Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 04:10 PM EDT

PDB ID	:	1TMF
Title	:	THREE-DIMENSIONAL STRUCTURE OF THEILER MURINE ENCEPHALOMYELITIS VIRUS (BEAN STRAIN)
Authors	:	Luo, M.; Toth, K.S.
Deposited on	:	1992-02-20
Resolution	:	3.50 Å(reported)

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

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

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

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

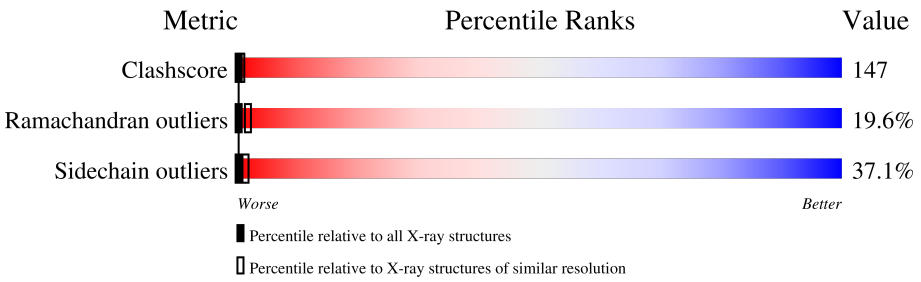
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	276	8% 28% 36% 29%
2	2	267	18% 40% 27% 15%
3	3	232	17% 33% 34% 16%
4	4	45	9% 24% 16% 20% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6260 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 THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	276	2156	1385	361	400	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	138	THR	MET	conflict	UNP P08544
1	139	ASP	THR	conflict	UNP P08544
1	140	THR	ARG	conflict	UNP P08544

- Molecule 2 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	267	2078	1299	367	404	8	0	0	0

- Molecule 3 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	232	1785	1148	288	338	11	0	0	0

- Molecule 4 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	4	31	241	148	40	53	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	12	ASN	GLN	conflict	UNP P13899
4	13	GLU	SER	conflict	UNP P13899
4	55	LEU	ILE	conflict	UNP P13899

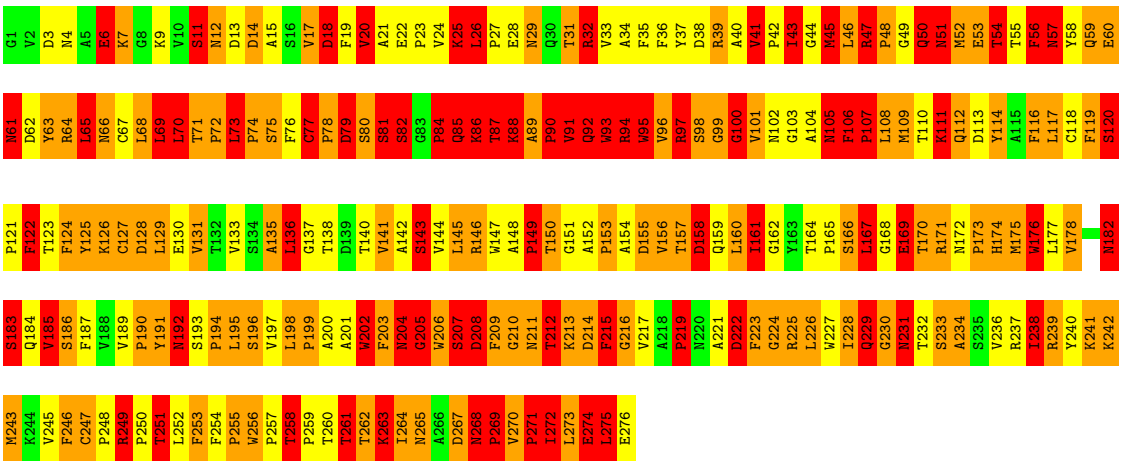
3 Residue-property plots (i)

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

Note EDS was not executed.

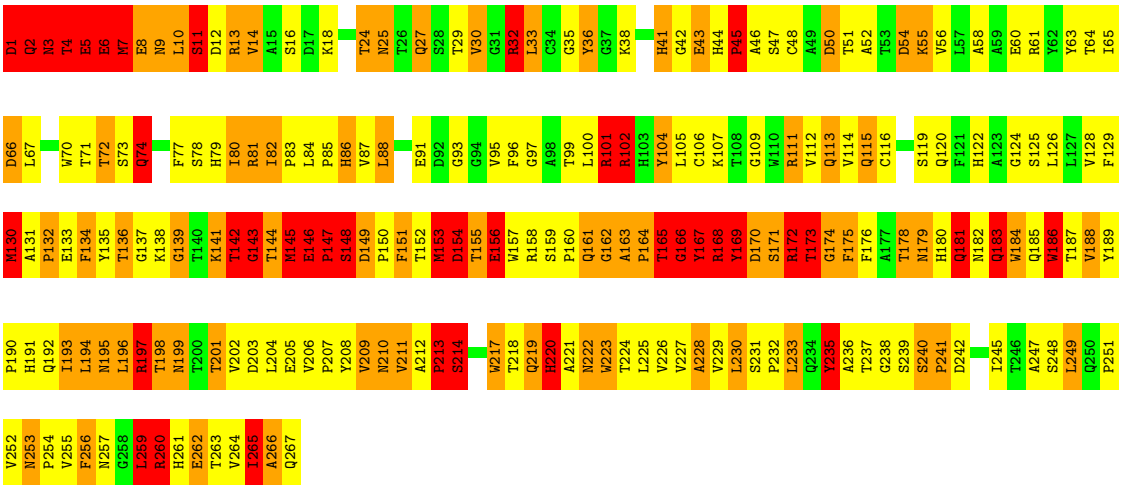
• Molecule 1: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1)

Chain 1: 8% 28% 36% 29%



• Molecule 2: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2)

Chain 2: 18% 40% 27% 15%



• Molecule 3: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3)

Chain 3: 17% 33% 34% 16%

S1 V7 R8 E9 H10 K11 G12 C13 F14 Y15 S16 T17 N18 P19 D20 T21 T22 V23 P24 T25 Y26 T29 P33 S34 D35 Y36 M37 L44 L45 E46 L47 C48 K49 L50 P51 T52 F53 L54 G55 N56 P57 N58 T59 N60 N61 K62 R63 Y64 P65 Y66 F67 S68 A69 T70 N71 S72

V73 P74 A75 T76 S77 M78 V79 D80 Y81 Q82 V83 A84 L85 S86 C87 S88 C89 M90 A91 N92 S93 M94 L95 A96 A97 V98 A99 R100 N101 F102 N103 Q104 Y105 R106 G107 S108 L109 N110 F111 L112 F113 V114 F115 T116 G117 A118 A119 M120 V121 K122 G123 K124 F125 L126 I127 A128 Y129 T130 P131 P132

G133 K136 P137 T138 T139 R140 D141 Q142 A143 M144 Q145 S146 T147 Y148 A149 I150 W151 D152 L153 G154 L155 N156 S157 S158 F159 N160 F161 T162 A163 P164 F165 I166 S167 P168 T169 H170 Y171 R172 Q173 T174 S175 Y176 T177 S178 P179 T180 I181 T182 S183 V184 D185 G186 W187 V188 T189 V190 W191 Q192 L193

T194 P195 L196 T197 Y198 T202 P203 T204 N205 S206 D207 I208 L209 T210 L211 V212 S213 A214 G215 D216 D217 F218 T219 L220 R221 M222 P223 I224 S225 P226 T227 K228 W229 V230 P231 Q232

- Molecule 4: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4)

Chain 4: 9% 24% 16% 20% 31%

N12 E13 S14 G15 N16 E17 G18 V19 I20 I21 N22 N23 F24 Y25 S26 N27 Q28 Y29 Q30 N31 S32 I33 D34 L35 S36 A37 SER GLY GLY ASN ALA GLY ASP ALA PRO GLN THR ASN GLY GLN L52 S53 N54 L55 L56

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	331.86Å 331.86Å 796.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6260	wwPDB-VP
Average B, all atoms ($Å^2$)	0.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	2.15	60/2222 (2.7%)	2.83	192/3039 (6.3%)
2	2	1.78	34/2136 (1.6%)	2.48	107/2922 (3.7%)
3	3	1.48	20/1840 (1.1%)	2.19	97/2525 (3.8%)
4	4	1.92	2/242 (0.8%)	3.39	16/326 (4.9%)
All	All	1.84	116/6440 (1.8%)	2.57	412/8812 (4.7%)

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	1	0	41
2	2	0	15
3	3	0	8
4	4	0	3
All	All	0	67

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	105	ASN	C-N	26.88	1.95	1.34
2	2	260	ARG	C-N	23.70	1.88	1.34
4	4	34	ASP	C-N	-22.21	0.82	1.34
1	1	272	ILE	CB-CG1	21.32	2.13	1.54
2	2	143	GLY	C-N	19.07	1.77	1.34
1	1	75	SER	C-N	18.03	1.75	1.34
1	1	26	LEU	C-N	15.75	1.64	1.34
1	1	251	THR	C-N	15.47	1.69	1.34
2	2	259	LEU	C-N	15.22	1.69	1.34
3	3	74	PRO	C-N	-14.83	0.99	1.34
2	2	147	PRO	C-N	13.58	1.65	1.34
1	1	27	PRO	C-N	-13.56	1.02	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	66	ASN	C-N	13.21	1.64	1.34
1	1	272	ILE	N-CA	-13.08	1.20	1.46
1	1	238	ILE	C-N	12.63	1.63	1.34
1	1	25	LYS	C-N	11.41	1.60	1.34
1	1	85	GLN	C-N	11.23	1.59	1.34
1	1	69	LEU	C-N	-11.21	1.08	1.34
1	1	95	TRP	C-N	11.09	1.59	1.34
3	3	164	PRO	C-N	-11.00	1.08	1.34
2	2	3	ASN	C-N	-10.98	1.08	1.34
1	1	219	PRO	C-N	10.59	1.58	1.34
2	2	7	MET	C-N	10.37	1.57	1.34
1	1	107	PRO	C-N	10.29	1.57	1.34
1	1	184	GLN	N-CA	10.29	1.67	1.46
1	1	14	ASP	C-N	-9.96	1.11	1.34
1	1	246	PHE	C-N	9.95	1.56	1.34
1	1	274	GLU	N-CA	-9.81	1.26	1.46
2	2	6	GLU	CG-CD	9.80	1.66	1.51
1	1	185	VAL	N-CA	9.21	1.64	1.46
1	1	153	PRO	C-N	-9.03	1.13	1.34
2	2	265	ILE	N-CA	8.98	1.64	1.46
2	2	2	GLN	C-N	-8.97	1.13	1.34
1	1	159	GLN	C-N	-8.86	1.13	1.34
4	4	55	LEU	C-N	8.82	1.54	1.34
2	2	10	LEU	N-CA	8.77	1.63	1.46
3	3	70	THR	C-N	8.71	1.54	1.34
3	3	29	THR	C-N	-8.54	1.14	1.34
2	2	213	PRO	C-N	-8.50	1.14	1.34
1	1	44	GLY	N-CA	8.47	1.58	1.46
2	2	11	SER	N-CA	8.39	1.63	1.46
2	2	213	PRO	CA-C	-8.30	1.36	1.52
1	1	271	PRO	CA-C	-8.15	1.36	1.52
1	1	273	LEU	C-N	-8.06	1.15	1.34
1	1	158	ASP	C-N	8.01	1.52	1.34
1	1	29	ASN	N-CA	-7.91	1.30	1.46
1	1	100	GLY	CA-C	7.89	1.64	1.51
1	1	12	ASN	C-N	-7.86	1.16	1.34
3	3	19	PRO	C-N	7.71	1.51	1.34
3	3	176	TYR	C-N	-7.66	1.16	1.34
3	3	47	LEU	C-N	-7.62	1.16	1.34
2	2	223	TRP	C-N	-7.56	1.16	1.34
1	1	100	GLY	N-CA	7.50	1.57	1.46
1	1	271	PRO	C-N	-7.50	1.16	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	5	GLU	N-CA	7.46	1.61	1.46
1	1	21	ALA	C-N	7.41	1.51	1.34
2	2	143	GLY	N-CA	-7.41	1.34	1.46
3	3	231	PRO	N-CA	-7.41	1.34	1.47
3	3	71	ASN	C-N	7.36	1.50	1.34
1	1	156	VAL	C-N	-7.15	1.17	1.34
1	1	57	ASN	C-N	7.09	1.50	1.34
3	3	180	THR	C-N	-6.93	1.18	1.34
1	1	237	ARG	C-N	6.92	1.50	1.34
1	1	176	TRP	N-CA	6.92	1.60	1.46
1	1	176	TRP	CB-CG	6.89	1.62	1.50
2	2	8	GLU	N-CA	-6.81	1.32	1.46
1	1	73	LEU	N-CA	-6.80	1.32	1.46
2	2	9	ASN	CA-C	6.79	1.70	1.52
1	1	69	LEU	N-CA	6.71	1.59	1.46
1	1	228	ILE	N-CA	6.66	1.59	1.46
1	1	184	GLN	CA-C	6.52	1.70	1.52
2	2	146	GLU	C-N	6.35	1.46	1.34
2	2	148	SER	N-CA	6.35	1.59	1.46
2	2	4	THR	CA-C	6.34	1.69	1.52
3	3	168	PRO	C-N	-6.34	1.19	1.34
1	1	117	LEU	C-N	6.29	1.48	1.34
1	1	271	PRO	C-O	6.23	1.35	1.23
1	1	184	GLN	C-N	6.22	1.48	1.34
2	2	6	GLU	CB-CG	6.10	1.63	1.52
2	2	186	TRP	CD1-NE1	6.07	1.48	1.38
2	2	6	GLU	CD-OE2	6.04	1.32	1.25
1	1	9	LYS	C-N	-6.00	1.20	1.34
1	1	129	LEU	N-CA	5.97	1.58	1.46
1	1	28	GLU	C-N	-5.95	1.20	1.34
1	1	183	SER	C-N	5.95	1.47	1.34
3	3	37	MET	C-N	-5.91	1.20	1.34
3	3	74	PRO	CA-C	-5.89	1.41	1.52
1	1	124	PHE	CB-CG	-5.88	1.41	1.51
2	2	4	THR	C-N	5.86	1.47	1.34
1	1	72	PRO	C-N	-5.84	1.20	1.34
1	1	46	LEU	CA-C	-5.72	1.38	1.52
2	2	164	PRO	N-CA	-5.70	1.37	1.47
2	2	217	TRP	N-CA	5.66	1.57	1.46
1	1	32	ARG	C-N	-5.65	1.21	1.34
1	1	230	GLY	N-CA	5.64	1.54	1.46
3	3	229	TRP	NE1-CE2	-5.62	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	216	GLY	N-CA	-5.59	1.37	1.46
2	2	214	SER	N-CA	-5.57	1.35	1.46
3	3	231	PRO	CA-C	-5.57	1.41	1.52
3	3	203	PRO	CA-C	-5.56	1.41	1.52
2	2	10	LEU	CA-C	5.49	1.67	1.52
3	3	92	ASN	N-CA	-5.45	1.35	1.46
2	2	6	GLU	CD-OE1	5.42	1.31	1.25
3	3	230	VAL	C-N	-5.39	1.24	1.34
1	1	272	ILE	CB-CG2	5.34	1.69	1.52
1	1	125	TYR	N-CA	5.33	1.57	1.46
1	1	6	GLU	C-N	-5.25	1.22	1.34
2	2	184	TRP	NE1-CE2	-5.25	1.30	1.37
2	2	5	GLU	C-N	5.23	1.46	1.34
1	1	72	PRO	CA-C	-5.21	1.42	1.52
3	3	11	LYS	C-N	5.20	1.42	1.33
1	1	56	PHE	N-CA	5.13	1.56	1.46
2	2	184	TRP	CB-CG	5.11	1.59	1.50
2	2	264	VAL	C-N	5.08	1.45	1.34
3	3	57	PRO	N-CA	5.07	1.55	1.47
1	1	205	GLY	C-N	5.00	1.45	1.34

