O	1:4:258:SER:N	2.54	0.40
1:2:124:ALA:C	1:2:126:LEU:H	2.24	0.40
1:3:315:ARG:HH11	1:3:315:ARG:HG2	1.86	0.40
1:1:111:GLU:OE2	1:1:250:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	346/361 (96%)	276 (80%)	48 (14%)	22 (6%)	2	10
1	2	346/361 (96%)	292 (84%)	40 (12%)	14 (4%)	4	21
1	3	340/361 (94%)	287 (84%)	39 (12%)	14 (4%)	3	20
1	4	329/361 (91%)	267 (81%)	49 (15%)	13 (4%)	4	21
1	5	345/361 (96%)	279 (81%)	54 (16%)	12 (4%)	4	24
1	6	339/361 (94%)	288 (85%)	41 (12%)	10 (3%)	6	29
All	All	2045/2166 (94%)	1689 (83%)	271 (13%)	85 (4%)	3	19

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	137	GLU
1	1	174	ALA
1	1	191	THR
1	1	257	ASP
1	1	300	PRO
1	1	313	THR
1	1	318	GLY
1	1	351	ASP
1	2	137	GLU
1	2	351	ASP
1	3	105	GLY
1	3	137	GLU
1	3	257	ASP
1	3	301	ILE
1	4	14	PRO
1	4	132	THR
1	4	137	GLU
1	4	140	ALA
1	4	324	MET
1	4	341	PRO
1	5	102	LEU
1	5	137	GLU
1	5	301	ILE
1	5	351	ASP
1	6	132	THR
1	6	137	GLU
1	6	257	ASP
1	6	346	MET
1	1	147	SER
1	1	306	SER

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Mol	Chain	Res	Type
1	1	309	ILE
1	1	317	ASP
1	1	353	PHE
1	2	18	LYS
1	2	257	ASP
1	2	307	ASP
1	3	100	GLU
1	3	132	THR
1	3	191	THR
1	3	300	PRO
1	4	130	SER
1	4	131	GLY
1	5	127	ASN
1	5	131	GLY
1	6	130	SER
1	6	131	GLY
1	1	131	GLY
1	1	360	MET
1	2	103	THR
1	2	215	ASN
1	2	353	PHE
1	3	346	MET
1	4	72	GLU
1	5	191	THR
1	5	257	ASP
1	5	300	PRO
1	6	18	LYS
1	6	101	ASP
1	1	182	ALA
1	1	255	LYS
1	1	346	MET
1	2	131	GLY
1	2	173	PRO
1	3	136	HIS
1	4	191	THR
1	6	72	GLU
1	1	173	PRO
1	2	181	ASN
1	3	124	ALA
1	3	193	HIS
1	5	58	PRO
1	6	181	ASN

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Mol	Chain	Res	Type
1	2	58	PRO
1	2	319	GLN
1	4	173	PRO
1	5	103	THR
1	5	132	THR
1	4	300	PRO
1	1	58	PRO
1	1	319	GLN
1	3	58	PRO
1	2	309	ILE
1	4	301	ILE
1	1	34	VAL
1	3	320	PRO

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	1	306/314 (98%)	250 (82%)	56 (18%)	2	9
1	2	306/314 (98%)	265 (87%)	41 (13%)	5	20
1	3	300/314 (96%)	254 (85%)	46 (15%)	3	14
1	4	289/314 (92%)	251 (87%)	38 (13%)	5	21
1	5	305/314 (97%)	251 (82%)	54 (18%)	2	10
1	6	299/314 (95%)	260 (87%)	39 (13%)	5	21
All	All	1805/1884 (96%)	1531 (85%)	274 (15%)	3	14

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	LYS
1	1	21	VAL
1	1	45	THR
1	1	76	THR
1	1	80	PRO

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Mol	Chain	Res	Type
1	1	92	ARG
1	1	97	ASN
1	1	98	ILE
1	1	100	GLU
1	1	104	CYS
1	1	114	THR
1	1	117	THR
1	1	122	VAL
1	1	127	ASN
1	1	128	LEU
1	1	132	THR
1	1	138	ASN
1	1	151	PHE
1	1	165	LEU
1	1	175	GLN
1	1	190	ASN
1	1	191	THR
1	1	201	ASN
1	1	211	ASP
1	1	214	LYS
1	1	218	THR
1	1	223	THR
1	1	229	ASN
1	1	239	THR
1	1	245	LEU
1	1	255	LYS
1	1	262	SER
1	1	270	PHE
1	1	276	THR
1	1	284	ARG
1	1	285	TYR
1	1	294	SER
1	1	295	VAL
1	1	296	LYS
1	1	299	TYR
1	1	304	LEU
1	1	306	SER
1	1	308	LEU
1	1	311	ARG
1	1	312	ARG
1	1	315	ARG
1	1	317	ASP