All (412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	34	ASP	O-C-N	-39.99	58.72	122.70
2	2	5	GLU	O-C-N	-31.94	71.59	122.70
2	2	8	GLU	O-C-N	-31.39	72.48	122.70
2	2	3	ASN	O-C-N	-29.43	75.61	122.70
1	1	271	PRO	O-C-N	25.77	163.93	122.70
1	1	107	PRO	O-C-N	-25.49	81.91	122.70
1	1	32	ARG	O-C-N	-21.44	88.40	122.70
1	1	273	LEU	O-C-N	21.36	156.87	122.70
2	2	147	PRO	O-C-N	-21.06	89.01	122.70
2	2	8	GLU	CA-C-N	20.60	162.51	117.20
4	4	34	ASP	CA-C-N	20.57	162.45	117.20
2	2	2	GLN	O-C-N	-20.35	90.14	122.70
3	3	74	PRO	O-C-N	20.28	155.15	122.70
1	1	85	GLN	O-C-N	19.99	154.69	122.70
1	1	182	ASN	O-C-N	-19.57	91.39	122.70
1	1	97	ARG	C-N-CA	18.58	168.16	121.70
1	1	272	ILE	CB-CA-C	-18.34	74.92	111.60
1	1	28	GLU	O-C-N	-18.27	93.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	105	ASN	CA-C-N	-18.23	77.08	117.20
2	2	6	GLU	O-C-N	-18.10	93.74	122.70
1	1	271	PRO	CA-C-N	-17.88	77.88	117.20
3	3	77	SER	O-C-N	17.83	151.23	122.70
2	2	8	GLU	C-N-CA	17.54	165.54	121.70
1	1	159	GLN	C-N-CA	17.44	165.31	121.70
1	1	215	PHE	O-C-N	17.40	152.78	123.20
1	1	107	PRO	CA-C-N	16.62	153.76	117.20
1	1	84	PRO	O-C-N	-16.61	96.12	122.70
1	1	26	LEU	O-C-N	-16.40	89.94	121.10
3	3	67	PHE	CA-CB-CG	16.40	153.26	113.90
1	1	272	ILE	CG1-CB-CG2	16.16	146.96	111.40
1	1	95	TRP	O-C-N	-15.89	97.28	122.70
1	1	215	PHE	CA-C-N	-15.89	84.42	116.20
1	1	97	ARG	O-C-N	-15.69	97.60	122.70
1	1	273	LEU	CA-C-N	-15.66	82.76	117.20
2	2	147	PRO	CA-C-N	15.63	151.58	117.20
1	1	107	PRO	C-N-CA	15.45	160.32	121.70
1	1	85	GLN	CA-C-N	-14.87	84.49	117.20
3	3	74	PRO	C-N-CA	14.49	157.92	121.70
3	3	74	PRO	CA-C-N	-14.31	85.72	117.20
2	2	235	TYR	O-C-N	14.29	145.56	122.70
1	1	65	LEU	C-N-CA	14.02	156.75	121.70
2	2	241	PRO	O-C-N	14.02	145.13	122.70
2	2	143	GLY	C-N-CA	-13.68	87.51	121.70
3	3	214	ALA	C-N-CA	13.45	150.55	122.30
4	4	34	ASP	C-N-CA	13.44	155.29	121.70
2	2	147	PRO	C-N-CA	13.39	155.17	121.70
3	3	64	TYR	O-C-N	-13.28	95.86	121.10
3	3	71	ASN	N-CA-CB	13.24	134.44	110.60
3	3	77	SER	CA-C-N	-13.22	88.11	117.20
3	3	184	VAL	O-C-N	13.13	143.71	122.70
2	2	1	ASP	O-C-N	-13.01	101.89	122.70
2	2	139	GLY	C-N-CA	12.71	153.49	121.70
4	4	55	LEU	O-C-N	-12.55	102.61	122.70
3	3	209	LEU	C-N-CA	12.55	153.07	121.70
1	1	100	GLY	C-N-CA	12.49	152.92	121.70
3	3	226	PRO	O-C-N	12.26	142.31	122.70
3	3	179	PRO	O-C-N	12.04	141.96	122.70
1	1	28	GLU	CA-C-N	11.81	143.18	117.20
2	2	6	GLU	CA-C-N	11.78	143.13	117.20
3	3	49	LYS	C-N-CA	11.74	151.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	274	GLU	O-C-N	11.73	141.46	122.70
2	2	5	GLU	CA-C-N	11.44	142.37	117.20
1	1	207	SER	O-C-N	11.40	140.94	122.70
2	2	2	GLN	CA-C-N	11.36	142.18	117.20
1	1	26	LEU	CA-C-N	11.21	148.48	117.10
1	1	88	LYS	C-N-CA	11.15	149.57	121.70
1	1	182	ASN	C-N-CA	11.07	149.38	121.70
1	1	182	ASN	CA-C-N	10.90	141.18	117.20
1	1	22	GLU	O-C-N	-10.72	100.74	121.10
3	3	231	PRO	O-C-N	10.67	139.78	122.70
3	3	70	THR	CA-C-N	-10.64	93.78	117.20
1	1	75	SER	O-C-N	-10.60	105.73	122.70
2	2	3	ASN	CA-C-N	10.60	140.51	117.20
1	1	26	LEU	C-N-CD	-10.53	97.44	120.60
3	3	71	ASN	O-C-N	-10.52	105.87	122.70
1	1	28	GLU	C-N-CA	10.51	147.97	121.70
2	2	235	TYR	CA-C-N	-10.49	94.11	117.20
1	1	22	GLU	C-N-CD	-10.49	97.52	120.60
1	1	205	GLY	C-N-CA	10.47	147.87	121.70
1	1	57	ASN	O-C-N	-10.46	105.97	122.70
1	1	21	ALA	C-N-CA	-10.36	95.81	121.70
3	3	67	PHE	CB-CA-C	-10.28	89.83	110.40
3	3	66	TYR	O-C-N	-10.27	106.27	122.70
2	2	146	GLU	CB-CA-C	-10.11	90.19	110.40
2	2	6	GLU	C-N-CA	9.90	146.45	121.70
1	1	97	ARG	CA-C-N	9.80	138.75	117.20
3	3	184	VAL	CA-C-N	-9.79	95.66	117.20
3	3	176	TYR	O-C-N	9.75	138.30	122.70
3	3	202	THR	O-C-N	9.65	139.44	121.10
1	1	246	PHE	O-C-N	-9.64	107.27	122.70
3	3	100	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	1	122	PHE	CA-C-N	-9.57	96.14	117.20
2	2	241	PRO	CA-C-N	-9.48	96.34	117.20
4	4	54	ASN	CB-CA-C	9.43	129.25	110.40
1	1	66	ASN	O-C-N	-9.41	107.65	122.70
2	2	142	THR	O-C-N	9.32	139.04	123.20
1	1	97	ARG	N-CA-CB	9.27	127.28	110.60
1	1	274	GLU	CA-C-N	-9.22	96.92	117.20
1	1	97	ARG	NE-CZ-NH2	9.21	124.90	120.30
3	3	59	THR	O-C-N	9.18	137.39	122.70
1	1	229	GLN	CB-CA-C	-9.14	92.12	110.40
1	1	205	GLY	O-C-N	-9.13	108.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	208	ASP	O-C-N	-9.07	108.19	122.70
1	1	153	PRO	O-C-N	9.06	137.20	122.70
2	2	4	THR	N-CA-CB	-9.03	93.14	110.30
1	1	219	PRO	C-N-CA	-9.02	99.16	121.70
1	1	46	LEU	C-N-CA	-9.00	99.20	121.70
3	3	64	TYR	CA-C-N	8.97	142.21	117.10
2	2	5	GLU	CB-CA-C	-8.92	92.57	110.40
2	2	232	PRO	O-C-N	8.83	136.83	122.70
1	1	274	GLU	N-CA-CB	8.77	126.39	110.60
1	1	84	PRO	CA-C-N	8.74	136.43	117.20
3	3	65	PRO	CB-CA-C	-8.70	90.26	112.00
1	1	222	ASP	C-N-CA	-8.64	100.10	121.70
3	3	76	THR	O-C-N	8.63	136.50	122.70
1	1	42	PRO	O-C-N	8.60	136.47	122.70
3	3	180	THR	C-N-CA	8.58	143.15	121.70
2	2	45	PRO	O-C-N	-8.55	109.03	122.70
3	3	222	MET	C-N-CD	8.49	146.22	128.40
1	1	66	ASN	C-N-CA	8.47	142.86	121.70
3	3	176	TYR	CA-C-N	-8.46	98.60	117.20
1	1	25	LYS	C-N-CA	-8.38	100.75	121.70
1	1	81	SER	O-C-N	-8.38	109.29	122.70
1	1	255	PRO	O-C-N	8.38	136.10	122.70
2	2	142	THR	CA-C-N	-8.34	99.51	116.20
3	3	178	SER	N-CA-C	-8.32	88.54	111.00
1	1	225	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	1	40	ALA	O-C-N	8.18	135.79	122.70
1	1	224	GLY	C-N-CA	8.09	141.93	121.70
1	1	174	HIS	N-CA-CB	-8.07	96.07	110.60
1	1	46	LEU	O-C-N	8.07	135.61	122.70
3	3	179	PRO	CA-C-N	-8.05	99.50	117.20
1	1	170	THR	O-C-N	8.00	135.51	122.70
3	3	226	PRO	CA-C-N	-8.00	99.60	117.20
1	1	146	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	1	273	LEU	C-N-CA	8.00	141.69	121.70
2	2	172	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	1	127	CYS	C-N-CA	7.96	141.59	121.70
1	1	237	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	1	207	SER	CA-C-N	-7.89	99.85	117.20
1	1	107	PRO	CA-N-CD	7.88	122.73	111.70
1	1	111	LYS	O-C-N	-7.88	110.10	122.70
2	2	169	TYR	O-C-N	-7.86	110.12	122.70
1	1	25	LYS	CA-C-N	-7.86	99.92	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	111	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	1	32	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	2	167	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	1	207	SER	C-N-CA	7.75	141.08	121.70
2	2	169	TYR	CB-CG-CD2	-7.72	116.37	121.00
2	2	6	GLU	OE1-CD-OE2	-7.72	114.04	123.30
2	2	4	THR	N-CA-C	7.67	131.70	111.00
3	3	106	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	1	171	ARG	NE-CZ-NH2	7.61	124.11	120.30
3	3	221	ARG	NE-CZ-NH2	7.60	124.10	120.30
2	2	32	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	1	39	ARG	NE-CZ-NH2	7.55	124.08	120.30
2	2	139	GLY	O-C-N	-7.52	110.67	122.70
3	3	77	SER	CB-CA-C	-7.45	95.94	110.10
2	2	158	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	1	12	ASN	O-C-N	-7.42	110.82	122.70
1	1	22	GLU	CA-C-N	7.42	137.87	117.10
3	3	140	ARG	NE-CZ-NH2	7.42	124.01	120.30
3	3	63	ARG	CB-CA-C	7.41	125.22	110.40
2	2	13	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	1	40	ALA	CA-C-N	-7.40	100.91	117.20
2	2	61	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	1	40	ALA	C-N-CA	-7.39	103.22	121.70
1	1	27	PRO	O-C-N	7.39	134.52	122.70
2	2	102	ARG	NE-CZ-NH2	7.38	123.99	120.30
3	3	71	ASN	CA-C-N	7.37	133.42	117.20
2	2	165	THR	O-C-N	7.36	135.70	123.20
3	3	81	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	1	47	ARG	NE-CZ-NH2	7.35	123.97	120.30
3	3	172	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	1	124	PHE	CB-CG-CD1	-7.33	115.67	120.80
2	2	101	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	2	145	MET	O-C-N	-7.32	110.98	122.70
3	3	8	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	1	173	PRO	O-C-N	7.31	134.40	122.70
2	2	74	GLN	O-C-N	7.30	134.39	122.70
3	3	63	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	2	81	ARG	NE-CZ-NH2	7.26	123.93	120.30
3	3	58	ASN	O-C-N	7.26	134.32	122.70
2	2	146	GLU	N-CA-C	7.26	130.59	111.00
3	3	64	TYR	C-N-CD	-7.25	104.65	120.60
3	3	202	THR	CA-C-N	-7.21	96.90	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	SER	O-C-N	7.21	135.46	123.20
1	1	106	PHE	O-C-N	-7.19	107.43	121.10
1	1	92	GLN	O-C-N	7.19	134.21	122.70
1	1	199	PRO	O-C-N	7.18	134.18	122.70
2	2	7	MET	CG-SD-CE	7.17	111.67	100.20
1	1	169	GLU	C-N-CA	-7.16	103.81	121.70
1	1	43	ILE	O-C-N	-7.15	111.05	123.20
1	1	56	PHE	C-N-CA	-7.14	103.84	121.70
1	1	100	GLY	O-C-N	-7.13	111.29	122.70
1	1	141	VAL	O-C-N	7.12	134.09	122.70
1	1	51	ASN	CB-CA-C	-7.12	96.17	110.40
1	1	71	THR	O-C-N	-7.11	107.59	121.10
4	4	54	ASN	O-C-N	-7.11	111.32	122.70
2	2	10	LEU	C-N-CA	7.11	139.47	121.70
2	2	260	ARG	NE-CZ-NH2	7.10	123.85	120.30
3	3	231	PRO	CA-C-N	-7.10	101.59	117.20
2	2	219	GLN	O-C-N	-7.09	111.36	122.70
3	3	82	GLN	O-C-N	7.08	134.03	122.70
1	1	107	PRO	CB-CA-C	7.08	129.69	112.00
2	2	186	TRP	CB-CG-CD2	-7.06	117.42	126.60
3	3	66	TYR	CA-C-N	7.05	132.72	117.20
1	1	75	SER	C-N-CA	-7.05	104.08	121.70
2	2	197	ARG	NE-CZ-NH2	7.03	123.81	120.30
3	3	203	PRO	O-C-N	7.03	133.94	122.70
2	2	45	PRO	CA-C-N	7.01	132.62	117.20
1	1	124	PHE	CD1-CG-CD2	7.00	127.40	118.30
1	1	120	SER	O-C-N	-6.98	107.84	121.10
1	1	57	ASN	CA-C-N	6.98	132.55	117.20
1	1	64	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	2	153	MET	CG-SD-CE	6.93	111.28	100.20
1	1	55	THR	O-C-N	-6.89	111.67	122.70
1	1	184	GLN	O-C-N	-6.88	111.69	122.70
2	2	148	SER	O-C-N	-6.87	111.71	122.70
3	3	178	SER	CB-CA-C	6.86	123.14	110.10
2	2	164	PRO	O-C-N	6.86	133.68	122.70
1	1	31	THR	C-N-CA	-6.83	104.63	121.70
3	3	94	MET	CG-SD-CE	6.82	111.11	100.20
3	3	187	TRP	N-CA-CB	6.78	122.81	110.60
3	3	70	THR	N-CA-C	6.77	129.28	111.00
3	3	59	THR	CA-C-N	-6.75	102.35	117.20
1	1	52	MET	CG-SD-CE	6.74	110.99	100.20
2	2	235	TYR	CB-CG-CD2	-6.74	116.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	46	LEU	CA-C-N	-6.72	102.42	117.20
1	1	272	ILE	CA-CB-CG2	-6.71	97.49	110.90
2	2	144	THR	O-C-N	6.70	133.41	122.70
1	1	192	ASN	O-C-N	-6.68	112.01	122.70
1	1	159	GLN	O-C-N	-6.68	112.02	122.70
1	1	249	ARG	NE-CZ-NH2	6.65	123.62	120.30
4	4	33	ILE	O-C-N	-6.64	112.08	122.70
2	2	260	ARG	C-N-CA	-6.64	105.10	121.70
3	3	69	ALA	CB-CA-C	-6.64	100.14	110.10
2	2	10	LEU	CB-CA-C	-6.64	97.59	110.20
1	1	106	PHE	CB-CA-C	6.60	123.61	110.40
4	4	54	ASN	N-CA-C	-6.59	93.22	111.00
4	4	55	LEU	CA-C-N	6.58	131.69	117.20
3	3	11	LYS	O-C-N	-6.58	112.02	123.20
1	1	79	ASP	O-C-N	6.54	133.16	122.70
2	2	228	ALA	O-C-N	6.54	133.17	122.70
1	1	271	PRO	C-N-CA	6.52	138.00	121.70
3	3	76	THR	CA-C-N	-6.51	102.87	117.20
3	3	33	PRO	O-C-N	6.49	133.08	122.70
3	3	209	LEU	O-C-N	-6.46	112.37	122.70
2	2	145	MET	C-N-CA	-6.44	105.59	121.70
1	1	45	MET	CG-SD-CE	6.44	110.50	100.20
1	1	243	MET	CG-SD-CE	6.40	110.44	100.20
2	2	10	LEU	N-CA-C	6.40	128.28	111.00
3	3	62	LYS	C-N-CA	-6.39	105.73	121.70
1	1	26	LEU	C-N-CA	6.38	148.82	122.00
2	2	24	THR	CB-CA-C	-6.36	94.43	111.60
1	1	31	THR	O-C-N	6.35	132.85	122.70
2	2	186	TRP	CG-CD2-CE3	-6.33	128.21	133.90
2	2	145	MET	CG-SD-CE	6.32	110.31	100.20
3	3	185	ASP	CB-CA-C	-6.32	97.76	110.40
2	2	1	ASP	C-N-CA	-6.30	105.96	121.70
1	1	185	VAL	C-N-CA	6.29	137.41	121.70
1	1	257	PRO	O-C-N	6.28	132.75	122.70
3	3	91	ALA	O-C-N	6.27	132.74	122.70
2	2	168	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	1	185	VAL	CB-CA-C	-6.26	99.51	111.40
1	1	231	ASN	C-N-CA	6.26	137.34	121.70
3	3	77	SER	N-CA-C	6.25	127.88	111.00
2	2	9	ASN	N-CA-CB	-6.23	99.39	110.60
2	2	165	THR	CA-C-N	-6.23	103.75	116.20
4	4	31	ASN	CB-CA-C	6.21	122.81	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	222	MET	CG-SD-CE	6.20	110.13	100.20
1	1	45	MET	CB-CA-C	-6.18	98.05	110.40
3	3	78	MET	CG-SD-CE	6.17	110.07	100.20
1	1	149	PRO	C-N-CA	6.16	137.10	121.70
1	1	59	GLN	O-C-N	6.16	132.55	122.70
2	2	186	TRP	N-CA-CB	-6.15	99.54	110.60
1	1	79	ASP	CA-C-N	-6.13	103.71	117.20
1	1	117	LEU	C-N-CA	-6.12	106.39	121.70
2	2	180	HIS	O-C-N	6.12	132.49	122.70
3	3	79	VAL	O-C-N	6.11	132.47	122.70
1	1	46	LEU	N-CA-CB	6.10	122.61	110.40
3	3	37	MET	CG-SD-CE	6.10	109.97	100.20
1	1	153	PRO	CA-C-N	-6.10	103.78	117.20
2	2	130	MET	CG-SD-CE	6.08	109.93	100.20
3	3	120	MET	CG-SD-CE	6.07	109.91	100.20
1	1	90	PRO	O-C-N	6.07	132.41	122.70
3	3	19	PRO	O-C-N	6.05	132.39	122.70
1	1	109	MET	CG-SD-CE	6.05	109.87	100.20
3	3	90	MET	CG-SD-CE	6.04	109.86	100.20
3	3	144	MET	CG-SD-CE	6.03	109.84	100.20
1	1	106	PHE	CA-CB-CG	-6.02	99.45	113.90
3	3	204	THR	N-CA-C	-6.02	94.75	111.00
1	1	74	PRO	O-C-N	6.01	132.32	122.70
1	1	239	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	1	117	LEU	O-C-N	6.00	132.30	122.70
1	1	50	GLN	O-C-N	5.99	132.29	122.70
3	3	100	ARG	NH1-CZ-NH2	-5.99	112.81	119.40
1	1	78	PRO	O-C-N	5.99	132.28	122.70
2	2	6	GLU	N-CA-CB	5.99	121.38	110.60
1	1	275	LEU	N-CA-C	5.96	127.10	111.00
2	2	214	SER	O-C-N	5.96	132.23	122.70
1	1	275	LEU	N-CA-CB	-5.95	98.51	110.40
1	1	155	ASP	O-C-N	5.94	132.20	122.70
3	3	65	PRO	N-CA-C	5.94	127.53	112.10
2	2	158	ARG	O-C-N	5.94	132.20	122.70
1	1	66	ASN	CA-C-N	5.93	130.24	117.20
1	1	22	GLU	C-N-CA	5.92	146.85	122.00
2	2	186	TRP	CB-CG-CD1	5.91	134.69	127.00
1	1	25	LYS	O-C-N	5.89	132.13	122.70
3	3	49	LYS	O-C-N	-5.86	113.32	122.70
2	2	180	HIS	CA-C-N	-5.84	104.35	117.20
2	2	165	THR	N-CA-C	-5.84	95.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	175	MET	CG-SD-CE	5.84	109.54	100.20
2	2	221	ALA	O-C-N	5.82	132.02	122.70
2	2	3	ASN	N-CA-C	5.81	126.69	111.00
1	1	57	ASN	C-N-CA	5.81	136.22	121.70
4	4	33	ILE	CB-CA-C	5.81	123.21	111.60
2	2	249	LEU	CB-CA-C	-5.80	99.17	110.20
1	1	64	ARG	O-C-N	5.80	131.98	122.70
2	2	232	PRO	CA-C-N	-5.79	104.46	117.20
2	2	181	GLN	O-C-N	5.79	131.96	122.70
3	3	64	TYR	CB-CA-C	-5.78	98.84	110.40
1	1	98	SER	CA-C-N	-5.76	104.68	116.20
4	4	32	SER	CB-CA-C	-5.76	99.16	110.10
1	1	42	PRO	CA-C-N	-5.75	104.54	117.20
1	1	170	THR	CA-C-N	-5.75	104.55	117.20
2	2	266	ALA	O-C-N	-5.74	113.51	122.70
3	3	71	ASN	C-N-CA	-5.74	107.34	121.70
1	1	167	LEU	O-C-N	5.73	132.95	123.20
1	1	94	ARG	CB-CA-C	-5.72	98.97	110.40
2	2	3	ASN	C-N-CA	5.72	135.99	121.70
1	1	149	PRO	O-C-N	-5.71	113.56	122.70
1	1	124	PHE	CB-CG-CD2	-5.71	116.81	120.80
2	2	209	VAL	O-C-N	-5.70	113.58	122.70
4	4	52	LEU	CB-CG-CD1	5.67	120.64	111.00
3	3	164	PRO	O-C-N	5.65	131.74	122.70
3	3	58	ASN	CA-C-N	-5.63	104.81	117.20
1	1	56	PHE	N-CA-CB	-5.63	100.46	110.60
2	2	218	THR	O-C-N	-5.63	113.69	122.70
3	3	66	TYR	N-CA-CB	5.63	120.73	110.60
3	3	77	SER	C-N-CA	5.61	135.74	121.70
2	2	209	VAL	C-N-CA	5.61	135.72	121.70
1	1	24	VAL	CB-CA-C	5.60	122.04	111.40
1	1	73	LEU	CB-CA-C	5.59	120.82	110.20
2	2	220	HIS	O-C-N	-5.58	113.77	122.70
3	3	36	TYR	CB-CA-C	-5.58	99.23	110.40
3	3	62	LYS	O-C-N	5.56	131.60	122.70
1	1	61	ASN	C-N-CA	5.56	135.60	121.70
1	1	105	ASN	O-C-N	-5.55	113.82	122.70
2	2	157	TRP	CB-CA-C	-5.55	99.30	110.40
2	2	186	TRP	CA-CB-CG	5.54	124.23	113.70
1	1	47	ARG	O-C-N	5.54	131.62	121.10
1	1	255	PRO	CA-C-N	-5.53	105.04	117.20
1	1	92	GLN	CA-C-N	-5.50	105.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	166	GLY	O-C-N	5.50	131.50	122.70
1	1	11	SER	O-C-N	5.49	131.48	122.70
1	1	202	TRP	CB-CA-C	-5.48	99.44	110.40
1	1	205	GLY	CA-C-N	5.47	129.24	117.20
1	1	20	VAL	CB-CA-C	-5.46	101.03	111.40
3	3	227	THR	N-CA-C	5.45	125.72	111.00
1	1	198	LEU	N-CA-CB	-5.45	99.50	110.40
3	3	222	MET	C-N-CA	-5.44	99.15	122.00
1	1	185	VAL	O-C-N	-5.43	114.01	122.70
1	1	93	TRP	O-C-N	-5.42	114.04	122.70
1	1	31	THR	CA-C-N	-5.40	105.32	117.20
3	3	10	HIS	C-N-CA	5.40	135.20	121.70
1	1	65	LEU	O-C-N	-5.38	114.09	122.70
4	4	31	ASN	O-C-N	-5.37	114.11	122.70
3	3	11	LYS	C-N-CA	-5.35	111.07	122.30
2	2	265	ILE	CB-CA-C	-5.34	100.91	111.60
3	3	230	VAL	CB-CA-C	-5.34	101.24	111.40
2	2	199	ASN	CB-CA-C	-5.32	99.76	110.40
2	2	186	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	1	167	LEU	CA-C-N	-5.31	105.58	116.20
2	2	198	THR	O-C-N	5.31	131.19	122.70
1	1	141	VAL	CA-C-N	-5.30	105.53	117.20
3	3	11	LYS	CA-C-N	5.29	126.78	116.20
1	1	174	HIS	CA-CB-CG	5.29	122.59	113.60
2	2	236	ALA	O-C-N	5.29	131.16	122.70
1	1	234	ALA	C-N-CA	5.28	134.90	121.70
1	1	27	PRO	CA-C-N	-5.27	105.61	117.20
1	1	137	GLY	O-C-N	5.27	131.13	122.70
1	1	208	ASP	CA-C-N	5.27	128.79	117.20
2	2	8	GLU	N-CA-CB	-5.25	101.14	110.60
1	1	173	PRO	C-N-CA	5.21	134.74	121.70
1	1	18	ASP	N-CA-CB	5.21	119.98	110.60
2	2	11	SER	N-CA-C	5.21	125.07	111.00
1	1	72	PRO	C-N-CA	-5.21	108.68	121.70
3	3	82	GLN	CA-C-N	-5.20	105.76	117.20
3	3	162	THR	O-C-N	5.20	131.01	122.70
3	3	229	TRP	CA-CB-CG	5.20	123.57	113.70
4	4	12	ASN	O-C-N	5.19	131.00	122.70
4	4	23	ASN	O-C-N	5.18	130.99	122.70
1	1	127	CYS	O-C-N	-5.17	114.43	122.70
1	1	268	ASN	C-N-CA	-5.16	100.32	122.00
3	3	76	THR	C-N-CA	5.16	134.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	176	TRP	CA-CB-CG	5.12	123.43	113.70
1	1	156	VAL	C-N-CA	5.12	134.50	121.70
2	2	11	SER	CB-CA-C	-5.12	100.38	110.10
3	3	231	PRO	CA-N-CD	5.11	118.85	111.70
1	1	162	GLY	C-N-CA	5.10	134.45	121.70
3	3	81	TYR	N-CA-CB	5.08	119.74	110.60
2	2	173	THR	O-C-N	5.07	131.82	123.20
1	1	94	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	1	162	GLY	O-C-N	5.06	130.79	122.70
2	2	10	LEU	O-C-N	5.05	130.79	122.70
1	1	124	PHE	CA-CB-CG	-5.05	101.78	113.90
1	1	17	VAL	CB-CA-C	-5.04	101.82	111.40
3	3	229	TRP	O-C-N	-5.04	114.64	122.70
1	1	59	GLN	C-N-CA	5.03	134.27	121.70
2	2	134	PHE	N-CA-CB	-5.02	101.57	110.60
2	2	169	TYR	CA-C-N	5.01	128.23	117.20

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	GLY	Peptide,Mainchain
1	1	107	PRO	Peptide,Mainchain
1	1	111	LYS	Mainchain
1	1	12	ASN	Mainchain
1	1	122	PHE	Mainchain
1	1	149	PRO	Peptide,Mainchain
1	1	158	ASP	Peptide,Mainchain
1	1	182	ASN	Mainchain
1	1	205	GLY	Peptide,Mainchain
1	1	246	PHE	Mainchain
1	1	25	LYS	Mainchain
1	1	261	THR	Peptide
1	1	263	LYS	Peptide
1	1	267	ASP	Peptide
1	1	269	PRO	Peptide
1	1	274	GLU	Peptide
1	1	275	LEU	Peptide
1	1	32	ARG	Peptide,Mainchain
1	1	56	PHE	Mainchain
1	1	57	ASN	Peptide
1	1	65	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	1	81	SER	Peptide,Mainchain
1	1	84	PRO	Peptide,Mainchain
1	1	86	LYS	Peptide
1	1	87	THR	Peptide
1	1	88	LYS	Peptide,Mainchain
1	1	95	TRP	Peptide,Mainchain
1	1	96	VAL	Peptide
1	1	97	ARG	Peptide,Mainchain
1	1	99	GLY	Peptide
2	2	1	ASP	Peptide,Mainchain
2	2	146	GLU	Peptide
2	2	197	ARG	Sidechain
2	2	2	GLN	Mainchain
2	2	220	HIS	Mainchain
2	2	238	GLY	Peptide
2	2	3	ASN	Peptide,Mainchain
2	2	4	THR	Peptide
2	2	5	GLU	Peptide,Mainchain
2	2	6	GLU	Peptide,Mainchain
2	2	8	GLU	Mainchain
3	3	100	ARG	Sidechain
3	3	178	SER	Peptide
3	3	180	THR	Peptide,Mainchain
3	3	222	MET	Mainchain
3	3	70	THR	Mainchain
3	3	73	VAL	Peptide
3	3	74	PRO	Peptide
4	4	34	ASP	Peptide,Mainchain
4	4	55	LEU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2156	0	2050	880	0
2	2	2078	0	1953	564	0
3	3	1785	0	1711	472	0
4	4	241	0	220	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6260	0	5934	1795	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 147.

All (1795) 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)
2:2:183:GLN:HB2	2:2:186:TRP:CZ3	1.31	1.64
3:3:7:VAL:CG2	3:3:11:LYS:HE2	1.18	1.62
1:1:192:ASN:HB3	3:3:222:MET:CE	1.17	1.61
1:1:192:ASN:CB	3:3:222:MET:HE1	1.14	1.61
1:1:108:LEU:CD1	1:1:112:GLN:HE22	0.98	1.59
1:1:68:LEU:HD21	1:1:70:LEU:CD1	1.34	1.56
3:3:83:VAL:CG1	3:3:186:GLY:HA3	1.24	1.56
1:1:274:GLU:HG2	1:1:275:LEU:CB	1.33	1.56
1:1:175:MET:CE	1:1:187:PHE:CG	1.89	1.55
1:1:146:ARG:CD	1:1:167:LEU:HD11	1.13	1.55
2:2:183:GLN:CA	2:2:186:TRP:CE3	1.84	1.55
1:1:274:GLU:CG	1:1:275:LEU:HB2	1.37	1.55
3:3:127:ILE:CG2	3:3:161:PHE:CE2	1.82	1.54
2:2:183:GLN:CB	2:2:186:TRP:CZ3	1.92	1.53
1:1:71:THR:CG2	1:1:92:GLN:NE2	1.67	1.52
1:1:175:MET:HE1	1:1:187:PHE:CD2	1.44	1.51
1:1:108:LEU:HD23	2:2:175:PHE:CE2	1.45	1.50
1:1:148:ALA:HB2	1:1:227:TRP:CH2	1.44	1.50
1:1:108:LEU:CD2	2:2:175:PHE:HE2	1.23	1.49
2:2:183:GLN:HA	2:2:186:TRP:CE3	1.39	1.49
3:3:7:VAL:HG23	3:3:11:LYS:CE	1.02	1.48
1:1:175:MET:HE1	1:1:187:PHE:CG	0.98	1.48
1:1:146:ARG:HD2	1:1:167:LEU:CD1	1.42	1.48
1:1:175:MET:HE1	1:1:187:PHE:CD1	1.49	1.47
1:1:146:ARG:HB3	1:1:227:TRP:CE3	1.48	1.46
2:2:183:GLN:CB	2:2:186:TRP:CE3	1.96	1.45
1:1:251:THR:C	1:1:252:LEU:N	1.69	1.45
1:1:47:ARG:HE	1:1:233:SER:CB	1.26	1.44
1:1:149:PRO:HB3	1:1:192:ASN:ND2	1.25	1.43
2:2:259:LEU:C	2:2:260:ARG:N	1.69	1.43
1:1:47:ARG:NE	1:1:233:SER:HB2	1.21	1.43
1:1:175:MET:CE	1:1:187:PHE:CD1	2.01	1.43
3:3:83:VAL:HG12	3:3:186:GLY:CA	1.46	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:GLY:O	1:1:101:VAL:CG2	1.67	1.41
2:2:67:LEU:CD2	2:2:82:ILE:CD1	1.99	1.41
1:1:254:PHE:CD1	1:1:255:PRO:HD2	1.53	1.40
2:2:145:MET:O	2:2:169:TYR:CE2	1.75	1.40
3:3:78:MET:CE	3:3:192:GLN:OE1	1.64	1.40
1:1:90:PRO:O	1:1:91:VAL:CG2	1.69	1.40
1:1:259:PRO:CB	1:1:260:THR:N	1.85	1.40
1:1:54:THR:O	1:1:160:LEU:CD2	1.68	1.39
1:1:75:SER:C	1:1:76:PHE:N	1.75	1.39
1:1:263:LYS:HG2	1:1:264:ILE:CA	1.50	1.39
2:2:70:TRP:CD1	2:2:233:LEU:HD21	1.58	1.39
1:1:108:LEU:CD2	2:2:175:PHE:CE2	2.02	1.38
1:1:251:THR:H	2:2:185:GLN:NE2	1.17	1.37
2:2:143:GLY:C	2:2:144:THR:N	1.77	1.37
2:2:136:THR:CG2	2:2:137:GLY:H	1.32	1.36
2:2:10:LEU:O	2:2:13:ARG:HB2	1.28	1.34
1:1:79:ASP:N	1:1:84:PRO:HB3	1.41	1.33
2:2:143:GLY:O	2:2:144:THR:HG22	1.26	1.33
1:1:6:GLU:HB3	2:2:193:ILE:CG2	1.58	1.33
3:3:48:CYS:SG	3:3:95:LEU:HB2	1.66	1.33
1:1:68:LEU:CD2	1:1:70:LEU:CD1	2.06	1.33
1:1:108:LEU:HD12	1:1:112:GLN:NE2	1.01	1.32
2:2:161:GLN:HB2	2:2:167:TYR:OH	1.16	1.32
2:2:67:LEU:HD11	2:2:247:ALA:CB	1.58	1.32
2:2:67:LEU:HD21	2:2:82:ILE:CD1	1.57	1.32
2:2:259:LEU:HD23	2:2:260:ARG:N	1.01	1.31
1:1:259:PRO:HB2	1:1:260:THR:N	0.99	1.31
3:3:78:MET:HE1	3:3:192:GLN:CG	1.58	1.31
1:1:186:SER:HB2	3:3:10:HIS:ND1	1.40	1.30
1:1:96:VAL:CG2	1:1:108:LEU:HD11	1.60	1.30
1:1:261:THR:OG1	1:1:262:THR:HA	1.27	1.30
1:1:47:ARG:NH2	1:1:233:SER:H	1.26	1.30
1:1:78:PRO:C	1:1:84:PRO:HB3	1.51	1.30
1:1:124:PHE:HZ	2:2:133:GLU:OE1	1.04	1.30
3:3:7:VAL:CG2	3:3:11:LYS:CE	1.86	1.30
2:2:166:GLY:O	2:2:179:ASN:ND2	1.64	1.29
2:2:52:ALA:HB1	2:2:256:PHE:O	1.32	1.29
1:1:146:ARG:CD	1:1:167:LEU:CD1	2.03	1.29
2:2:259:LEU:CD2	2:2:260:ARG:N	1.95	1.29
1:1:124:PHE:CZ	2:2:133:GLU:OE1	1.85	1.27
1:1:68:LEU:CD2	1:1:70:LEU:HD11	1.61	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:268:ASN:HD22	1:1:269:PRO:CD	1.46	1.27
3:3:8:ARG:O	3:3:11:LYS:HG3	1.32	1.27
1:1:130:GLU:OE1	1:1:241:LYS:NZ	1.62	1.27
1:1:149:PRO:CB	1:1:192:ASN:HD22	1.45	1.27
2:2:260:ARG:C	2:2:261:HIS:N	1.88	1.27
1:1:72:PRO:O	1:1:73:LEU:HD13	1.32	1.27
1:1:105:ASN:OD1	2:2:175:PHE:CE1	1.88	1.27
1:1:251:THR:N	2:2:185:GLN:HE22	1.30	1.27
1:1:211:ASN:O	1:1:213:LYS:N	1.67	1.26
1:1:272:ILE:CG1	1:1:272:ILE:CB	2.13	1.26
2:2:70:TRP:CG	2:2:233:LEU:HD21	1.69	1.26
1:1:71:THR:HG21	1:1:92:GLN:CD	1.56	1.26
1:1:74:PRO:O	1:1:92:GLN:HG3	1.11	1.25
1:1:258:THR:OG1	1:1:259:PRO:HD3	1.10	1.25
1:1:47:ARG:HH21	1:1:233:SER:N	1.35	1.25
2:2:43:GLU:O	2:2:107:LYS:NZ	1.69	1.25
1:1:258:THR:OG1	1:1:259:PRO:CD	1.83	1.24
1:1:263:LYS:CG	1:1:264:ILE:HA	1.68	1.24
3:3:127:ILE:O	3:3:148:TYR:HB2	1.32	1.23
3:3:86:SER:HB2	3:3:175:SER:CB	1.68	1.22
3:3:54:LEU:O	3:3:54:LEU:HD22	1.35	1.22
3:3:78:MET:HE2	3:3:192:GLN:OE1	1.11	1.22
1:1:45:MET:CB	1:1:64:ARG:HG2	1.40	1.22
1:1:74:PRO:O	1:1:92:GLN:CG	1.87	1.20
3:3:84:ALA:O	3:3:86:SER:N	1.73	1.20
1:1:122:PHE:CD2	1:1:245:VAL:HG21	1.76	1.20
3:3:69:ALA:O	3:3:70:THR:CG2	1.88	1.20
1:1:274:GLU:OE2	1:1:275:LEU:HD22	1.38	1.19
1:1:96:VAL:HG21	1:1:112:GLN:OE1	1.04	1.19
2:2:183:GLN:HA	2:2:186:TRP:CD2	1.75	1.19
1:1:97:ARG:HD2	2:2:172:ARG:HD2	1.25	1.19
2:2:67:LEU:CD1	2:2:247:ALA:CB	2.21	1.18
3:3:109:LEU:O	3:3:162:THR:HG23	1.43	1.18
1:1:48:PRO:HD3	1:1:233:SER:OG	1.36	1.18
1:1:122:PHE:CG	1:1:245:VAL:CG2	2.27	1.18
3:3:86:SER:HB2	3:3:175:SER:HB3	1.22	1.18
2:2:6:GLU:OE1	2:2:9:ASN:HA	1.41	1.17
1:1:46:LEU:HD23	1:1:228:ILE:HG22	1.22	1.17
1:1:105:ASN:C	1:1:106:PHE:N	1.95	1.17
1:1:68:LEU:CG	1:1:70:LEU:HD13	1.75	1.17
1:1:273:LEU:CD1	1:1:274:GLU:HA	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:259:LEU:C	2:2:259:LEU:HD23	1.65	1.17
1:1:192:ASN:CB	3:3:222:MET:CE	1.89	1.17
2:2:145:MET:O	2:2:169:TYR:CZ	1.97	1.17
1:1:47:ARG:CZ	1:1:233:SER:HB2	1.73	1.16
1:1:72:PRO:O	1:1:73:LEU:CD1	1.93	1.16
3:3:67:PHE:HZ	3:3:125:PHE:CE2	1.61	1.16
1:1:186:SER:CB	3:3:10:HIS:CE1	2.28	1.16
3:3:127:ILE:HG21	3:3:161:PHE:CD2	1.79	1.16
1:1:96:VAL:CG2	1:1:112:GLN:OE1	1.92	1.16
3:3:48:CYS:SG	3:3:95:LEU:CB	2.33	1.16
3:3:77:SER:OG	3:3:78:MET:N	1.72	1.16
1:1:131:VAL:HG11	1:1:187:PHE:CE1	1.81	1.16
2:2:112:VAL:HG22	2:2:249:LEU:CD2	1.76	1.16
3:3:78:MET:HE2	3:3:192:GLN:CD	1.64	1.16
2:2:112:VAL:HG22	2:2:249:LEU:HD22	1.25	1.16
3:3:176:TYR:OH	3:3:226:PRO:HB3	1.45	1.16
1:1:186:SER:HB2	3:3:10:HIS:CE1	1.81	1.15
2:2:259:LEU:HD23	2:2:260:ARG:CA	1.77	1.15
2:2:9:ASN:O	2:2:27:GLN:O	1.63	1.15
1:1:77:CYS:SG	1:1:85:GLN:HG3	1.87	1.14
1:1:206:TRP:O	2:2:219:GLN:NE2	1.77	1.14
1:1:47:ARG:NH2	1:1:233:SER:N	1.94	1.14
1:1:78:PRO:C	1:1:84:PRO:CB	2.15	1.14
2:2:143:GLY:O	2:2:144:THR:CG2	1.96	1.14
2:2:67:LEU:HD23	2:2:82:ILE:HD12	1.15	1.13
1:1:251:THR:N	2:2:185:GLN:NE2	1.90	1.13
2:2:7:MET:HA	2:2:120:GLN:OE1	1.47	1.13
2:2:82:ILE:HG22	2:2:225:LEU:HB3	1.24	1.13
2:2:24:THR:CG2	2:2:25:ASN:N	2.03	1.13
3:3:127:ILE:CG2	3:3:161:PHE:HE2	1.31	1.13
3:3:198:TYR:O	3:3:198:TYR:HD1	1.31	1.13
1:1:77:CYS:HB3	1:1:85:GLN:OE1	1.47	1.12
2:2:168:ARG:HG2	2:2:169:TYR:N	1.50	1.13
2:2:171:SER:O	2:2:172:ARG:HG2	1.48	1.13
3:3:127:ILE:HG23	3:3:161:PHE:HE2	0.96	1.13
2:2:67:LEU:CD1	2:2:247:ALA:HB2	1.76	1.12
3:3:54:LEU:O	3:3:54:LEU:CD2	1.97	1.12
3:3:126:LEU:HD21	3:3:148:TYR:HD2	1.06	1.12
2:2:136:THR:HG22	2:2:137:GLY:H	1.05	1.12
1:1:94:ARG:HG3	1:1:217:VAL:CG2	1.80	1.12
2:2:5:GLU:HB3	2:2:6:GLU:HG2	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:268:ASN:ND2	1:1:269:PRO:HD2	1.65	1.11
3:3:69:ALA:O	3:3:70:THR:HG23	0.96	1.11
2:2:71:THR:C	2:2:233:LEU:HD13	1.70	1.11
3:3:112:LEU:HD21	3:3:211:LEU:HD12	1.31	1.11
1:1:4:ASN:O	1:1:7:LYS:CD	1.99	1.11
1:1:71:THR:HG22	1:1:92:GLN:NE2	1.49	1.11
3:3:127:ILE:CG2	3:3:161:PHE:CD2	2.33	1.11
1:1:6:GLU:CB	2:2:193:ILE:HG22	1.78	1.10
2:2:45:PRO:O	2:2:47:SER:N	1.84	1.10
3:3:202:THR:HB	3:3:203:PRO:HD2	1.29	1.10
3:3:34:SER:O	3:3:35:ASP:HB2	1.30	1.10
3:3:99:ALA:HA	3:3:220:LEU:CD2	1.80	1.10
1:1:146:ARG:HB3	1:1:227:TRP:CZ3	1.86	1.10
3:3:78:MET:CE	3:3:192:GLN:CG	2.27	1.10
3:3:78:MET:CE	3:3:192:GLN:CD	2.18	1.10
1:1:96:VAL:HG22	1:1:108:LEU:HD11	1.11	1.09
3:3:99:ALA:HA	3:3:220:LEU:HD21	1.10	1.09
2:2:67:LEU:HD11	2:2:247:ALA:HB3	1.26	1.09
1:1:142:ALA:HB3	1:1:231:ASN:HB2	1.20	1.09
2:2:13:ARG:NH2	2:2:198:THR:O	1.84	1.09
2:2:129:PHE:HZ	2:2:186:TRP:CD1	1.70	1.09
1:1:250:PRO:HB3	2:2:185:GLN:HB2	1.31	1.09
3:3:48:CYS:SG	3:3:95:LEU:HA	1.91	1.09
3:3:229:TRP:O	3:3:230:VAL:HB	1.30	1.09
2:2:136:THR:HG22	2:2:137:GLY:N	1.61	1.09
2:2:129:PHE:CZ	2:2:186:TRP:CD1	2.41	1.08
3:3:52:THR:O	3:3:53:PHE:HB2	1.47	1.08
3:3:198:TYR:O	3:3:198:TYR:CD1	2.04	1.08
1:1:101:VAL:HG21	1:1:104:ALA:HB2	1.34	1.08
1:1:141:VAL:HG12	1:1:142:ALA:O	1.52	1.08
1:1:250:PRO:CA	2:2:185:GLN:HE21	1.66	1.08
1:1:93:TRP:O	1:1:94:ARG:CB	1.98	1.08
1:1:105:ASN:OD1	2:2:175:PHE:HE1	1.26	1.08
2:2:161:GLN:CB	2:2:167:TYR:OH	2.02	1.08
1:1:148:ALA:HB2	1:1:227:TRP:CZ2	1.89	1.07
1:1:221:ALA:O	1:1:222:ASP:HB2	1.28	1.07
3:3:127:ILE:HG22	3:3:161:PHE:CE2	1.61	1.07
3:3:83:VAL:HG11	3:3:186:GLY:HA3	1.35	1.07
3:3:99:ALA:O	3:3:174:THR:HG21	1.53	1.07
2:2:146:GLU:HG3	2:2:146:GLU:O	1.36	1.07
2:2:183:GLN:HB3	2:2:186:TRP:CZ3	1.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:THR:HG21	1:1:92:GLN:NE2	1.37	1.07
1:1:122:PHE:CB	1:1:245:VAL:CG2	2.32	1.07
1:1:250:PRO:HA	2:2:185:GLN:HE21	1.13	1.07
1:1:46:LEU:HD23	1:1:228:ILE:CG2	1.83	1.07
1:1:146:ARG:CG	1:1:167:LEU:CD1	2.31	1.07
2:2:24:THR:HG22	2:2:25:ASN:N	1.70	1.06
2:2:52:ALA:HB2	2:2:257:ASN:HB3	1.11	1.06
1:1:264:ILE:HG12	1:1:265:ASN:H	0.95	1.06
2:2:134:PHE:HD2	2:2:224:THR:HG21	1.18	1.06
2:2:134:PHE:CD2	2:2:224:THR:HG21	1.88	1.06
1:1:175:MET:CE	1:1:187:PHE:CD2	2.23	1.06
1:1:261:THR:CG2	1:1:262:THR:HB	1.85	1.06
3:3:126:LEU:HD21	3:3:148:TYR:CD2	1.91	1.06
1:1:68:LEU:HD23	1:1:226:LEU:CD2	1.85	1.06
1:1:174:HIS:HB3	3:3:16:SER:CB	1.87	1.05
3:3:230:VAL:O	3:3:230:VAL:HG12	1.26	1.05
1:1:105:ASN:CA	1:1:106:PHE:N	2.19	1.05
1:1:133:VAL:HG22	1:1:185:VAL:HG12	1.29	1.05
1:1:54:THR:C	1:1:160:LEU:HD21	1.74	1.05
1:1:192:ASN:CA	3:3:222:MET:CE	2.35	1.05
3:3:230:VAL:O	3:3:230:VAL:CG1	1.97	1.05
1:1:71:THR:HG21	1:1:92:GLN:OE1	1.54	1.04
1:1:90:PRO:C	1:1:91:VAL:HG23	1.74	1.04
1:1:96:VAL:HG23	1:1:110:THR:CG2	1.87	1.04
1:1:108:LEU:HD21	2:2:175:PHE:CE2	1.89	1.04
1:1:122:PHE:CG	1:1:245:VAL:HG23	1.91	1.04
1:1:175:MET:HE3	1:1:187:PHE:CD1	1.87	1.04
2:2:143:GLY:C	2:2:144:THR:CA	2.25	1.04
3:3:214:ALA:HB1	3:3:218:PHE:CG	1.92	1.04
1:1:47:ARG:CG	1:1:48:PRO:HD2	1.88	1.04
1:1:148:ALA:CB	1:1:227:TRP:CH2	2.40	1.04
1:1:268:ASN:ND2	1:1:269:PRO:CD	2.19	1.04
2:2:136:THR:CG2	2:2:137:GLY:N	2.06	1.04
1:1:125:TYR:CE1	1:1:199:PRO:O	2.10	1.04
2:2:112:VAL:HG21	2:2:130:MET:HE3	1.33	1.04
3:3:126:LEU:CD2	3:3:148:TYR:HD2	1.70	1.04
2:2:172:ARG:O	2:2:173:THR:OG1	1.75	1.03
3:3:52:THR:HG21	3:3:94:MET:H	1.23	1.03
3:3:8:ARG:HH11	3:3:8:ARG:CG	1.70	1.03
1:1:4:ASN:O	1:1:7:LYS:HD2	1.57	1.03
1:1:46:LEU:CD2	1:1:228:ILE:CG2	2.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:ARG:HG3	1:1:48:PRO:CD	1.87	1.03
1:1:192:ASN:CA	3:3:222:MET:HE3	1.89	1.03
3:3:127:ILE:O	3:3:148:TYR:CB	2.06	1.03
1:1:47:ARG:HA	1:1:233:SER:OG	1.57	1.02
1:1:35:PHE:HE1	1:1:39:ARG:HH12	1.04	1.02
1:1:79:ASP:CA	1:1:84:PRO:HB3	1.89	1.02
1:1:196:SER:O	1:1:197:VAL:HG13	1.59	1.02
3:3:73:VAL:HG22	3:3:74:PRO:O	1.57	1.02
4:4:33:ILE:O	4:4:34:ASP:HB2	1.55	1.02
1:1:150:THR:HG21	1:1:222:ASP:O	1.60	1.02
3:3:8:ARG:O	3:3:11:LYS:CG	2.08	1.02
3:3:8:ARG:NH1	3:3:8:ARG:HG2	1.59	1.02
2:2:150:PRO:O	2:2:151:PHE:CD1	2.13	1.02
3:3:48:CYS:HB2	3:3:98:VAL:HG11	1.41	1.02
3:3:79:VAL:HG12	3:3:190:VAL:HG12	1.36	1.02
2:2:67:LEU:HD21	2:2:82:ILE:HD13	1.02	1.01
2:2:206:VAL:HG11	2:2:223:TRP:CH2	1.95	1.01