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Mol	Chain	Res	Type
1	1	321	MET
1	1	329	GLU
1	1	334	TYR
1	1	344	PRO
1	1	345	ASP
1	1	346	MET
1	1	352	GLU
1	1	353	PHE
1	1	359	ARG
1	2	15	LYS
1	2	23	VAL
1	2	33	GLU
1	2	35	LEU
1	2	76	THR
1	2	81	ASP
1	2	100	GLU
1	2	102	LEU
1	2	107	ILE
1	2	114	THR
1	2	127	ASN
1	2	132	THR
1	2	165	LEU
1	2	183	THR
1	2	185	ASP
1	2	188	GLN
1	2	191	THR
1	2	201	ASN
1	2	205	VAL
1	2	214	LYS
1	2	218	THR
1	2	221	PHE
1	2	223	THR
1	2	225	THR
1	2	229	ASN
1	2	231	PRO
1	2	233	VAL
1	2	261	VAL
1	2	262	SER
1	2	270	PHE
1	2	273	THR
1	2	276	THR
1	2	280	LYS

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Mol	Chain	Res	Type
1	2	289	THR
1	2	302	SER
1	2	307	ASP
1	2	312	ARG
1	2	353	PHE
1	2	356	THR
1	2	359	ARG
1	2	360	MET
1	3	21	VAL
1	3	41	VAL
1	3	43	SER
1	3	45	THR
1	3	76	THR
1	3	84	GLN
1	3	99	ASN
1	3	101	ASP
1	3	102	LEU
1	3	114	THR
1	3	122	VAL
1	3	127	ASN
1	3	132	THR
1	3	138	ASN
1	3	151	PHE
1	3	165	LEU
1	3	173	PRO
1	3	175	GLN
1	3	190	ASN
1	3	191	THR
1	3	209	VAL
1	3	213	SER
1	3	214	LYS
1	3	218	THR
1	3	221	PHE
1	3	223	THR
1	3	229	ASN
1	3	250	VAL
1	3	262	SER
1	3	273	THR
1	3	274	SER
1	3	280	LYS
1	3	285	TYR
1	3	303	PHE

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Mol	Chain	Res	Type
1	3	305	LEU
1	3	307	ASP
1	3	308	LEU
1	3	312	ARG
1	3	315	ARG
1	3	322	ILE
1	3	324	MET
1	3	325	SER
1	3	347	ILE
1	3	348	ARG
1	3	350	ILE
1	3	355	GLN
1	4	14	PRO
1	4	45	THR
1	4	76	THR
1	4	103	THR
1	4	114	THR
1	4	127	ASN
1	4	135	THR
1	4	137	GLU
1	4	138	ASN
1	4	151	PHE
1	4	173	PRO
1	4	184	VAL
1	4	190	ASN
1	4	191	THR
1	4	201	ASN
1	4	218	THR
1	4	229	ASN
1	4	230	VAL
1	4	233	VAL
1	4	245	LEU
1	4	250	VAL
1	4	262	SER
1	4	270	PHE
1	4	273	THR
1	4	274	SER
1	4	276	THR
1	4	280	LYS
1	4	284	ARG
1	4	293	ARG
1	4	295	VAL

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Mol	Chain	Res	Type
1	4	301	ILE
1	4	305	LEU
1	4	310	ASN
1	4	311	ARG
1	4	312	ARG
1	4	316	VAL
1	4	322	ILE
1	4	334	TYR
1	5	16	LYS
1	5	28	ILE
1	5	33	GLU
1	5	45	THR
1	5	48	GLU
1	5	49	CYS
1	5	65	LEU
1	5	76	THR
1	5	84	GLN
1	5	114	THR
1	5	117	THR
1	5	122	VAL
1	5	127	ASN
1	5	132	THR
1	5	137	GLU
1	5	138	ASN
1	5	151	PHE
1	5	152	PHE
1	5	165	LEU
1	5	173	PRO
1	5	184	VAL
1	5	189	MET
1	5	190	ASN
1	5	191	THR
1	5	201	ASN
1	5	218	THR
1	5	221	PHE
1	5	223	THR
1	5	225	THR
1	5	229	ASN
1	5	236	ILE
1	5	239	THR
1	5	245	LEU
1	5	255	LYS