1:1:77:CYS:SG	1:1:85:GLN:CG	2.47	1.01
1:1:154:ALA:HB1	1:1:225:ARG:HD3	1.41	1.01
1:1:122:PHE:CG	1:1:245:VAL:HG21	1.93	1.01
1:1:226:LEU:HG	1:1:226:LEU:O	1.58	1.01
2:2:146:GLU:HA	2:2:169:TYR:HE2	1.20	1.01
2:2:194:LEU:HD23	2:2:199:ASN:HB3	1.40	1.01
1:1:90:PRO:O	1:1:91:VAL:HG23	0.83	1.01
1:1:146:ARG:CB	1:1:227:TRP:CE3	2.41	1.01
1:1:192:ASN:HA	3:3:222:MET:HE3	1.38	1.01
3:3:77:SER:OG	3:3:78:MET:SD	2.15	1.01
1:1:273:LEU:HD12	1:1:274:GLU:HA	1.01	1.00
2:2:82:ILE:CG2	2:2:225:LEU:HB3	1.91	1.00
1:1:45:MET:HB3	1:1:64:ARG:HG2	1.37	1.00
1:1:94:ARG:O	1:1:95:TRP:HB3	1.61	1.00
2:2:38:LYS:O	2:2:207:PRO:HG3	1.60	1.00
3:3:91:ALA:O	3:3:92:ASN:HB2	1.57	1.00
1:1:254:PHE:CD1	1:1:255:PRO:CD	2.44	1.00
1:1:261:THR:OG1	1:1:262:THR:CA	2.08	1.00
2:2:67:LEU:HD23	2:2:82:ILE:CD1	1.75	1.00
2:2:168:ARG:HG2	2:2:169:TYR:H	0.85	1.00
3:3:24:PRO:O	3:3:25:ILE:HG22	1.61	1.00
3:3:78:MET:HE1	3:3:192:GLN:HG3	1.42	1.00
1:1:89:ALA:HB1	1:1:225:ARG:NH2	1.77	1.00
2:2:82:ILE:HG22	2:2:82:ILE:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:196:LEU:HD23	3:3:196:LEU:O	1.61	1.00
1:1:86:LYS:O	1:1:88:LYS:O	1.80	1.00
2:2:136:THR:HG23	2:2:137:GLY:H	1.22	1.00
1:1:268:ASN:HD22	1:1:269:PRO:N	1.58	1.00
1:1:99:GLY:C	1:1:101:VAL:HG22	1.82	0.99
1:1:175:MET:SD	1:1:187:PHE:CE2	2.56	0.99
2:2:70:TRP:CG	2:2:233:LEU:CD2	2.45	0.99
3:3:48:CYS:SG	3:3:95:LEU:CA	2.49	0.99
3:3:99:ALA:CA	3:3:220:LEU:HD21	1.92	0.99
1:1:275:LEU:HG	1:1:276:GLU:HA	1.41	0.99
2:2:113:GLN:HG3	2:2:203:ASP:OD1	1.61	0.99
4:4:26:SER:O	4:4:29:TYR:N	1.95	0.99
2:2:161:GLN:HB2	2:2:167:TYR:HH	1.20	0.99
1:1:96:VAL:HG23	1:1:110:THR:HG23	1.43	0.99
1:1:146:ARG:CG	1:1:167:LEU:HD12	1.93	0.99
1:1:221:ALA:O	1:1:222:ASP:CB	2.08	0.99
2:2:162:GLY:O	2:2:163:ALA:HB2	1.60	0.99
1:1:215:PHE:N	2:2:146:GLU:OE1	1.95	0.99
1:1:254:PHE:HD1	1:1:255:PRO:CD	1.74	0.99
1:1:264:ILE:HG12	1:1:265:ASN:N	1.77	0.99
2:2:72:THR:N	2:2:233:LEU:HD13	1.75	0.98
3:3:85:LEU:HD21	3:3:99:ALA:HB1	1.42	0.98
1:1:175:MET:CE	1:1:187:PHE:CE1	2.46	0.98
1:1:261:THR:HG23	1:1:262:THR:CB	1.93	0.98
3:3:138:THR:HG22	3:3:142:GLN:HE22	1.28	0.98
1:1:131:VAL:HG21	1:1:187:PHE:CZ	1.98	0.98
3:3:54:LEU:H	3:3:54:LEU:HD13	1.28	0.98
3:3:176:TYR:HH	3:3:226:PRO:HB3	1.13	0.98
1:1:273:LEU:HD12	1:1:274:GLU:CA	1.93	0.98
2:2:82:ILE:CG2	2:2:82:ILE:O	2.09	0.98
2:2:183:GLN:HB2	2:2:186:TRP:CE3	1.79	0.98
1:1:68:LEU:CD2	1:1:236:VAL:HG11	1.92	0.98
2:2:161:GLN:O	2:2:163:ALA:N	1.97	0.98
1:1:174:HIS:HB3	3:3:16:SER:HB3	1.41	0.98
2:2:99:THR:HG23	2:2:256:PHE:HE2	1.26	0.98
2:2:6:GLU:OE2	2:2:13:ARG:NH1	1.95	0.98
2:2:213:PRO:O	2:2:214:SER:HB2	1.64	0.98
2:2:259:LEU:C	2:2:259:LEU:CD2	2.28	0.98
3:3:127:ILE:HG23	3:3:161:PHE:CE2	1.74	0.98
3:3:176:TYR:OH	3:3:226:PRO:CB	2.11	0.97
1:1:105:ASN:HA	1:1:106:PHE:N	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:67:LEU:CD2	2:2:82:ILE:HD12	1.80	0.97
3:3:70:THR:O	3:3:72:SER:N	1.96	0.97
3:3:103:ASN:HB2	3:3:224:ILE:HD12	1.45	0.97
1:1:250:PRO:HB3	2:2:185:GLN:CB	1.93	0.97
1:1:54:THR:HA	1:1:160:LEU:HD11	1.45	0.97
1:1:68:LEU:HG	1:1:70:LEU:HD13	1.40	0.97
1:1:261:THR:HG23	1:1:262:THR:HB	0.97	0.97
3:3:8:ARG:HH11	3:3:8:ARG:HG2	0.82	0.97
2:2:217:TRP:CE3	2:2:217:TRP:O	2.18	0.97
1:1:133:VAL:CG2	1:1:185:VAL:HG12	1.93	0.96
3:3:7:VAL:CG2	3:3:11:LYS:NZ	2.26	0.96
2:2:67:LEU:CD1	2:2:247:ALA:HB3	1.89	0.96
1:1:186:SER:HB3	3:3:10:HIS:CE1	1.97	0.96
2:2:83:PRO:O	2:2:87:VAL:HG12	1.64	0.96
1:1:53:GLU:OE2	1:1:164:THR:CA	2.12	0.96
1:1:146:ARG:CG	1:1:167:LEU:HD11	1.93	0.96
1:1:148:ALA:HB2	1:1:227:TRP:HH2	1.20	0.96
3:3:224:ILE:HG22	3:3:225:SER:H	1.29	0.96
1:1:46:LEU:HD22	1:1:228:ILE:HB	1.46	0.96
1:1:68:LEU:HD23	1:1:226:LEU:HD22	1.45	0.96
2:2:67:LEU:HD11	2:2:247:ALA:HB2	1.40	0.96
1:1:194:PRO:O	3:3:169:THR:HG23	1.64	0.96
2:2:252:VAL:HG22	2:2:253:ASN:OD1	1.65	0.96
1:1:6:GLU:HB3	2:2:193:ILE:HG22	0.96	0.96
1:1:77:CYS:CB	1:1:85:GLN:OE1	2.13	0.96
1:1:146:ARG:HB3	1:1:227:TRP:HE3	1.18	0.96
3:3:176:TYR:HH	3:3:226:PRO:CB	1.78	0.95
3:3:67:PHE:CZ	3:3:125:PHE:CE2	2.54	0.95
2:2:24:THR:HG23	2:2:25:ASN:N	1.80	0.95
2:2:260:ARG:HG2	2:2:261:HIS:N	1.81	0.95
3:3:52:THR:O	3:3:53:PHE:CB	2.11	0.95
1:1:53:GLU:O	1:1:54:THR:OG1	1.85	0.95
1:1:78:PRO:O	1:1:84:PRO:O	1.85	0.95
1:1:105:ASN:CG	2:2:175:PHE:CE1	2.39	0.95
3:3:34:SER:O	3:3:35:ASP:CB	2.14	0.95
3:3:83:VAL:CG1	3:3:186:GLY:CA	2.20	0.95
2:2:70:TRP:HD1	2:2:74:GLN:HE22	1.08	0.95
3:3:48:CYS:HG	3:3:95:LEU:HB2	1.19	0.95
1:1:175:MET:HE3	1:1:187:PHE:CE1	2.01	0.95
2:2:183:GLN:CA	2:2:186:TRP:HE3	1.42	0.95
2:2:222:ASN:H	2:2:222:ASN:ND2	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:VAL:CG1	1:1:187:PHE:CE1	2.50	0.95
3:3:224:ILE:CG2	3:3:225:SER:H	1.80	0.95
1:1:68:LEU:HD21	1:1:70:LEU:HD11	0.97	0.94
1:1:99:GLY:O	1:1:101:VAL:HG22	0.77	0.94
1:1:154:ALA:O	1:1:227:TRP:NE1	1.99	0.94
3:3:87:CYS:SG	3:3:88:SER:N	2.40	0.94
3:3:161:PHE:HD1	3:3:162:THR:H	1.03	0.94
1:1:68:LEU:HD22	1:1:236:VAL:HG11	1.49	0.94
1:1:268:ASN:HD22	1:1:269:PRO:HD2	1.18	0.94
2:2:192:GLN:HG2	2:2:202:VAL:HG23	1.48	0.94
3:3:100:ARG:HG3	3:3:226:PRO:HG3	1.47	0.94
1:1:68:LEU:HD21	1:1:70:LEU:HD12	1.48	0.94
2:2:195:ASN:O	2:2:197:ARG:N	2.01	0.94
1:1:135:ALA:O	1:1:136:LEU:HB2	1.68	0.94
1:1:208:ASP:H	2:2:219:GLN:NE2	1.65	0.94
2:2:155:THR:O	2:2:156:GLU:HB2	1.67	0.94
1:1:203:PHE:CE2	1:1:219:PRO:HD3	2.02	0.93
1:1:268:ASN:ND2	1:1:269:PRO:N	2.15	0.93
3:3:17:THR:O	3:3:19:PRO:HD3	1.67	0.93
3:3:112:LEU:CD2	3:3:211:LEU:HD12	1.96	0.93
1:1:96:VAL:HG21	1:1:112:GLN:CD	1.87	0.93
3:3:74:PRO:HG3	3:3:78:MET:SD	2.08	0.93
3:3:112:LEU:HD23	3:3:211:LEU:HB2	1.47	0.93
1:1:94:ARG:O	1:1:95:TRP:CB	2.15	0.93
2:2:70:TRP:HD1	2:2:74:GLN:NE2	1.66	0.93
1:1:48:PRO:CD	1:1:233:SER:OG	2.17	0.93
1:1:76:PHE:HB3	1:1:93:TRP:HZ3	1.33	0.93
1:1:78:PRO:O	1:1:84:PRO:CB	2.17	0.93
1:1:142:ALA:O	1:1:143:SER:HB2	1.67	0.92
3:3:86:SER:CB	3:3:175:SER:HB3	1.99	0.92
3:3:7:VAL:HG23	3:3:11:LYS:CD	1.98	0.92
1:1:4:ASN:O	1:1:7:LYS:HD3	1.68	0.92
2:2:95:VAL:O	2:2:99:THR:HG22	1.70	0.92
2:2:185:GLN:O	2:2:188:VAL:HG12	1.70	0.92
3:3:78:MET:HE1	3:3:192:GLN:HG2	1.49	0.92
1:1:51:ASN:OD1	1:1:53:GLU:O	1.87	0.92
1:1:54:THR:O	1:1:160:LEU:HD21	0.74	0.92
1:1:108:LEU:CD1	1:1:112:GLN:NE2	1.80	0.92
2:2:52:ALA:CB	2:2:257:ASN:HB3	1.99	0.92
1:1:156:VAL:O	1:1:156:VAL:HG12	1.68	0.91
2:2:183:GLN:C	2:2:186:TRP:HE3	1.72	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:264:ILE:CG1	1:1:265:ASN:H	1.80	0.91
2:2:252:VAL:CG2	2:2:253:ASN:OD1	2.18	0.91
3:3:138:THR:HG22	3:3:142:GLN:NE2	1.85	0.91
1:1:71:THR:CG2	1:1:92:GLN:CD	2.22	0.91
1:1:208:ASP:OD1	2:2:219:GLN:OE1	1.87	0.91
1:1:94:ARG:O	1:1:95:TRP:CE3	2.24	0.91
1:1:141:VAL:O	1:1:178:VAL:HG23	1.70	0.91
2:2:70:TRP:CD2	2:2:233:LEU:CD2	2.53	0.91
1:1:68:LEU:HG	1:1:68:LEU:O	1.71	0.91
1:1:142:ALA:CB	1:1:231:ASN:HB2	1.99	0.91
1:1:96:VAL:CG2	1:1:112:GLN:CD	2.37	0.91
1:1:97:ARG:NH1	2:2:172:ARG:HB3	1.86	0.91
2:2:41:HIS:O	2:2:43:GLU:N	2.03	0.91
2:2:149:ASP:OD2	2:2:152:THR:OG1	1.89	0.91
1:1:248:PRO:HB2	2:2:188:VAL:HG23	1.52	0.91
2:2:136:THR:HG21	2:2:150:PRO:HA	1.52	0.91
1:1:46:LEU:HD22	1:1:228:ILE:CB	2.02	0.90
1:1:51:ASN:OD1	1:1:54:THR:OG1	1.89	0.90
3:3:78:MET:CE	3:3:192:GLN:HG2	1.99	0.90
3:3:218:PHE:CE2	3:3:220:LEU:HD13	2.07	0.90
4:4:15:GLY:O	4:4:17:GLU:HB2	1.72	0.90
1:1:258:THR:HG1	1:1:259:PRO:HD3	1.36	0.90
1:1:146:ARG:HG3	1:1:167:LEU:HD12	1.52	0.90
2:2:10:LEU:HG	2:2:11:SER:H	1.36	0.90
3:3:175:SER:O	3:3:176:TYR:HD1	1.52	0.89
1:1:97:ARG:HD2	2:2:172:ARG:CD	2.02	0.89
2:2:112:VAL:HG21	2:2:130:MET:CE	2.02	0.89
1:1:186:SER:CB	3:3:10:HIS:ND1	2.30	0.89
1:1:96:VAL:CG2	1:1:110:THR:CG2	2.51	0.89
1:1:171:ARG:HB3	3:3:225:SER:HB2	1.55	0.89
1:1:36:PHE:HD2	1:1:37:TYR:CD1	1.90	0.89
4:4:35:LEU:HD12	4:4:36:SER:H	1.39	0.88
1:1:142:ALA:HB3	1:1:231:ASN:CB	2.02	0.88
3:3:51:PRO:HB2	3:3:211:LEU:HB3	1.54	0.88
1:1:45:MET:CB	1:1:64:ARG:CG	2.37	0.88
1:1:69:LEU:CD1	1:1:91:VAL:HA	2.03	0.88
1:1:71:THR:CG2	1:1:92:GLN:OE1	2.21	0.88
1:1:248:PRO:HB2	2:2:188:VAL:CG2	2.03	0.88
2:2:168:ARG:CG	2:2:169:TYR:H	1.81	0.88
1:1:36:PHE:CD2	1:1:37:TYR:CE1	2.61	0.88
1:1:105:ASN:OD1	2:2:175:PHE:CD1	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:108:LEU:HD21	2:2:175:PHE:CD2	2.07	0.88
1:1:203:PHE:CE2	1:1:219:PRO:CD	2.56	0.88
1:1:64:ARG:HH22	1:1:136:LEU:HD11	1.38	0.88
3:3:85:LEU:HD21	3:3:99:ALA:CB	2.04	0.88
1:1:274:GLU:HG2	1:1:275:LEU:HB3	1.49	0.87
2:2:254:PRO:HB2	2:2:256:PHE:HE1	1.39	0.87
1:1:78:PRO:O	1:1:84:PRO:CA	2.22	0.87
2:2:150:PRO:O	2:2:151:PHE:CG	2.28	0.87
2:2:193:ILE:O	2:2:199:ASN:ND2	2.08	0.87
1:1:72:PRO:HB3	1:1:113:ASP:HB2	1.54	0.87
3:3:79:VAL:HG22	3:3:80:ASP:H	1.39	0.87
1:1:101:VAL:CG2	1:1:104:ALA:HB2	2.03	0.87
2:2:5:GLU:HB3	2:2:6:GLU:CG	2.03	0.87
3:3:174:THR:O	3:3:175:SER:HB2	1.71	0.87
1:1:93:TRP:O	1:1:94:ARG:HB2	1.11	0.87
1:1:141:VAL:CG2	1:1:232:THR:HB	1.97	0.87
2:2:161:GLN:C	2:2:163:ALA:H	1.78	0.87
1:1:68:LEU:CD2	1:1:70:LEU:HD13	1.96	0.86
3:3:79:VAL:HG12	3:3:190:VAL:CG1	2.05	0.86
1:1:175:MET:SD	1:1:187:PHE:CD2	2.67	0.86
3:3:67:PHE:CE1	3:3:208:ILE:HG21	2.10	0.86
1:1:154:ALA:CB	1:1:225:ARG:HH11	1.88	0.86
2:2:136:THR:CG2	2:2:150:PRO:HA	2.06	0.86
3:3:202:THR:CB	3:3:203:PRO:HD2	2.05	0.86
1:1:259:PRO:O	1:1:260:THR:HG22	1.73	0.86
1:1:64:ARG:HH22	1:1:136:LEU:CD1	1.87	0.86
1:1:261:THR:HG1	1:1:262:THR:HA	1.39	0.86
3:3:54:LEU:CD1	3:3:210:THR:C	2.44	0.86
3:3:221:ARG:O	3:3:222:MET:HB2	1.74	0.86
2:2:260:ARG:NH1	3:3:133:GLY:HA3	1.89	0.86
2:2:101:ARG:HB3	2:2:217:TRP:HZ2	1.40	0.85
1:1:76:PHE:HB3	1:1:93:TRP:CZ3	2.12	0.85
3:3:218:PHE:HE2	3:3:220:LEU:HD13	1.41	0.85
2:2:112:VAL:CG2	2:2:130:MET:HE3	2.07	0.85
1:1:108:LEU:HD23	2:2:175:PHE:HE2	0.83	0.85
1:1:194:PRO:O	3:3:169:THR:CG2	2.23	0.85
1:1:194:PRO:HB2	3:3:169:THR:HG21	1.58	0.85
3:3:44:LEU:O	3:3:47:LEU:HB3	1.76	0.85
1:1:108:LEU:HD13	1:1:110:THR:HG22	1.59	0.85
2:2:48:CYS:SG	2:2:257:ASN:ND2	2.49	0.85
2:2:67:LEU:CD2	2:2:82:ILE:HD13	1.84	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:63:TYR:CD2	2:2:88:LEU:CD1	2.60	0.85
1:1:51:ASN:CG	1:1:54:THR:OG1	2.15	0.85
1:1:258:THR:HG23	1:1:259:PRO:HD2	1.59	0.85
1:1:129:LEU:CD1	1:1:240:TYR:HD1	1.89	0.85
1:1:186:SER:OG	3:3:9:GLU:OE1	1.95	0.85
2:2:67:LEU:CD2	2:2:82:ILE:HD11	2.07	0.85
1:1:175:MET:HE1	1:1:187:PHE:CE2	2.12	0.84
2:2:52:ALA:CB	2:2:256:PHE:O	2.23	0.84
3:3:191:TRP:N	3:3:191:TRP:CD1	2.45	0.84
3:3:83:VAL:HG13	3:3:83:VAL:O	1.75	0.84
1:1:186:SER:CB	3:3:10:HIS:HE1	1.89	0.84
2:2:63:TYR:CD2	2:2:88:LEU:HD12	2.12	0.84
3:3:176:TYR:OH	3:3:226:PRO:CA	2.25	0.84
1:1:79:ASP:OD1	1:1:79:ASP:O	1.96	0.84
3:3:161:PHE:HD1	3:3:162:THR:N	1.75	0.84
3:3:202:THR:HB	3:3:203:PRO:CD	2.08	0.84
1:1:206:TRP:C	2:2:219:GLN:HE21	1.81	0.84
3:3:127:ILE:HG13	3:3:190:VAL:HG23	1.60	0.84
1:1:35:PHE:HE1	1:1:39:ARG:NH1	1.61	0.84
1:1:47:ARG:HG3	1:1:48:PRO:HD2	0.93	0.84
1:1:122:PHE:HB2	1:1:245:VAL:CG2	2.06	0.84
2:2:132:PRO:HD3	2:2:223:TRP:CZ3	2.13	0.84
3:3:48:CYS:CB	3:3:98:VAL:HG11	2.07	0.84
3:3:127:ILE:HG21	3:3:161:PHE:CE2	1.91	0.84
2:2:5:GLU:OE2	2:2:13:ARG:HD2	1.77	0.83
1:1:25:LYS:O	1:1:26:LEU:HG	1.79	0.83
1:1:37:TYR:OH	1:1:119:PHE:HB3	1.79	0.83
1:1:68:LEU:HB3	1:1:226:LEU:CD2	2.07	0.83
2:2:33:LEU:HD13	2:2:191:HIS:O	1.77	0.83
2:2:167:TYR:HD1	2:2:167:TYR:H	1.24	0.83
2:2:183:GLN:HB2	2:2:186:TRP:HZ3	1.00	0.83
1:1:36:PHE:CE2	1:1:37:TYR:HE1	1.97	0.83
1:1:186:SER:HB3	3:3:10:HIS:HE1	1.38	0.83
2:2:24:THR:HG23	2:2:25:ASN:H	1.38	0.83
4:4:33:ILE:O	4:4:34:ASP:CB	2.19	0.83
1:1:171:ARG:NH1	3:3:101:ASN:OD1	2.11	0.83
2:2:7:MET:CA	2:2:120:GLN:OE1	2.26	0.83
1:1:94:ARG:HG3	1:1:217:VAL:HG22	1.60	0.83
2:2:101:ARG:NH1	2:2:262:GLU:OE2	2.11	0.83
3:3:121:VAL:HG13	3:3:122:LYS:N	1.93	0.83
1:1:173:PRO:HB3	3:3:17:THR:HG21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:ARG:HH21	1:1:233:SER:CA	1.90	0.82
1:1:108:LEU:CD1	1:1:110:THR:HG22	2.10	0.82
2:2:70:TRP:CD1	2:2:233:LEU:CD2	2.54	0.82
3:3:70:THR:HG22	3:3:196:LEU:HD22	1.59	0.82
3:3:214:ALA:HB1	3:3:218:PHE:CB	2.10	0.82
1:1:191:TYR:C	1:1:191:TYR:HD1	1.82	0.82
2:2:146:GLU:HA	2:2:169:TYR:CE2	2.08	0.82
3:3:79:VAL:CG1	3:3:190:VAL:HG12	2.09	0.82
1:1:53:GLU:C	1:1:54:THR:OG1	2.15	0.82
1:1:69:LEU:O	1:1:71:THR:N	2.12	0.82
3:3:99:ALA:O	3:3:174:THR:CG2	2.27	0.82
2:2:162:GLY:O	2:2:163:ALA:CB	2.24	0.82
1:1:78:PRO:O	1:1:84:PRO:C	2.18	0.81
1:1:35:PHE:CE1	1:1:39:ARG:NH1	2.46	0.81
3:3:103:ASN:HB3	3:3:222:MET:HB3	1.62	0.81
3:3:210:THR:O	3:3:211:LEU:HD23	1.80	0.81
2:2:171:SER:O	2:2:172:ARG:CG	2.27	0.81
2:2:32:ARG:NH2	2:2:111:ARG:NE	2.28	0.81
2:2:70:TRP:CD2	2:2:233:LEU:HD23	2.13	0.81
2:2:129:PHE:O	2:2:226:VAL:HG12	1.81	0.81
1:1:46:LEU:HB3	1:1:228:ILE:HG21	1.61	0.81
2:2:63:TYR:HD2	2:2:88:LEU:CD1	1.93	0.81
1:1:265:ASN:OD1	1:1:276:GLU:O	1.99	0.81
2:2:172:ARG:C	2:2:173:THR:OG1	2.17	0.81
2:2:174:GLY:O	2:2:175:PHE:HB2	1.79	0.81
3:3:165:PHE:CZ	3:3:172:ARG:HG3	2.16	0.81
1:1:94:ARG:HG3	1:1:217:VAL:HG23	1.61	0.81
2:2:82:ILE:HG22	2:2:225:LEU:CB	2.10	0.80
2:2:222:ASN:ND2	2:2:222:ASN:N	2.27	0.80
2:2:222:ASN:N	2:2:222:ASN:HD22	1.79	0.80
3:3:52:THR:HG21	3:3:94:MET:N	1.95	0.80
3:3:83:VAL:HG13	3:3:185:ASP:O	1.80	0.80
1:1:145:LEU:HD21	1:1:226:LEU:CD1	2.12	0.80
1:1:175:MET:CE	1:1:187:PHE:CE2	2.64	0.80
3:3:83:VAL:CG1	3:3:83:VAL:O	2.29	0.80
1:1:148:ALA:CB	1:1:227:TRP:CZ2	2.63	0.80
2:2:259:LEU:CD2	2:2:260:ARG:CA	2.50	0.80
1:1:6:GLU:CB	2:2:193:ILE:CG2	2.50	0.80
1:1:269:PRO:O	1:1:270:VAL:HG12	1.82	0.80
2:2:63:TYR:HD2	2:2:88:LEU:HD12	1.44	0.80
3:3:224:ILE:HG22	3:3:225:SER:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:LEU:HD21	1:1:226:LEU:HD13	1.64	0.80
1:1:53:GLU:OE2	1:1:164:THR:HA	1.80	0.80
1:1:128:ASP:CB	4:4:31:ASN:OD1	2.30	0.79
1:1:174:HIS:HB3	3:3:16:SER:HB2	1.63	0.79
1:1:250:PRO:CA	2:2:185:GLN:NE2	2.45	0.79
2:2:67:LEU:HD13	2:2:247:ALA:HB2	1.64	0.79
2:2:131:ALA:HB1	2:2:189:TYR:CE1	2.17	0.79
1:1:47:ARG:HH21	1:1:233:SER:H	0.81	0.79
3:3:7:VAL:HG22	3:3:11:LYS:NZ	1.96	0.79
1:1:161:ILE:O	1:1:161:ILE:HG22	1.79	0.79
1:1:250:PRO:HA	2:2:185:GLN:NE2	1.94	0.79
2:2:64:THR:HG23	2:2:248:SER:HB3	1.64	0.79
3:3:45:LEU:O	3:3:49:LYS:CG	2.31	0.79
1:1:203:PHE:HE2	1:1:219:PRO:HD3	1.47	0.79
2:2:126:LEU:HD11	2:2:245:ILE:HD11	1.64	0.79
2:2:206:VAL:CG1	2:2:223:TRP:CH2	2.65	0.79
1:1:258:THR:CB	1:1:259:PRO:CD	2.61	0.79
2:2:168:ARG:CG	2:2:169:TYR:N	2.39	0.79
3:3:78:MET:HE3	3:3:192:GLN:OE1	1.78	0.79
1:1:98:SER:O	1:1:109:MET:N	2.15	0.78
1:1:105:ASN:ND2	2:2:175:PHE:CD1	2.51	0.78
2:2:143:GLY:C	2:2:144:THR:CG2	2.51	0.78
1:1:108:LEU:CD1	1:1:110:THR:CG2	2.61	0.78
1:1:146:ARG:CB	1:1:227:TRP:CZ3	2.65	0.78
1:1:185:VAL:CG1	1:1:185:VAL:O	2.30	0.78
3:3:73:VAL:HG13	3:3:73:VAL:O	1.83	0.78
1:1:37:TYR:HE2	1:1:122:PHE:CE2	2.02	0.78
1:1:110:THR:HG23	1:1:112:GLN:NE2	1.99	0.78
1:1:263:LYS:HG2	1:1:264:ILE:N	1.98	0.78
3:3:115:PHE:CD2	3:3:153:LEU:HD21	2.18	0.78
3:3:129:TYR:HE1	3:3:186:GLY:HA2	1.49	0.78
3:3:69:ALA:C	3:3:70:THR:HG23	2.01	0.78
1:1:52:MET:O	1:1:53:GLU:HB2	1.81	0.78
1:1:101:VAL:HG21	1:1:104:ALA:CB	2.13	0.78
2:2:10:LEU:O	2:2:13:ARG:CB	2.22	0.78
2:2:109:GLY:O	2:2:252:VAL:HG12	1.84	0.78
2:2:173:THR:HG22	2:2:174:GLY:N	1.99	0.78
1:1:6:GLU:HB3	2:2:193:ILE:HG21	1.63	0.77
1:1:182:ASN:CB	3:3:12:GLY:HA3	2.15	0.77
1:1:271:PRO:HB2	1:1:272:ILE:C	2.02	0.77
2:2:70:TRP:CD2	2:2:233:LEU:HD21	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:126:LEU:HD11	2:2:245:ILE:CD1	2.15	0.77
2:2:182:ASN:C	2:2:184:TRP:H	1.84	0.77
1:1:168:GLY:HA2	1:1:174:HIS:HE1	1.49	0.77
2:2:81:ARG:CZ	2:2:136:THR:HA	2.15	0.77
2:2:134:PHE:CD2	2:2:224:THR:CG2	2.65	0.77
1:1:90:PRO:C	1:1:91:VAL:CG2	2.34	0.77
3:3:71:ASN:O	3:3:195:PRO:HB3	1.85	0.77
2:2:145:MET:O	2:2:169:TYR:OH	2.02	0.77
1:1:96:VAL:HG22	1:1:108:LEU:CD1	2.06	0.77
1:1:146:ARG:HB2	1:1:167:LEU:HG	1.66	0.77
3:3:67:PHE:CE1	3:3:208:ILE:CG2	2.64	0.77
3:3:175:SER:O	3:3:176:TYR:CD1	2.37	0.77
1:1:34:ALA:O	1:1:38:ASP:HB2	1.85	0.76
2:2:70:TRP:NE1	2:2:233:LEU:HD21	1.99	0.76
1:1:194:PRO:HB2	3:3:169:THR:CG2	2.15	0.76
1:1:271:PRO:HB2	1:1:272:ILE:O	1.84	0.76
1:1:36:PHE:CE2	1:1:37:TYR:CE1	2.72	0.76
1:1:96:VAL:CG2	1:1:108:LEU:CD1	2.54	0.76
1:1:191:TYR:C	1:1:191:TYR:CD1	2.58	0.76
2:2:146:GLU:CA	2:2:169:TYR:HE2	1.96	0.76
2:2:217:TRP:O	2:2:217:TRP:HE3	1.63	0.76
3:3:95:LEU:O	3:3:96:ALA:CB	2.33	0.76
2:2:139:GLY:HA3	2:2:148:SER:HB2	1.68	0.76
2:2:213:PRO:O	2:2:214:SER:CB	2.32	0.76
1:1:79:ASP:HB3	1:1:93:TRP:CZ2	2.20	0.76
2:2:138:LYS:HD2	2:2:152:THR:HG21	1.67	0.76
2:2:173:THR:CG2	2:2:174:GLY:H	1.95	0.76
1:1:209:PHE:C	1:1:211:ASN:N	2.35	0.76
3:3:116:THR:HB	3:3:207:ASP:O	1.84	0.76
2:2:125:SER:HB3	2:2:230:LEU:CD2	2.14	0.76
2:2:260:ARG:CG	2:2:261:HIS:N	2.49	0.76
1:1:122:PHE:CB	1:1:245:VAL:HG22	2.14	0.76
1:1:154:ALA:HB1	1:1:225:ARG:CD	2.16	0.76
2:2:129:PHE:HZ	2:2:186:TRP:NE1	1.83	0.76
1:1:129:LEU:HD11	1:1:240:TYR:CD1	2.21	0.76
3:3:7:VAL:CB	3:3:11:LYS:HE2	2.14	0.76
1:1:108:LEU:HD11	1:1:112:GLN:NE2	1.99	0.76
1:1:263:LYS:HG2	1:1:264:ILE:HA	0.78	0.76
1:1:271:PRO:HB2	1:1:272:ILE:CG1	2.16	0.76
2:2:70:TRP:CE2	2:2:233:LEU:CD2	2.69	0.76
2:2:80:ILE:HG22	2:2:227:VAL:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:75:SER:C	1:1:76:PHE:CA	2.55	0.75
2:2:10:LEU:HG	2:2:11:SER:N	2.01	0.75
2:2:99:THR:HG23	2:2:256:PHE:CE2	2.16	0.75
2:2:3:ASN:CG	2:2:11:SER:HB2	2.05	0.75
1:1:182:ASN:HB3	3:3:12:GLY:HA3	1.68	0.75
1:1:270:VAL:HG22	1:1:271:PRO:N	2.00	0.75
2:2:183:GLN:HB3	2:2:186:TRP:CE3	2.09	0.75
3:3:54:LEU:H	3:3:210:THR:HG22	1.49	0.75
3:3:84:ALA:C	3:3:86:SER:H	1.90	0.75
2:2:1:ASP:O	2:2:2:GLN:HB2	1.87	0.75
2:2:45:PRO:C	2:2:47:SER:H	1.89	0.75
3:3:47:LEU:O	3:3:50:LEU:HD12	1.87	0.75
3:3:149:ALA:HB1	3:3:159:PHE:HZ	1.50	0.75
1:1:56:PHE:CZ	1:1:227:TRP:HB3	2.22	0.75
1:1:79:ASP:HA	1:1:84:PRO:CB	2.16	0.75
3:3:222:MET:O	3:3:223:PRO:C	2.19	0.75
1:1:48:PRO:HD3	1:1:233:SER:HG	1.52	0.74
1:1:50:GLN:HE22	1:1:57:ASN:N	1.85	0.74
1:1:122:PHE:CD2	1:1:245:VAL:CG2	2.57	0.74
3:3:126:LEU:CD2	3:3:148:TYR:CD2	2.63	0.74
1:1:175:MET:HE1	1:1:187:PHE:CE1	2.15	0.74
3:3:86:SER:CB	3:3:175:SER:CB	2.59	0.74
3:3:115:PHE:CG	3:3:153:LEU:HD21	2.22	0.74
3:3:138:THR:CG2	3:3:142:GLN:NE2	2.50	0.74
2:2:70:TRP:CD1	2:2:74:GLN:NE2	2.52	0.74
2:2:99:THR:CG2	2:2:256:PHE:HE2	1.99	0.74
1:1:47:ARG:NE	1:1:233:SER:CB	2.06	0.74
1:1:169:GLU:HG2	3:3:228:LYS:HE3	1.69	0.74
2:2:195:ASN:H	2:2:199:ASN:HB2	1.53	0.74
1:1:53:GLU:OE1	1:1:165:PRO:HD3	1.88	0.74
1:1:62:ASP:O	1:1:63:TYR:CD2	2.40	0.74
3:3:77:SER:OG	3:3:78:MET:CB	2.36	0.74
1:1:97:ARG:H	1:1:110:THR:CG2	2.00	0.74
1:1:101:VAL:HB	1:1:103:GLY:H	1.52	0.74
1:1:209:PHE:C	1:1:211:ASN:H	1.90	0.74
2:2:52:ALA:HB2	2:2:257:ASN:CB	2.05	0.74
3:3:218:PHE:HE2	3:3:220:LEU:CD1	2.01	0.74
1:1:47:ARG:NH2	1:1:233:SER:HB2	2.01	0.74
1:1:238:ILE:O	1:1:238:ILE:HG12	1.86	0.74
1:1:69:LEU:HD22	1:1:92:GLN:NE2	2.03	0.74
1:1:185:VAL:O	1:1:185:VAL:HG13	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:192:ASN:HA	3:3:222:MET:CE	2.08	0.74
3:3:73:VAL:O	3:3:73:VAL:CG1	2.35	0.74
2:2:85:PRO:HD3	2:2:222:ASN:HD21	1.52	0.74
3:3:83:VAL:HG12	3:3:186:GLY:HA3	0.74	0.74
3:3:95:LEU:O	3:3:96:ALA:HB2	1.88	0.74
1:1:35:PHE:O	1:1:39:ARG:NH2	2.21	0.73
2:2:97:GLY:O	2:2:100:LEU:HB3	1.88	0.73
2:2:192:GLN:CG	2:2:202:VAL:HG23	2.16	0.73
4:4:15:GLY:O	4:4:16:ASN:C	2.25	0.73
3:3:15:TYR:HB2	3:3:18:ASN:HB2	1.69	0.73
3:3:45:LEU:C	3:3:47:LEU:H	1.91	0.73
1:1:50:GLN:HE22	1:1:57:ASN:H	1.33	0.73
1:1:94:ARG:HD3	1:1:217:VAL:HG23	1.68	0.73
1:1:123:THR:O	1:1:124:PHE:CD1	2.41	0.73
1:1:79:ASP:CA	1:1:84:PRO:CB	2.67	0.73
1:1:129:LEU:HD22	1:1:223:PHE:CZ	2.24	0.73
3:3:155:LEU:CD1	3:3:155:LEU:C	2.57	0.73
1:1:46:LEU:CD2	1:1:228:ILE:HB	2.18	0.73
2:2:101:ARG:HB3	2:2:217:TRP:CZ2	2.22	0.73
1:1:258:THR:CG2	1:1:259:PRO:HD2	2.19	0.73
1:1:274:GLU:HG3	1:1:275:LEU:HB2	1.63	0.73
1:1:94:ARG:CG	1:1:217:VAL:CG2	2.65	0.73
2:2:50:ASP:OD1	3:3:166:ILE:HG12	1.89	0.73
1:1:36:PHE:CD2	1:1:37:TYR:CD1	2.77	0.73
1:1:72:PRO:O	1:1:73:LEU:HD12	1.85	0.73
3:3:90:MET:O	3:3:96:ALA:CB	2.37	0.73
1:1:46:LEU:CD2	1:1:228:ILE:CB	2.65	0.73
2:2:129:PHE:CE1	2:2:226:VAL:HG11	2.24	0.73
2:2:131:ALA:CB	2:2:189:TYR:CE1	2.72	0.73
3:3:62:LYS:HD3	3:3:64:TYR:OH	1.89	0.73
1:1:146:ARG:O	1:1:227:TRP:CE3	2.41	0.72
2:2:71:THR:C	2:2:233:LEU:CD1	2.56	0.72
1:1:46:LEU:HD22	1:1:228:ILE:CG2	2.16	0.72
1:1:68:LEU:HB3	1:1:226:LEU:HD23	1.70	0.72
1:1:94:ARG:O	1:1:95:TRP:CD2	2.41	0.72
2:2:10:LEU:CG	2:2:11:SER:H	2.02	0.72
3:3:7:VAL:CG2	3:3:11:LYS:CD	2.60	0.72
1:1:197:VAL:HG23	2:2:211:VAL:HA	1.72	0.72
1:1:275:LEU:HG	1:1:276:GLU:CA	2.18	0.72
1:1:45:MET:HB3	1:1:64:ARG:CG	2.15	0.72
1:1:54:THR:CA	1:1:160:LEU:HD11	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:96:VAL:HG23	1:1:110:THR:HG21	1.71	0.72
1:1:141:VAL:HG22	1:1:232:THR:HB	1.70	0.72
2:2:5:GLU:CB	2:2:6:GLU:HG2	2.12	0.72
2:2:84:LEU:HD21	2:2:249:LEU:HD13	1.71	0.72
2:2:143:GLY:O	2:2:144:THR:CA	2.38	0.72
3:3:51:PRO:CB	3:3:211:LEU:HB3	2.20	0.72
1:1:52:MET:O	1:1:53:GLU:CB	2.36	0.72
1:1:79:ASP:HA	1:1:84:PRO:HB3	1.69	0.72
1:1:117:LEU:HG	1:1:117:LEU:O	1.87	0.72
3:3:165:PHE:CE2	3:3:167:SER:HB3	2.25	0.72
1:1:92:GLN:O	1:1:217:VAL:HG11	1.88	0.72
1:1:150:THR:CG2	1:1:222:ASP:O	2.37	0.72
2:2:143:GLY:C	2:2:144:THR:HA	2.09	0.71
2:2:88:LEU:O	2:2:93:GLY:HA3	1.90	0.71
1:1:68:LEU:CB	1:1:226:LEU:HD23	2.20	0.71
1:1:72:PRO:C	1:1:73:LEU:HD13	2.10	0.71
1:1:105:ASN:ND2	2:2:175:PHE:CE1	2.57	0.71
2:2:167:TYR:HD1	2:2:167:TYR:N	1.80	0.71
2:2:167:TYR:CD1	2:2:167:TYR:N	2.40	0.71
3:3:126:LEU:HD23	3:3:127:ILE:N	2.04	0.71
2:2:139:GLY:HA3	2:2:148:SER:CB	2.21	0.71
1:1:51:ASN:OD1	1:1:51:ASN:O	2.08	0.71
1:1:263:LYS:CG	1:1:264:ILE:CA	2.46	0.71
3:3:218:PHE:CE2	3:3:220:LEU:CD1	2.73	0.71
1:1:36:PHE:HE2	1:1:37:TYR:HE1	1.36	0.71
1:1:68:LEU:HB3	1:1:226:LEU:HD21	1.71	0.71
2:2:111:ARG:HG3	2:2:205:GLU:HG3	1.72	0.71
3:3:77:SER:OG	3:3:78:MET:CA	2.39	0.71
1:1:131:VAL:HG13	1:1:187:PHE:CD1	2.26	0.71
1:1:254:PHE:HD1	1:1:255:PRO:HD2	0.99	0.71
3:3:94:MET:O	3:3:97:ALA:N	2.18	0.71
1:1:131:VAL:CG2	1:1:187:PHE:CZ	2.74	0.71
2:2:35:GLY:O	2:2:36:TYR:HB2	1.91	0.71
2:2:79:HIS:HA	2:2:228:ALA:CB	2.21	0.71
2:2:182:ASN:C	2:2:184:TRP:N	2.44	0.71
3:3:176:TYR:OH	3:3:226:PRO:HA	1.89	0.71
1:1:96:VAL:HG23	1:1:112:GLN:CD	2.11	0.70
1:1:68:LEU:HD23	1:1:226:LEU:HD23	1.71	0.70
2:2:254:PRO:HB2	2:2:256:PHE:CE1	2.24	0.70
2:2:195:ASN:O	2:2:198:THR:N	2.23	0.70