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Mol	Chain	Res	Type
1	5	262	SER
1	5	270	PHE
1	5	273	THR
1	5	274	SER
1	5	280	LYS
1	5	284	ARG
1	5	296	LYS
1	5	297	ASN
1	5	301	ILE
1	5	302	SER
1	5	305	LEU
1	5	312	ARG
1	5	316	VAL
1	5	322	ILE
1	5	324	MET
1	5	332	ARG
1	5	346	MET
1	5	348	ARG
1	5	353	PHE
1	5	359	ARG
1	6	15	LYS
1	6	21	VAL
1	6	35	LEU
1	6	55	MET
1	6	68	SER
1	6	76	THR
1	6	98	ILE
1	6	102	LEU
1	6	114	THR
1	6	127	ASN
1	6	134	LYS
1	6	151	PHE
1	6	165	LEU
1	6	173	PRO
1	6	184	VAL
1	6	190	ASN
1	6	191	THR
1	6	201	ASN
1	6	214	LYS
1	6	218	THR
1	6	223	THR
1	6	229	ASN

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Mol	Chain	Res	Type
1	6	250	VAL
1	6	255	LYS
1	6	262	SER
1	6	273	THR
1	6	274	SER
1	6	276	THR
1	6	278	GLN
1	6	284	ARG
1	6	298	PRO
1	6	301	ILE
1	6	303	PHE
1	6	312	ARG
1	6	314	GLN
1	6	315	ARG
1	6	324	MET
1	6	345	ASP
1	6	350	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	HIS
1	1	97	ASN
1	1	99	ASN
1	1	127	ASN
1	1	133	GLN
1	1	136	HIS
1	1	162	GLN
1	1	167	ASN
1	1	181	ASN
1	1	190	ASN
1	1	201	ASN
1	1	229	ASN
1	1	235	HIS
1	1	277	GLN
1	1	319	GLN
1	1	327	GLN
1	2	22	GLN
1	2	61	HIS
1	2	99	ASN
1	2	127	ASN
1	2	129	HIS

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Mol	Chain	Res	Type
1	2	162	GLN
1	2	167	ASN
1	2	175	GLN
1	2	181	ASN
1	2	190	ASN
1	2	201	ASN
1	2	229	ASN
1	2	235	HIS
1	2	272	ASN
1	2	277	GLN
1	2	278	GLN
1	2	319	GLN
1	2	327	GLN
1	3	22	GLN
1	3	61	HIS
1	3	99	ASN
1	3	127	ASN
1	3	129	HIS
1	3	162	GLN
1	3	167	ASN
1	3	175	GLN
1	3	181	ASN
1	3	187	GLN
1	3	188	GLN
1	3	190	ASN
1	3	201	ASN
1	3	229	ASN
1	3	235	HIS
1	3	277	GLN
1	3	319	GLN
1	3	327	GLN
1	4	61	HIS
1	4	99	ASN
1	4	127	ASN
1	4	129	HIS
1	4	136	HIS
1	4	162	GLN
1	4	167	ASN
1	4	175	GLN
1	4	181	ASN
1	4	190	ASN
1	4	201	ASN

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Mol	Chain	Res	Type
1	4	229	ASN
1	4	235	HIS
1	4	277	GLN
1	4	319	GLN
1	4	327	GLN
1	5	61	HIS
1	5	99	ASN
1	5	127	ASN
1	5	129	HIS
1	5	162	GLN
1	5	175	GLN
1	5	190	ASN
1	5	201	ASN
1	5	229	ASN
1	5	272	ASN
1	5	277	GLN
1	5	278	GLN
1	5	319	GLN
1	5	327	GLN
1	6	22	GLN
1	6	99	ASN
1	6	106	ASN
1	6	127	ASN
1	6	162	GLN
1	6	175	GLN
1	6	181	ASN
1	6	190	ASN
1	6	201	ASN
1	6	229	ASN
1	6	277	GLN
1	6	310	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.