1:1:72:PRO:HB3	1:1:113:ASP:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:146:ARG:HB2	1:1:167:LEU:CG	2.21	0.70
1:1:175:MET:CE	1:1:187:PHE:CZ	2.74	0.70
3:3:161:PHE:CD1	3:3:162:THR:N	2.55	0.70
1:1:129:LEU:CD1	1:1:240:TYR:CD1	2.73	0.70
3:3:54:LEU:H	3:3:54:LEU:CD1	2.04	0.70
1:1:146:ARG:CB	1:1:227:TRP:HE3	1.89	0.70
2:2:84:LEU:HD11	2:2:130:MET:HE2	1.72	0.70
2:2:146:GLU:HB3	2:2:169:TYR:OH	1.91	0.70
3:3:112:LEU:HD21	3:3:211:LEU:CD1	2.16	0.70
2:2:3:ASN:ND2	2:2:12:ASP:H	1.90	0.70
3:3:181:ILE:O	3:3:182:THR:HB	1.92	0.70
1:1:113:ASP:OD2	1:1:116:PHE:HB3	1.92	0.70
1:1:174:HIS:CB	3:3:16:SER:CB	2.67	0.70
3:3:77:SER:C	3:3:79:VAL:H	1.93	0.70
1:1:36:PHE:HD2	1:1:37:TYR:CE1	2.03	0.69
1:1:45:MET:HA	1:1:234:ALA:O	1.92	0.69
1:1:94:ARG:O	1:1:95:TRP:CG	2.45	0.69
2:2:165:THR:HG22	2:2:176:PHE:CB	2.21	0.69
3:3:121:VAL:CG1	3:3:122:LYS:N	2.55	0.69
1:1:125:TYR:O	1:1:198:LEU:HB3	1.92	0.69
3:3:54:LEU:O	3:3:54:LEU:HD23	1.92	0.69
1:1:78:PRO:C	1:1:84:PRO:HB2	2.12	0.69
3:3:18:ASN:HD22	3:3:18:ASN:C	1.96	0.69
3:3:73:VAL:CG2	3:3:74:PRO:O	2.36	0.69
3:3:229:TRP:O	3:3:230:VAL:CB	2.15	0.69
3:3:14:PHE:C	3:3:14:PHE:CD1	2.64	0.69
1:1:91:VAL:HG22	1:1:225:ARG:NH2	2.08	0.69
2:2:173:THR:HG22	2:2:174:GLY:H	1.56	0.69
2:2:182:ASN:O	2:2:185:GLN:N	2.19	0.69
2:2:259:LEU:C	2:2:260:ARG:CA	2.61	0.69
1:1:110:THR:O	1:1:111:LYS:C	2.29	0.69
1:1:150:THR:HG21	1:1:223:PHE:HA	1.73	0.69
2:2:3:ASN:OD1	2:2:11:SER:HB2	1.92	0.69
3:3:24:PRO:O	3:3:25:ILE:CG2	2.39	0.69
3:3:83:VAL:HG12	3:3:186:GLY:C	2.11	0.69
1:1:122:PHE:HB2	1:1:245:VAL:HG22	1.72	0.69
1:1:154:ALA:HB2	1:1:225:ARG:HH11	1.58	0.69
2:2:132:PRO:HA	2:2:223:TRP:HA	1.73	0.69
3:3:155:LEU:C	3:3:155:LEU:HD12	2.13	0.69
1:1:97:ARG:CD	2:2:172:ARG:HD2	2.15	0.69
1:1:171:ARG:HB3	3:3:225:SER:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:5:GLU:OE2	2:2:13:ARG:CD	2.41	0.69
1:1:32:ARG:O	1:1:34:ALA:N	2.26	0.68
2:2:70:TRP:CE2	2:2:233:LEU:HD21	2.28	0.68
1:1:25:LYS:C	1:1:26:LEU:HG	2.12	0.68
1:1:46:LEU:CD2	1:1:228:ILE:HG21	2.23	0.68
1:1:273:LEU:HD12	1:1:274:GLU:N	2.08	0.68
2:2:192:GLN:HB3	2:2:202:VAL:CG2	2.24	0.68
2:2:194:LEU:HA	2:2:199:ASN:HD22	1.57	0.68
2:2:71:THR:H	2:2:74:GLN:NE2	1.89	0.68
2:2:71:THR:O	2:2:73:SER:N	2.27	0.68
3:3:74:PRO:HG3	3:3:78:MET:CE	2.23	0.68
1:1:108:LEU:HD11	1:1:110:THR:CG2	2.24	0.68
2:2:146:GLU:CB	2:2:169:TYR:OH	2.41	0.68
2:2:188:VAL:CG2	2:2:188:VAL:O	2.42	0.68
3:3:79:VAL:CG2	3:3:80:ASP:H	2.06	0.68
1:1:127:CYS:SG	1:1:240:TYR:HB3	2.33	0.68
1:1:131:VAL:HG21	1:1:187:PHE:CE2	2.28	0.68
1:1:203:PHE:HE2	1:1:219:PRO:CD	2.02	0.68
2:2:71:THR:H	2:2:74:GLN:HE22	1.41	0.68
1:1:94:ARG:CG	1:1:217:VAL:HG23	2.23	0.68
1:1:161:ILE:O	1:1:161:ILE:CG2	2.40	0.68
1:1:271:PRO:HG2	1:1:272:ILE:C	2.14	0.68
1:1:68:LEU:CG	1:1:226:LEU:HD23	2.24	0.67
1:1:79:ASP:OD2	1:1:95:TRP:HZ2	1.75	0.67
2:2:32:ARG:CZ	2:2:111:ARG:HE	2.06	0.67
1:1:69:LEU:HD13	1:1:91:VAL:HA	1.76	0.67
1:1:79:ASP:HB3	1:1:93:TRP:HZ2	1.57	0.67
1:1:196:SER:O	1:1:197:VAL:CG1	2.39	0.67
1:1:259:PRO:O	1:1:260:THR:CG2	2.42	0.67
1:1:274:GLU:HG2	1:1:275:LEU:HB2	0.68	0.67
1:1:68:LEU:CD2	1:1:226:LEU:CD2	2.67	0.67
1:1:100:GLY:CA	1:1:109:MET:SD	2.83	0.67
3:3:61:ASN:HD21	3:3:63:ARG:NH2	1.92	0.67
3:3:77:SER:C	3:3:79:VAL:N	2.46	0.67
1:1:75:SER:O	1:1:76:PHE:HA	1.95	0.67
1:1:62:ASP:O	1:1:63:TYR:HB2	1.94	0.67
1:1:131:VAL:CG2	1:1:187:PHE:CE2	2.78	0.67
1:1:175:MET:HE2	1:1:187:PHE:CG	2.21	0.67
2:2:112:VAL:HG22	2:2:249:LEU:HD23	1.76	0.67
1:1:146:ARG:CB	1:1:167:LEU:CD1	2.72	0.67
1:1:192:ASN:CG	3:3:222:MET:HE1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:210:ASN:ND2	2:2:211:VAL:H	1.93	0.67
3:3:103:ASN:HB3	3:3:222:MET:CB	2.25	0.67
3:3:79:VAL:HG22	3:3:80:ASP:N	2.09	0.67
2:2:183:GLN:HA	2:2:186:TRP:CG	2.29	0.66
1:1:37:TYR:HB3	1:1:240:TYR:HD2	1.60	0.66
1:1:149:PRO:CB	1:1:192:ASN:ND2	2.22	0.66
1:1:211:ASN:O	1:1:212:THR:C	2.27	0.66
3:3:165:PHE:CE2	3:3:167:SER:CB	2.78	0.66
1:1:96:VAL:CG2	1:1:110:THR:HG21	2.23	0.66
2:2:141:LYS:HG3	2:2:148:SER:N	2.10	0.66
1:1:94:ARG:CD	1:1:217:VAL:HG23	2.26	0.66
1:1:130:GLU:HG2	1:1:239:ARG:CD	2.25	0.66
1:1:133:VAL:CG2	1:1:133:VAL:O	2.43	0.66
2:2:230:LEU:HD23	2:2:230:LEU:C	2.16	0.66
3:3:54:LEU:CD1	3:3:211:LEU:N	2.58	0.66
3:3:93:SER:O	3:3:97:ALA:HB2	1.96	0.66
1:1:156:VAL:O	1:1:156:VAL:CG1	2.42	0.66
1:1:168:GLY:HA2	1:1:174:HIS:CE1	2.31	0.66
3:3:110:ASN:HB2	3:3:162:THR:OG1	1.96	0.66
3:3:121:VAL:O	3:3:122:LYS:HG3	1.95	0.66
1:1:146:ARG:NE	1:1:167:LEU:HD11	2.07	0.66
1:1:150:THR:CG2	1:1:223:PHE:HA	2.26	0.66
1:1:254:PHE:CE1	1:1:255:PRO:HD2	2.23	0.66
4:4:32:SER:O	4:4:33:ILE:C	2.34	0.66
1:1:203:PHE:CZ	1:1:219:PRO:HD3	2.30	0.66
3:3:144:MET:HG2	3:3:145:GLN:N	2.08	0.66
1:1:142:ALA:HA	1:1:178:VAL:HB	1.77	0.65
1:1:209:PHE:O	1:1:211:ASN:N	2.28	0.65
3:3:109:LEU:O	3:3:162:THR:CG2	2.35	0.65
1:1:130:GLU:HB3	1:1:239:ARG:CG	2.26	0.65
2:2:210:ASN:HD21	2:2:220:HIS:CE1	2.14	0.65
1:1:215:PHE:CD1	1:1:215:PHE:C	2.70	0.65
3:3:70:THR:O	3:3:71:ASN:C	2.34	0.65
3:3:126:LEU:HD23	3:3:127:ILE:H	1.60	0.65
1:1:121:PRO:O	1:1:122:PHE:HB3	1.95	0.65
3:3:63:ARG:HG2	3:3:63:ARG:HH11	1.61	0.65
1:1:37:TYR:HE2	1:1:122:PHE:HE2	1.44	0.65
1:1:46:LEU:CB	1:1:228:ILE:HG21	2.25	0.65
1:1:197:VAL:O	2:2:211:VAL:HG22	1.97	0.65
2:2:24:THR:C	2:2:25:ASN:HD22	2.00	0.65
3:3:124:LYS:HE2	3:3:152:ASP:OD1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:LEU:HD23	1:1:70:LEU:HD11	1.70	0.65
1:1:15:ALA:C	1:1:17:VAL:H	2.00	0.65
1:1:68:LEU:CD1	1:1:70:LEU:HD13	2.27	0.65
1:1:116:PHE:CD1	1:1:116:PHE:O	2.49	0.65
1:1:146:ARG:C	1:1:227:TRP:CE3	2.70	0.65
2:2:114:VAL:HG22	2:2:202:VAL:HG12	1.79	0.64
3:3:77:SER:O	3:3:79:VAL:O	2.16	0.64
3:3:103:ASN:CB	3:3:222:MET:HB3	2.28	0.64
2:2:6:GLU:OE1	2:2:9:ASN:CA	2.32	0.64
2:2:79:HIS:HA	2:2:228:ALA:HB2	1.79	0.64
2:2:97:GLY:O	2:2:101:ARG:HG3	1.97	0.64
1:1:95:TRP:HB2	2:2:168:ARG:HG3	1.79	0.64
3:3:81:TYR:O	3:3:188:VAL:HG12	1.98	0.64
2:2:252:VAL:HG23	2:2:253:ASN:OD1	1.98	0.64
3:3:45:LEU:O	3:3:49:LYS:HG3	1.97	0.64
1:1:122:PHE:CD1	1:1:245:VAL:HG23	2.32	0.64
1:1:130:GLU:HB3	1:1:239:ARG:HG3	1.80	0.64
2:2:3:ASN:ND2	2:2:11:SER:HB2	2.13	0.64
1:1:205:GLY:HA2	2:2:219:GLN:O	1.98	0.64
1:1:249:ARG:HG2	1:1:250:PRO:O	1.98	0.64
2:2:142:THR:CG2	2:2:142:THR:O	2.46	0.64
2:2:206:VAL:HG11	2:2:223:TRP:CZ3	2.31	0.64
3:3:115:PHE:CZ	3:3:121:VAL:HG11	2.32	0.64
1:1:20:VAL:HG12	1:1:20:VAL:O	1.99	0.63
1:1:191:TYR:CD1	1:1:191:TYR:O	2.52	0.63
1:1:191:TYR:HE1	1:1:193:SER:O	1.81	0.63
2:2:32:ARG:NH2	2:2:111:ARG:HE	1.94	0.63
2:2:165:THR:HG22	2:2:176:PHE:HB3	1.79	0.63
2:2:260:ARG:NH2	2:2:263:THR:OG1	2.31	0.63
4:4:27:ASN:H	4:4:27:ASN:ND2	1.95	0.63
1:1:251:THR:C	1:1:252:LEU:CA	2.66	0.63
2:2:1:ASP:O	2:2:2:GLN:CB	2.33	0.63
2:2:208:TYR:OH	2:2:212:ALA:O	2.15	0.63
3:3:100:ARG:CG	3:3:226:PRO:HG3	2.23	0.63
3:3:114:VAL:HG12	3:3:209:LEU:O	1.98	0.63
1:1:206:TRP:C	2:2:219:GLN:NE2	2.47	0.63
1:1:274:GLU:OE2	1:1:275:LEU:CD2	2.32	0.63
2:2:112:VAL:CG2	2:2:249:LEU:CD2	2.65	0.63
2:2:142:THR:O	2:2:142:THR:HG23	1.97	0.63
1:1:94:ARG:NH2	1:1:95:TRP:CZ3	2.66	0.63
1:1:97:ARG:H	1:1:110:THR:HG21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:TYR:CE2	1:1:198:LEU:HD23	2.33	0.63
2:2:129:PHE:O	2:2:226:VAL:CG1	2.46	0.63
3:3:86:SER:O	3:3:87:CYS:O	2.17	0.63
1:1:47:ARG:HA	1:1:233:SER:HG	1.63	0.63
1:1:63:TYR:HB3	1:1:76:PHE:CZ	2.34	0.63
1:1:146:ARG:HB2	1:1:167:LEU:CD1	2.28	0.63
1:1:174:HIS:CB	3:3:16:SER:HB3	2.24	0.63
3:3:100:ARG:HD2	3:3:226:PRO:HG2	1.79	0.63
1:1:108:LEU:CG	2:2:175:PHE:HE2	2.07	0.63
1:1:128:ASP:CG	4:4:31:ASN:OD1	2.37	0.63
3:3:62:LYS:O	3:3:63:ARG:C	2.37	0.63
3:3:65:PRO:O	3:3:209:LEU:HD12	1.98	0.63
1:1:192:ASN:CG	3:3:222:MET:CE	2.67	0.63
1:1:46:LEU:O	1:1:233:SER:CB	2.46	0.63
1:1:172:ASN:OD1	3:3:224:ILE:HG12	1.98	0.63
2:2:112:VAL:CG2	2:2:130:MET:CE	2.72	0.63
2:2:183:GLN:O	2:2:186:TRP:HE3	1.82	0.63
3:3:115:PHE:CE2	3:3:153:LEU:HD21	2.34	0.63
1:1:68:LEU:CG	1:1:70:LEU:CD1	2.48	0.62
1:1:133:VAL:HG22	1:1:185:VAL:CG1	2.17	0.62
1:1:274:GLU:CD	1:1:275:LEU:HD22	2.15	0.62
2:2:165:THR:HG22	2:2:176:PHE:CA	2.29	0.62
3:3:100:ARG:C	3:3:102:PHE:H	2.00	0.62
4:4:53:SER:HB3	4:4:54:ASN:O	1.98	0.62
1:1:124:PHE:HZ	2:2:133:GLU:CD	2.00	0.62
3:3:118:ALA:O	3:3:121:VAL:HB	2.00	0.62
2:2:134:PHE:HB3	2:2:224:THR:CG2	2.29	0.62
3:3:81:TYR:O	3:3:188:VAL:CG1	2.47	0.62
1:1:150:THR:HB	1:1:224:GLY:H	1.63	0.62
1:1:151:GLY:C	3:3:103:ASN:HD21	2.03	0.62
1:1:250:PRO:C	2:2:185:GLN:NE2	2.53	0.62
1:1:259:PRO:O	1:1:260:THR:N	2.33	0.62
1:1:62:ASP:O	1:1:63:TYR:CB	2.46	0.62
2:2:32:ARG:HA	2:2:203:ASP:O	2.00	0.62
2:2:101:ARG:CB	2:2:217:TRP:HZ2	2.12	0.62
2:2:260:ARG:C	2:2:261:HIS:CA	2.67	0.62
2:2:96:PHE:O	2:2:100:LEU:HB2	1.99	0.62
2:2:64:THR:HG23	2:2:248:SER:CB	2.30	0.62
2:2:155:THR:O	2:2:155:THR:OG1	2.16	0.62
3:3:77:SER:HB2	3:3:191:TRP:HB3	1.82	0.62
2:2:77:PHE:CD1	2:2:186:TRP:CZ3	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:86:HIS:CE1	2:2:217:TRP:O	2.52	0.62
3:3:181:ILE:O	3:3:182:THR:CB	2.47	0.62
2:2:195:ASN:C	2:2:197:ARG:H	2.01	0.61
4:4:27:ASN:HD22	4:4:27:ASN:N	1.98	0.61
1:1:37:TYR:HD2	1:1:243:MET:SD	2.23	0.61
3:3:122:LYS:O	3:3:197:THR:N	2.31	0.61
1:1:79:ASP:HA	1:1:84:PRO:CA	2.30	0.61
2:2:143:GLY:O	2:2:144:THR:CB	2.49	0.61
3:3:18:ASN:C	3:3:18:ASN:ND2	2.51	0.61
1:1:130:GLU:HG2	1:1:239:ARG:HD2	1.81	0.61
1:1:250:PRO:HB3	2:2:185:GLN:HB3	1.82	0.61
2:2:111:ARG:HG3	2:2:205:GLU:CG	2.29	0.61
1:1:41:VAL:HG12	1:1:238:ILE:HG12	1.82	0.61
1:1:273:LEU:CG	1:1:274:GLU:HA	2.29	0.61
2:2:112:VAL:HG13	2:2:249:LEU:HD23	1.80	0.61
2:2:143:GLY:O	2:2:144:THR:HA	2.01	0.61
2:2:2:GLN:O	2:2:3:ASN:O	2.17	0.61
2:2:195:ASN:C	2:2:197:ARG:N	2.51	0.61
4:4:22:ASN:HD22	4:4:22:ASN:N	1.98	0.61
1:1:146:ARG:HD2	1:1:167:LEU:CG	2.28	0.61
1:1:203:PHE:CE1	1:1:205:GLY:HA3	2.36	0.61
3:3:95:LEU:HD13	3:3:214:ALA:HB2	1.83	0.61
3:3:184:VAL:CG2	3:3:185:ASP:H	2.14	0.61
1:1:71:THR:O	1:1:73:LEU:N	2.33	0.61
1:1:141:VAL:O	1:1:178:VAL:CG2	2.47	0.61
3:3:139:THR:O	3:3:142:GLN:N	2.33	0.61
1:1:191:TYR:CE1	1:1:193:SER:O	2.54	0.61
2:2:125:SER:HB3	2:2:230:LEU:HD21	1.82	0.61
2:2:125:SER:CB	2:2:230:LEU:CD2	2.78	0.61
1:1:91:VAL:HG22	1:1:225:ARG:HH21	1.65	0.61
2:2:81:ARG:CZ	2:2:136:THR:CA	2.79	0.61
1:1:63:TYR:OH	1:1:109:MET:CE	2.49	0.60
1:1:201:ALA:O	2:2:178:THR:CG2	2.49	0.60
1:1:213:LYS:NZ	3:3:179:PRO:HG2	2.15	0.60
2:2:109:GLY:O	2:2:252:VAL:CG1	2.49	0.60
2:2:166:GLY:C	2:2:179:ASN:ND2	2.52	0.60
1:1:75:SER:O	1:1:76:PHE:CA	2.48	0.60
1:1:121:PRO:HB3	1:1:249:ARG:O	2.01	0.60
2:2:210:ASN:ND2	2:2:220:HIS:HE1	1.98	0.60
4:4:23:ASN:HD22	4:4:30:GLN:NE2	1.97	0.60
1:1:46:LEU:O	1:1:233:SER:OG	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:77:SER:CB	3:3:191:TRP:HB3	2.32	0.60
3:3:127:ILE:HG21	3:3:161:PHE:HD2	1.60	0.60
4:4:35:LEU:HD12	4:4:36:SER:N	2.13	0.60
1:1:173:PRO:HB3	3:3:17:THR:CG2	2.31	0.60
3:3:82:GLN:HA	3:3:187:TRP:HA	1.83	0.60
1:1:64:ARG:NH2	1:1:136:LEU:CD1	2.63	0.60
3:3:18:ASN:HD22	3:3:19:PRO:N	2.00	0.60
1:1:73:LEU:HB3	1:1:74:PRO:HD2	1.84	0.60
1:1:113:ASP:OD2	1:1:116:PHE:CB	2.48	0.60
1:1:129:LEU:HD13	1:1:240:TYR:HD1	1.65	0.60
1:1:182:ASN:CG	3:3:12:GLY:HA3	2.22	0.60
4:4:23:ASN:HD22	4:4:30:GLN:HE22	1.50	0.60
1:1:60:GLU:HG2	1:1:61:ASN:N	2.07	0.60
1:1:122:PHE:HB3	1:1:245:VAL:CG2	2.28	0.60
1:1:170:THR:HB	1:1:172:ASN:H	1.67	0.60
1:1:182:ASN:O	1:1:183:SER:OG	2.18	0.60
1:1:146:ARG:CB	1:1:167:LEU:HD12	2.31	0.60
1:1:274:GLU:CG	1:1:275:LEU:N	2.65	0.60
2:2:79:HIS:CA	2:2:228:ALA:HB2	2.32	0.60
1:1:131:VAL:CG1	1:1:187:PHE:CD1	2.84	0.60
1:1:215:PHE:H	2:2:146:GLU:CD	2.02	0.60
3:3:52:THR:CG2	3:3:93:SER:HA	2.32	0.59
1:1:56:PHE:HZ	1:1:227:TRP:HB3	1.64	0.59
1:1:272:ILE:CG1	1:1:272:ILE:HB	2.24	0.59
1:1:274:GLU:CD	1:1:275:LEU:HB2	2.18	0.59
2:2:146:GLU:CA	2:2:169:TYR:CE2	2.77	0.59
2:2:129:PHE:CZ	2:2:226:VAL:HG11	2.37	0.59
2:2:185:GLN:C	2:2:187:THR:H	2.04	0.59
3:3:77:SER:OG	3:3:78:MET:HB2	2.02	0.59
1:1:133:VAL:HG22	1:1:133:VAL:O	2.02	0.59
2:2:261:HIS:ND1	2:2:261:HIS:O	2.33	0.59
1:1:68:LEU:CD2	1:1:226:LEU:HD23	2.30	0.59
3:3:45:LEU:O	3:3:49:LYS:HG2	2.01	0.59
1:1:15:ALA:O	1:1:19:PHE:O	2.19	0.59
1:1:108:LEU:CD1	1:1:110:THR:HG23	2.32	0.59
1:1:271:PRO:CB	1:1:272:ILE:C	2.71	0.59
3:3:180:THR:HG23	3:3:180:THR:O	2.03	0.59
3:3:184:VAL:HG22	3:3:185:ASP:H	1.66	0.59
1:1:71:THR:O	1:1:71:THR:HG23	2.03	0.59
2:2:212:ALA:O	2:2:214:SER:N	2.35	0.59
1:1:141:VAL:O	1:1:178:VAL:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:83:VAL:CG1	3:3:185:ASP:O	2.49	0.59
1:1:106:PHE:HE1	1:1:114:TYR:CZ	2.20	0.59
1:1:108:LEU:HD13	1:1:110:THR:CG2	2.29	0.59
1:1:79:ASP:OD2	1:1:95:TRP:CZ2	2.55	0.58
1:1:144:VAL:HG11	1:1:167:LEU:O	2.03	0.58
1:1:208:ASP:H	2:2:219:GLN:HE22	1.46	0.58
2:2:146:GLU:O	2:2:146:GLU:CG	2.27	0.58
1:1:121:PRO:O	1:1:122:PHE:CB	2.50	0.58
1:1:269:PRO:O	1:1:270:VAL:CG1	2.51	0.58
3:3:126:LEU:HD13	3:3:140:ARG:HG3	1.84	0.58
1:1:56:PHE:O	1:1:57:ASN:CB	2.46	0.58
1:1:154:ALA:CB	1:1:225:ARG:NH1	2.63	0.58
1:1:212:THR:O	1:1:212:THR:OG1	2.17	0.58
3:3:90:MET:O	3:3:96:ALA:HB1	2.02	0.58
2:2:256:PHE:N	2:2:256:PHE:CD1	2.71	0.58
1:1:94:ARG:NH2	1:1:95:TRP:HZ3	2.02	0.58
1:1:122:PHE:HB2	1:1:245:VAL:HG23	1.82	0.58
1:1:238:ILE:O	1:1:238:ILE:CG1	2.51	0.58
1:1:6:GLU:HA	2:2:193:ILE:HB	1.86	0.58
1:1:142:ALA:O	1:1:232:THR:HG22	2.02	0.58
1:1:249:ARG:HG3	1:1:250:PRO:HD2	1.84	0.58
2:2:132:PRO:HA	2:2:222:ASN:O	2.04	0.58
1:1:201:ALA:O	2:2:178:THR:HG22	2.04	0.58
2:2:80:ILE:HG23	2:2:80:ILE:O	2.04	0.58
2:2:104:TYR:HA	2:2:260:ARG:NH1	2.19	0.58
2:2:229:VAL:HG13	2:2:229:VAL:O	2.04	0.58
2:2:260:ARG:CZ	3:3:133:GLY:HA3	2.33	0.58
3:3:24:PRO:C	3:3:25:ILE:CG2	2.72	0.58
3:3:57:PRO:HA	3:3:63:ARG:HA	1.86	0.58
3:3:106:ARG:HG3	3:3:107:GLY:N	2.18	0.58
1:1:108:LEU:CD1	1:1:112:GLN:CD	2.68	0.58
1:1:186:SER:OG	3:3:9:GLU:CD	2.42	0.58
1:1:274:GLU:CG	1:1:275:LEU:CB	2.25	0.58
2:2:3:ASN:HB3	2:2:12:ASP:HB2	1.86	0.58
3:3:149:ALA:HB1	3:3:159:PHE:CZ	2.38	0.58
1:1:41:VAL:O	1:1:41:VAL:CG1	2.51	0.57
1:1:142:ALA:N	1:1:231:ASN:OD1	2.36	0.57
3:3:7:VAL:HG22	3:3:11:LYS:HZ1	1.69	0.57
3:3:115:PHE:CD1	3:3:153:LEU:HD21	2.39	0.57
3:3:219:THR:O	3:3:219:THR:HG22	2.04	0.57
1:1:63:TYR:CZ	1:1:109:MET:SD	2.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:LEU:HD21	1:1:226:LEU:HD12	1.87	0.57
1:1:203:PHE:CE2	1:1:219:PRO:HD2	2.37	0.57
1:1:186:SER:O	3:3:15:TYR:OH	2.18	0.57
2:2:255:VAL:O	2:2:255:VAL:HG13	2.03	0.57
2:2:259:LEU:CD2	2:2:260:ARG:HA	2.34	0.57
1:1:6:GLU:OE1	2:2:195:ASN:HB2	2.04	0.57
3:3:7:VAL:C	3:3:11:LYS:HE2	2.23	0.57
1:1:95:TRP:CD1	1:1:97:ARG:NH2	2.73	0.57
1:1:171:ARG:HD2	3:3:224:ILE:O	2.04	0.57
1:1:33:VAL:HG21	1:1:245:VAL:HG12	1.86	0.57
1:1:178:VAL:O	1:1:178:VAL:HG13	2.05	0.57
2:2:210:ASN:ND2	2:2:220:HIS:CE1	2.73	0.57
3:3:143:ALA:HB2	3:3:191:TRP:CZ2	2.40	0.57
1:1:6:GLU:O	2:2:192:GLN:HG3	2.04	0.57
1:1:47:ARG:HH21	1:1:233:SER:CB	2.16	0.57
1:1:273:LEU:HD12	1:1:275:LEU:H	1.68	0.57
2:2:50:ASP:OD1	3:3:166:ILE:CG1	2.53	0.57
3:3:51:PRO:HA	3:3:212:VAL:O	2.04	0.57
3:3:106:ARG:CG	3:3:107:GLY:N	2.66	0.57
2:2:24:THR:HG22	2:2:25:ASN:CA	2.35	0.57
2:2:80:ILE:O	2:2:80:ILE:CG2	2.53	0.57
2:2:134:PHE:CE1	2:2:181:GLN:NE2	2.73	0.57
2:2:230:LEU:HG	2:2:230:LEU:O	2.04	0.57
3:3:48:CYS:SG	3:3:95:LEU:CD1	2.93	0.57
4:4:27:ASN:H	4:4:27:ASN:HD22	1.51	0.56
1:1:46:LEU:HD23	1:1:66:ASN:O	2.05	0.56
1:1:122:PHE:CB	1:1:245:VAL:HG23	2.19	0.56
1:1:141:VAL:HA	1:1:231:ASN:OD1	2.06	0.56
2:2:41:HIS:C	2:2:43:GLU:N	2.59	0.56
2:2:107:LYS:HD3	2:2:255:VAL:HG11	1.86	0.56
2:2:70:TRP:NE1	2:2:229:VAL:HG21	2.21	0.56
1:1:47:ARG:NH2	1:1:233:SER:CB	2.69	0.56
1:1:129:LEU:HD22	1:1:223:PHE:CE1	2.39	0.56
1:1:271:PRO:HG2	1:1:273:LEU:N	2.21	0.56
3:3:127:ILE:O	3:3:148:TYR:CA	2.53	0.56
1:1:100:GLY:HA2	1:1:109:MET:SD	2.46	0.56
1:1:154:ALA:O	1:1:227:TRP:CE2	2.57	0.56
4:4:26:SER:O	4:4:27:ASN:C	2.43	0.56
1:1:144:VAL:HB	1:1:229:GLN:HG3	1.88	0.56
2:2:41:HIS:CD2	2:2:43:GLU:HG3	2.41	0.56
2:2:70:TRP:CZ2	2:2:229:VAL:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:131:ALA:HB2	2:2:189:TYR:CD1	2.41	0.56
3:3:132:PRO:HG2	3:3:185:ASP:OD2	2.06	0.56
3:3:210:THR:O	3:3:211:LEU:CD2	2.54	0.56
1:1:76:PHE:CB	1:1:93:TRP:CZ3	2.88	0.56
4:4:19:VAL:HG22	4:4:21:ILE:HG23	1.87	0.56
1:1:251:THR:HG22	1:1:252:LEU:N	2.20	0.56
1:1:273:LEU:CG	1:1:274:GLU:N	2.68	0.56
2:2:142:THR:O	2:2:144:THR:N	2.39	0.56
2:2:194:LEU:HA	2:2:199:ASN:ND2	2.19	0.56
3:3:52:THR:O	3:3:53:PHE:CG	2.58	0.56
3:3:129:TYR:O	3:3:146:SER:OG	2.19	0.56
1:1:79:ASP:CG	1:1:93:TRP:HE1	2.08	0.56
1:1:129:LEU:HD22	1:1:223:PHE:HZ	1.69	0.56
1:1:192:ASN:CB	3:3:222:MET:HE2	2.22	0.56
3:3:116:THR:HG23	3:3:116:THR:O	2.06	0.56
1:1:124:PHE:CE1	2:2:133:GLU:OE1	2.54	0.55
1:1:191:TYR:CE1	1:1:193:SER:HB3	2.41	0.55
2:2:80:ILE:HG22	2:2:227:VAL:C	2.27	0.55
2:2:183:GLN:C	2:2:186:TRP:CE3	2.58	0.55
3:3:198:TYR:CD1	3:3:198:TYR:C	2.73	0.55
1:1:108:LEU:CD2	2:2:175:PHE:CD2	2.70	0.55
1:1:175:MET:SD	1:1:187:PHE:CZ	3.00	0.55
2:2:78:SER:OG	2:2:160:PRO:HD3	2.07	0.55
2:2:114:VAL:HG22	2:2:202:VAL:CG1	2.36	0.55
1:1:77:CYS:SG	1:1:85:GLN:OE1	2.64	0.55
1:1:146:ARG:HG3	1:1:167:LEU:CD1	2.20	0.55
1:1:173:PRO:CB	3:3:17:THR:HG21	2.35	0.55
1:1:3:ASP:OD2	1:1:11:SER:OG	2.24	0.55
1:1:69:LEU:HD22	1:1:92:GLN:HE21	1.68	0.55
1:1:108:LEU:HD23	2:2:175:PHE:CZ	2.28	0.55
1:1:142:ALA:O	1:1:232:THR:CG2	2.54	0.55
1:1:208:ASP:HA	2:2:219:GLN:CD	2.27	0.55
1:1:263:LYS:CG	1:1:264:ILE:N	2.65	0.55
2:2:70:TRP:HE1	2:2:229:VAL:HG21	1.71	0.55
3:3:48:CYS:SG	3:3:48:CYS:O	2.64	0.55
4:4:54:ASN:O	4:4:55:LEU:HB2	2.06	0.55
1:1:106:PHE:CE1	1:1:114:TYR:OH	2.55	0.55
2:2:170:ASP:O	2:2:171:SER:HB3	2.05	0.55
1:1:99:GLY:HA3	1:1:107:PRO:HB2	1.87	0.55
1:1:133:VAL:CG2	1:1:185:VAL:CG1	2.78	0.55
1:1:151:GLY:O	3:3:103:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:ALA:CB	1:1:225:ARG:CD	2.85	0.55
1:1:182:ASN:HB3	3:3:12:GLY:CA	2.37	0.55
3:3:157:SER:OG	3:3:158:SER:N	2.39	0.55
1:1:37:TYR:CE2	1:1:122:PHE:HE2	2.23	0.55
1:1:130:GLU:HG2	1:1:239:ARG:NH1	2.22	0.55
3:3:14:PHE:CD1	3:3:15:TYR:N	2.75	0.55
1:1:79:ASP:O	1:1:79:ASP:CG	2.45	0.55
1:1:146:ARG:NH2	1:1:170:THR:CA	2.64	0.55
1:1:251:THR:HG22	1:1:252:LEU:H	1.72	0.55
3:3:54:LEU:HD11	3:3:210:THR:C	1.95	0.55
3:3:100:ARG:HD2	3:3:226:PRO:CG	2.37	0.55
3:3:165:PHE:HZ	3:3:172:ARG:HG3	1.67	0.55
1:1:74:PRO:O	1:1:92:GLN:HG2	1.95	0.55
1:1:209:PHE:O	1:1:210:GLY:C	2.46	0.55
2:2:81:ARG:NH1	2:2:136:THR:CA	2.70	0.55
2:2:134:PHE:HB3	2:2:224:THR:HG22	1.88	0.55
3:3:85:LEU:CD2	3:3:99:ALA:HB1	2.28	0.55
1:1:67:CYS:SG	1:1:227:TRP:CD1	3.00	0.54
1:1:135:ALA:O	1:1:136:LEU:CB	2.46	0.54
3:3:116:THR:O	3:3:116:THR:CG2	2.56	0.54
3:3:45:LEU:O	3:3:47:LEU:N	2.39	0.54
3:3:70:THR:HG21	3:3:205:ASN:H	1.72	0.54
2:2:25:ASN:N	2:2:25:ASN:HD22	2.05	0.54
2:2:30:VAL:HG12	2:2:199:ASN:OD1	2.08	0.54
2:2:106:CYS:SG	2:2:107:LYS:N	2.81	0.54
1:1:64:ARG:NH2	1:1:136:LEU:HG	2.22	0.54
1:1:77:CYS:SG	1:1:85:GLN:CD	2.84	0.54
1:1:148:ALA:HA	1:1:172:ASN:HD21	1.73	0.54
2:2:77:PHE:CD1	2:2:186:TRP:HZ3	2.25	0.54
2:2:84:LEU:CD2	2:2:249:LEU:HD13	2.38	0.54
2:2:104:TYR:O	2:2:104:TYR:HD1	1.90	0.54
4:4:15:GLY:O	4:4:17:GLU:N	2.41	0.54
1:1:33:VAL:HG21	1:1:245:VAL:CG1	2.37	0.54
1:1:18:ASP:OD2	1:1:19:PHE:HE1	1.91	0.54
1:1:116:PHE:CD1	1:1:116:PHE:C	2.81	0.54
1:1:175:MET:HE1	1:1:187:PHE:CZ	2.41	0.54
2:2:84:LEU:HD11	2:2:130:MET:CE	2.38	0.54
2:2:112:VAL:HG13	2:2:249:LEU:CD2	2.38	0.54
3:3:115:PHE:HZ	3:3:121:VAL:HG11	1.73	0.54
3:3:166:ILE:O	3:3:166:ILE:HG22	2.08	0.54
1:1:68:LEU:HD11	1:1:70:LEU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:52:THR:HG21	3:3:93:SER:HA	1.89	0.54
3:3:78:MET:HE1	3:3:192:GLN:CD	2.01	0.54
4:4:19:VAL:HG13	4:4:21:ILE:O	2.06	0.54
1:1:121:PRO:O	1:1:122:PHE:CD2	2.61	0.54
1:1:186:SER:OG	3:3:9:GLU:OE2	2.25	0.54
2:2:124:GLY:HA2	2:2:231:SER:O	2.08	0.54
3:3:104:GLN:HG2	3:3:171:TYR:HB3	1.90	0.54
1:1:101:VAL:HB	1:1:103:GLY:O	2.08	0.54
1:1:129:LEU:CD2	1:1:223:PHE:CE1	2.90	0.54
3:3:121:VAL:HG13	3:3:122:LYS:H	1.70	0.54
1:1:37:TYR:OH	1:1:119:PHE:CD2	2.61	0.54
2:2:256:PHE:N	2:2:256:PHE:HD1	2.05	0.54
1:1:95:TRP:CD1	1:1:95:TRP:C	2.82	0.53
1:1:96:VAL:HG23	1:1:108:LEU:HD11	1.79	0.53
1:1:18:ASP:OD2	1:1:19:PHE:CE1	2.61	0.53
1:1:96:VAL:CG2	1:1:112:GLN:NE2	2.71	0.53
1:1:214:ASP:N	2:2:146:GLU:OE2	2.41	0.53
2:2:85:PRO:O	2:2:87:VAL:N	2.40	0.53
3:3:184:VAL:HG22	3:3:185:ASP:N	2.23	0.53
3:3:230:VAL:O	3:3:231:PRO:O	2.25	0.53
1:1:133:VAL:CG1	1:1:185:VAL:HG12	2.38	0.53
1:1:68:LEU:HD11	1:1:70:LEU:CD1	2.38	0.53
1:1:62:ASP:O	1:1:63:TYR:HD2	1.86	0.53
1:1:128:ASP:HB3	4:4:31:ASN:OD1	2.09	0.53
1:1:174:HIS:CB	3:3:16:SER:HB2	2.36	0.53
3:3:54:LEU:HD11	3:3:211:LEU:N	2.21	0.53
3:3:63:ARG:HG2	3:3:63:ARG:NH1	2.22	0.53
3:3:110:ASN:ND2	3:3:160:ASN:OD1	2.41	0.53
3:3:112:LEU:CD2	3:3:211:LEU:CD1	2.79	0.53
1:1:94:ARG:O	1:1:95:TRP:HE3	1.82	0.53
1:1:106:PHE:CE1	1:1:114:TYR:CZ	2.97	0.53
1:1:216:GLY:O	1:1:217:VAL:C	2.47	0.53
1:1:15:ALA:C	1:1:17:VAL:N	2.62	0.53
3:3:129:TYR:CE1	3:3:186:GLY:HA2	2.37	0.53
1:1:125:TYR:O	1:1:198:LEU:CB	2.57	0.53
2:2:259:LEU:HD21	2:2:260:ARG:O	2.09	0.53
2:2:3:ASN:O	2:2:5:GLU:CD	2.47	0.53
3:3:106:ARG:HD2	3:3:170:HIS:O	2.08	0.53
3:3:224:ILE:CG2	3:3:225:SER:N	2.52	0.53
1:1:131:VAL:HG11	1:1:187:PHE:CZ	2.40	0.53
2:2:142:THR:C	2:2:144:THR:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:86:SER:HB2	3:3:175:SER:HB2	1.83	0.53
1:1:241:LYS:O	1:1:242:LYS:HB2	2.09	0.52
3:3:7:VAL:HG21	3:3:11:LYS:HD3	1.91	0.52
3:3:165:PHE:CZ	3:3:172:ARG:CG	2.90	0.52
1:1:133:VAL:HG13	1:1:185:VAL:HG12	1.90	0.52
3:3:127:ILE:HG22	3:3:161:PHE:CZ	2.34	0.52
1:1:146:ARG:HB2	1:1:167:LEU:HD12	1.91	0.52
1:1:215:PHE:HB3	2:2:147:PRO:HD3	1.91	0.52
2:2:32:ARG:CZ	2:2:111:ARG:NE	2.70	0.52
1:1:46:LEU:O	1:1:233:SER:HB3	2.08	0.52
1:1:126:LYS:O	1:1:243:MET:HA	2.08	0.52
3:3:108:SER:OG	3:3:217:ASP:CB	2.58	0.52
1:1:207:SER:HA	2:2:219:GLN:HE22	1.75	0.52
1:1:131:VAL:HG22	1:1:187:PHE:CE2	2.44	0.52
1:1:171:ARG:HD2	3:3:225:SER:HB2	1.92	0.52
1:1:219:PRO:HG3	3:3:182:THR:HG21	1.91	0.52
1:1:251:THR:CG2	1:1:252:LEU:H	2.23	0.52
1:1:129:LEU:HD23	1:1:223:PHE:HE1	1.75	0.52
3:3:48:CYS:C	3:3:49:LYS:HG2	2.29	0.52
3:3:52:THR:CG2	3:3:94:MET:H	2.08	0.52
2:2:126:LEU:HD11	2:2:245:ILE:HD13	1.92	0.52
3:3:103:ASN:HB2	3:3:224:ILE:CD1	2.30	0.52
1:1:152:ALA:HB2	3:3:224:ILE:HD13	1.91	0.52
1:1:202:TRP:HA	1:1:202:TRP:HE3	1.75	0.52
1:1:251:THR:CG2	1:1:252:LEU:N	2.73	0.52
1:1:271:PRO:CG	1:1:272:ILE:C	2.78	0.52
2:2:141:LYS:CG	2:2:148:SER:HA	2.40	0.52
1:1:89:ALA:CB	1:1:225:ARG:NH2	2.65	0.52
1:1:166:SER:C	1:1:168:GLY:N	2.63	0.52
3:3:98:VAL:CG1	3:3:99:ALA:N	2.73	0.52
2:2:259:LEU:CA	2:2:260:ARG:N	2.68	0.51
3:3:116:THR:OG1	3:3:209:LEU:HD22	2.10	0.51
4:4:27:ASN:ND2	4:4:27:ASN:N	2.55	0.51
1:1:96:VAL:HG13	2:2:175:PHE:CD2	2.46	0.51
2:2:131:ALA:CB	2:2:189:TYR:CD1	2.94	0.51
2:2:192:GLN:HB3	2:2:202:VAL:HG23	1.92	0.51
1:1:256:TRP:CE3	1:1:256:TRP:HA	2.45	0.51
1:1:268:ASN:HD21	1:1:269:PRO:HD2	1.68	0.51
1:1:274:GLU:HG2	1:1:275:LEU:N	2.18	0.51
2:2:125:SER:CB	2:2:230:LEU:HD21	2.40	0.51
2:2:149:ASP:OD2	2:2:152:THR:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:45:LEU:C	3:3:47:LEU:N	2.61	0.51
3:3:91:ALA:O	3:3:92:ASN:CB	2.42	0.51
1:1:142:ALA:H	1:1:231:ASN:CB	2.24	0.51
2:2:5:GLU:C	2:2:6:GLU:HG2	2.29	0.51
3:3:93:SER:O	3:3:97:ALA:CB	2.59	0.51
3:3:114:VAL:HG13	3:3:209:LEU:HB2	1.90	0.51
3:3:115:PHE:CZ	3:3:117:GLY:HA3	2.46	0.51
1:1:89:ALA:HB1	1:1:225:ARG:HH21	1.67	0.51
3:3:67:PHE:HZ	3:3:125:PHE:HE2	1.45	0.51
3:3:130:THR:HA	3:3:146:SER:OG	2.11	0.51
1:1:63:TYR:CZ	1:1:109:MET:HE3	2.46	0.51
1:1:96:VAL:HG22	1:1:110:THR:CG2	2.37	0.51
1:1:191:TYR:HD1	1:1:191:TYR:O	1.93	0.51
2:2:67:LEU:HD12	2:2:247:ALA:HB3	1.85	0.51
3:3:193:LEU:HG	3:3:193:LEU:O	2.10	0.51
1:1:68:LEU:HD22	1:1:236:VAL:CG1	2.33	0.51
1:1:157:THR:CG2	1:1:157:THR:O	2.58	0.51
1:1:193:SER:C	1:1:195:LEU:H	2.14	0.51
2:2:10:LEU:CG	2:2:11:SER:N	2.69	0.51
2:2:134:PHE:CD1	2:2:181:GLN:NE2	2.79	0.51
2:2:183:GLN:HB3	2:2:186:TRP:CH2	2.42	0.51
3:3:54:LEU:HD13	3:3:210:THR:C	2.25	0.51
3:3:129:TYR:HE1	3:3:186:GLY:CA	2.23	0.51
1:1:68:LEU:HD23	1:1:236:VAL:HG11	1.87	0.51
1:1:105:ASN:CG	2:2:175:PHE:CD1	2.75	0.51
2:2:139:GLY:CA	2:2:148:SER:HB2	2.40	0.51
3:3:14:PHE:CE1	3:3:15:TYR:O	2.64	0.51
3:3:23:VAL:HG23	3:3:24:PRO:HD2	1.92	0.51
3:3:207:ASP:N	3:3:207:ASP:OD1	2.43	0.51
1:1:41:VAL:HG12	1:1:41:VAL:O	2.10	0.51
1:1:76:PHE:CD2	1:1:110:THR:HA	2.45	0.51
1:1:94:ARG:HG2	1:1:202:TRP:CH2	2.46	0.51
1:1:264:ILE:HG23	1:1:265:ASN:HB2	1.93	0.51
2:2:86:HIS:CD2	2:2:86:HIS:H	2.28	0.51
1:1:51:ASN:ND2	1:1:54:THR:OG1	2.44	0.50
1:1:78:PRO:HD3	1:1:89:ALA:O	2.11	0.50
1:1:276:GLU:O	1:1:276:GLU:HG2	2.11	0.50
2:2:206:VAL:CG1	2:2:223:TRP:CZ2	2.94	0.50
3:3:79:VAL:CG2	3:3:80:ASP:N	2.72	0.50
4:4:24:PHE:O	4:4:25:TYR:O	2.29	0.50
2:2:161:GLN:CG	2:2:167:TYR:OH	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:122:PHE:CB	1:1:245:VAL:HG21	2.24	0.50
2:2:104:TYR:CD1	2:2:104:TYR:C	2.84	0.50
3:3:210:THR:C	3:3:211:LEU:HG	2.32	0.50
1:1:45:MET:O	1:1:46:LEU:HD12	2.11	0.50
1:1:68:LEU:CD1	1:1:70:LEU:CD1	2.88	0.50
1:1:142:ALA:CA	1:1:178:VAL:HB	2.40	0.50
1:1:215:PHE:C	1:1:215:PHE:HD1	2.15	0.50
2:2:85:PRO:HD3	2:2:222:ASN:ND2	2.21	0.50
2:2:134:PHE:HB3	2:2:224:THR:HG21	1.92	0.50
1:1:130:GLU:HB3	1:1:239:ARG:HG2	1.93	0.50
2:2:84:LEU:HD21	2:2:249:LEU:CD1	2.42	0.50
2:2:195:ASN:O	2:2:196:LEU:C	2.49	0.50
1:1:146:ARG:O	1:1:227:TRP:HE3	1.95	0.50
2:2:41:HIS:O	2:2:41:HIS:ND1	2.44	0.50
2:2:67:LEU:CG	2:2:82:ILE:HD11	2.41	0.50
2:2:79:HIS:CB	2:2:228:ALA:HB2	2.41	0.50
2:2:201:THR:HG23	2:2:202:VAL:N	2.26	0.50
2:2:210:ASN:HD22	2:2:211:VAL:N	2.09	0.50
3:3:117:GLY:HA2	3:3:206:SER:OG	2.12	0.50
3:3:182:THR:O	3:3:183:SER:C	2.49	0.50
1:1:37:TYR:HE2	1:1:122:PHE:CZ	2.29	0.50
1:1:14:ASP:OD2	1:1:23:PRO:HG3	2.12	0.50
1:1:35:PHE:O	1:1:39:ARG:CZ	2.60	0.50
1:1:202:TRP:HA	1:1:202:TRP:CE3	2.46	0.50
2:2:66:ASP:OD1	2:2:66:ASP:N	2.45	0.50
3:3:77:SER:O	3:3:79:VAL:N	2.45	0.50
3:3:86:SER:HB2	3:3:175:SER:OG	2.09	0.50
1:1:35:PHE:O	1:1:35:PHE:HD1	1.91	0.50
1:1:97:ARG:N	1:1:110:THR:HG21	2.24	0.50
1:1:210:GLY:O	1:1:212:THR:N	2.44	0.50
1:1:215:PHE:N	2:2:146:GLU:CD	2.62	0.50
3:3:174:THR:O	3:3:174:THR:HG22	2.11	0.50
1:1:94:ARG:HG2	1:1:202:TRP:HH2	1.77	0.49
1:1:129:LEU:CD2	1:1:223:PHE:HE1	2.24	0.49
1:1:211:ASN:C	1:1:213:LYS:N	2.53	0.49
1:1:264:ILE:O	1:1:265:ASN:O	2.30	0.49
3:3:47:LEU:HD21	3:3:94:MET:CG	2.42	0.49
1:1:131:VAL:HG13	1:1:187:PHE:O	2.12	0.49
1:1:250:PRO:CB	2:2:185:GLN:HE21	2.22	0.49
1:1:146:ARG:NH2	1:1:170:THR:HA	2.27	0.49
2:2:70:TRP:NE1	2:2:233:LEU:CD2	2.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:210:ASN:HD22	2:2:211:VAL:H	1.59	0.49
3:3:144:MET:C	3:3:146:SER:H	2.15	0.49
1:1:37:TYR:OH	1:1:119:PHE:HD2	1.95	0.49
1:1:95:TRP:CZ3	2:2:169:TYR:HE1	2.31	0.49
3:3:44:LEU:O	3:3:47:LEU:CB	2.54	0.49
1:1:96:VAL:CG2	1:1:110:THR:HG23	2.24	0.49
1:1:97:ARG:HD2	2:2:172:ARG:HH11	1.77	0.49
2:2:50:ASP:HB3	2:2:257:ASN:HB2	1.94	0.49
2:2:84:LEU:CD1	2:2:130:MET:CE	2.89	0.49
3:3:84:ALA:C	3:3:86:SER:N	2.51	0.49
3:3:106:ARG:HA	3:3:165:PHE:CE1	2.48	0.49
3:3:230:VAL:C	3:3:231:PRO:O	2.49	0.49
1:1:99:GLY:CA	1:1:107:PRO:HB2	2.42	0.49
1:1:253:PHE:HB2	2:2:164:PRO:HG2	1.95	0.49
2:2:3:ASN:O	2:2:5:GLU:HG3	2.12	0.49
2:2:81:ARG:NH1	2:2:136:THR:HA	2.26	0.49
2:2:136:THR:HG23	2:2:137:GLY:N	2.01	0.49
3:3:61:ASN:HD21	3:3:63:ARG:HH22	1.59	0.49
2:2:188:VAL:O	2:2:188:VAL:HG22	2.12	0.49
2:2:265:ILE:HG12	2:2:266:ALA:N	2.27	0.49
3:3:103:ASN:CB	3:3:224:ILE:HD12	2.31	0.49
1:1:37:TYR:HB3	1:1:240:TYR:CD2	2.45	0.49
1:1:50:GLN:CG	1:1:50:GLN:O	2.61	0.49
1:1:96:VAL:HG13	2:2:175:PHE:HD2	1.77	0.49
1:1:133:VAL:HG13	1:1:185:VAL:CG1	2.42	0.49
2:2:259:LEU:HD22	3:3:145:GLN:O	2.13	0.49
3:3:7:VAL:HG21	3:3:11:LYS:CD	2.42	0.49
3:3:214:ALA:CB	3:3:218:PHE:CG	2.81	0.49
1:1:54:THR:C	1:1:160:LEU:HD11	2.33	0.49
2:2:67:LEU:HD12	2:2:247:ALA:CB	2.31	0.49
4:4:26:SER:O	4:4:29:TYR:HB2	2.13	0.49
1:1:50:GLN:O	1:1:50:GLN:HG2	2.13	0.49
1:1:122:PHE:HZ	1:1:243:MET:HE1	1.78	0.49
2:2:82:ILE:O	2:2:82:ILE:HG23	2.06	0.49
1:1:37:TYR:CE2	1:1:122:PHE:CE2	2.91	0.48
1:1:63:TYR:OH	1:1:109:MET:SD	2.71	0.48
1:1:76:PHE:CB	1:1:93:TRP:HZ3	2.14	0.48
1:1:201:ALA:O	2:2:178:THR:HG21	2.13	0.48
2:2:192:GLN:CB	2:2:202:VAL:HG23	2.43	0.48
1:1:146:ARG:HD2	1:1:167:LEU:HD11	0.49	0.48
1:1:160:LEU:HD22	1:1:164:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:251:THR:H	2:2:185:GLN:HE22	0.55	0.48
2:2:81:ARG:NH2	2:2:136:THR:C	2.66	0.48
2:2:153:MET:O	2:2:154:ASP:C	2.51	0.48
1:1:35:PHE:O	1:1:35:PHE:CD1	2.67	0.48
2:2:80:ILE:CG2	2:2:227:VAL:HB	2.43	0.48
2:2:84:LEU:CD1	2:2:130:MET:HE2	2.41	0.48
3:3:20:ASP:C	3:3:20:ASP:OD1	2.51	0.48
1:1:63:TYR:CZ	1:1:109:MET:CE	2.96	0.48
1:1:97:ARG:HG2	2:2:172:ARG:HH11	1.77	0.48
3:3:115:PHE:CE2	3:3:117:GLY:HA3	2.49	0.48
3:3:115:PHE:CD1	3:3:153:LEU:HD11	2.48	0.48
3:3:161:PHE:O	3:3:162:THR:OG1	2.23	0.48
1:1:35:PHE:O	1:1:39:ARG:NE	2.46	0.48
1:1:54:THR:HA	1:1:160:LEU:CD1	2.31	0.48
1:1:101:VAL:CB	1:1:103:GLY:O	2.61	0.48
1:1:125:TYR:HE1	1:1:199:PRO:O	1.89	0.48
2:2:178:THR:HG22	2:2:178:THR:O	2.14	0.48
1:1:144:VAL:CG1	1:1:167:LEU:O	2.61	0.48
3:3:116:THR:CB	3:3:207:ASP:O	2.58	0.48
2:2:78:SER:O	2:2:228:ALA:HB1	2.13	0.48
2:2:81:ARG:CZ	2:2:136:THR:C	2.82	0.48
1:1:124:PHE:CZ	2:2:133:GLU:CD	2.80	0.48
1:1:171:ARG:CD	3:3:224:ILE:O	2.62	0.48
1:1:261:THR:CB	1:1:262:THR:CA	2.90	0.48
2:2:83:PRO:HA	2:2:224:THR:HA	1.96	0.48
3:3:76:THR:O	3:3:191:TRP:CZ3	2.67	0.48
1:1:71:THR:HG23	1:1:92:GLN:NE2	2.07	0.48
2:2:161:GLN:C	2:2:163:ALA:N	2.41	0.48
3:3:14:PHE:HD1	3:3:15:TYR:N	2.10	0.48
2:2:11:SER:O	2:2:14:VAL:HG13	2.13	0.48
2:2:77:PHE:HD1	2:2:186:TRP:CZ3	2.31	0.48
1:1:73:LEU:HD21	1:1:116:PHE:HE1	1.79	0.47
1:1:219:PRO:C	1:1:221:ALA:H	2.18	0.47
2:2:13:ARG:HA	2:2:29:THR:HG22	1.96	0.47
2:2:261:HIS:CE1	3:3:142:GLN:OE1	2.67	0.47
3:3:54:LEU:HD22	3:3:54:LEU:C	2.21	0.47
3:3:108:SER:H	3:3:217:ASP:HB3	1.79	0.47
1:1:56:PHE:CD1	1:1:229:GLN:NE2	2.82	0.47
2:2:73:SER:OG	2:2:74:GLN:N	2.48	0.47
2:2:165:THR:HG22	2:2:176:PHE:HA	1.96	0.47
3:3:51:PRO:CB	3:3:211:LEU:CB	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:37:TYR:O	1:1:240:TYR:CD2	2.67	0.47
1:1:146:ARG:C	1:1:227:TRP:HE3	2.17	0.47
3:3:100:ARG:C	3:3:102:PHE:N	2.68	0.47
1:1:125:TYR:CD2	1:1:198:LEU:HD23	2.49	0.47
1:1:145:LEU:CD2	1:1:226:LEU:HD12	2.45	0.47
2:2:35:GLY:O	2:2:36:TYR:CB	2.62	0.47
1:1:147:TRP:CE2	1:1:189:VAL:HG21	2.50	0.47
3:3:149:ALA:CB	3:3:159:PHE:CZ	2.97	0.47
1:1:219:PRO:O	1:1:221:ALA:N	2.47	0.47
1:1:258:THR:OG1	1:1:259:PRO:HD2	2.00	0.47
1:1:271:PRO:CG	1:1:272:ILE:CA	2.88	0.47
2:2:131:ALA:O	2:2:132:PRO:O	2.32	0.47
2:2:182:ASN:O	2:2:184:TRP:N	2.47	0.47
3:3:78:MET:HB2	3:3:190:VAL:O	2.13	0.47
1:1:51:ASN:OD1	1:1:51:ASN:C	2.54	0.47
1:1:156:VAL:C	1:1:158:ASP:H	2.18	0.47
1:1:213:LYS:HZ3	3:3:179:PRO:HG2	1.78	0.47
2:2:33:LEU:HD23	2:2:35:GLY:HA2	1.97	0.47
2:2:79:HIS:HA	2:2:228:ALA:HB1	1.96	0.47
2:2:141:LYS:HG2	2:2:148:SER:HA	1.97	0.47
3:3:114:VAL:CG1	3:3:209:LEU:HB2	2.45	0.47
1:1:45:MET:HB3	1:1:64:ARG:CD	2.45	0.47
1:1:131:VAL:HG22	1:1:131:VAL:O	2.15	0.47
2:2:24:THR:C	2:2:25:ASN:ND2	2.66	0.47
2:2:143:GLY:C	2:2:144:THR:HG23	2.33	0.47
3:3:52:THR:HG21	3:3:93:SER:CA	2.45	0.47
3:3:89:CYS:O	3:3:91:ALA:N	2.48	0.47
3:3:108:SER:OG	3:3:217:ASP:HB3	2.14	0.47
4:4:32:SER:C	4:4:33:ILE:O	2.53	0.47
2:2:136:THR:CG2	2:2:150:PRO:CA	2.87	0.47
3:3:66:TYR:CD2	3:3:207:ASP:HB3	2.49	0.47
3:3:138:THR:CG2	3:3:142:GLN:HE21	2.28	0.47
3:3:178:SER:O	3:3:179:PRO:O	2.33	0.47
1:1:105:ASN:CG	2:2:175:PHE:HE1	1.97	0.46
1:1:130:GLU:CG	1:1:239:ARG:NH1	2.79	0.46
1:1:154:ALA:HB3	1:1:225:ARG:HH11	1.77	0.46
3:3:47:LEU:C	3:3:49:LYS:H	2.16	0.46
3:3:139:THR:O	3:3:142:GLN:HB2	2.15	0.46
3:3:165:PHE:CE1	3:3:172:ARG:HG3	2.49	0.46
1:1:96:VAL:CA	1:1:110:THR:HG21	2.45	0.46
3:3:174:THR:O	3:3:174:THR:CG2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:67:CYS:SG	1:1:227:TRP:HD1	2.38	0.46
1:1:264:ILE:HG23	1:1:265:ASN:N	2.29	0.46
2:2:81:ARG:NH2	2:2:136:THR:O	2.48	0.46
2:2:179:ASN:HD22	2:2:179:ASN:H	1.62	0.46
3:3:95:LEU:O	3:3:95:LEU:HG	2.08	0.46
3:3:126:LEU:CD2	3:3:127:ILE:N	2.76	0.46
3:3:149:ALA:CB	3:3:159:PHE:HZ	2.24	0.46
1:1:53:GLU:H	1:1:165:PRO:HB3	1.80	0.46
2:2:208:TYR:CE2	2:2:213:PRO:HA	2.50	0.46
3:3:106:ARG:HG3	3:3:107:GLY:H	1.80	0.46
1:1:78:PRO:CD	1:1:89:ALA:O	2.64	0.46
1:1:146:ARG:NE	1:1:167:LEU:CD1	2.73	0.46
2:2:189:TYR:O	2:2:190:PRO:C	2.52	0.46
1:1:6:GLU:OE1	2:2:198:THR:HB	2.16	0.46
1:1:170:THR:HB	1:1:172:ASN:N	2.31	0.46
1:1:249:ARG:HG2	1:1:250:PRO:N	2.25	0.46
2:2:77:PHE:CE1	2:2:183:GLN:O	2.69	0.46
2:2:109:GLY:C	2:2:252:VAL:HG12	2.35	0.46
2:2:137:GLY:O	2:2:138:LYS:HB3	2.15	0.46
2:2:255:VAL:O	2:2:255:VAL:CG1	2.64	0.46
1:1:90:PRO:O	1:1:91:VAL:HG22	1.96	0.46
1:1:208:ASP:HA	2:2:219:GLN:NE2	2.30	0.46
1:1:249:ARG:CG	1:1:250:PRO:HD2	2.44	0.46
1:1:269:PRO:O	1:1:270:VAL:CB	2.64	0.46
3:3:184:VAL:CG2	3:3:185:ASP:N	2.78	0.46
1:1:259:PRO:C	1:1:260:THR:N	2.69	0.46
2:2:183:GLN:O	2:2:186:TRP:CE3	2.64	0.46
3:3:110:ASN:OD1	3:3:213:SER:HB2	2.16	0.46
1:1:97:ARG:H	1:1:110:THR:HG22	1.76	0.46
1:1:201:ALA:HA	2:2:178:THR:CG2	2.45	0.46
2:2:64:THR:HA	2:2:248:SER:HA	1.98	0.46
2:2:100:LEU:O	2:2:217:TRP:NE1	2.48	0.46
3:3:54:LEU:N	3:3:210:THR:HG22	2.26	0.46
3:3:105:TYR:HA	3:3:219:THR:O	2.16	0.46
1:1:98:SER:O	1:1:109:MET:HB2	2.17	0.45
1:1:128:ASP:HB2	1:1:241:LYS:O	2.16	0.45
2:2:71:THR:C	2:2:73:SER:H	2.19	0.45
2:2:136:THR:HG22	2:2:150:PRO:HA	1.96	0.45
3:3:70:THR:HG22	3:3:196:LEU:CD2	2.36	0.45
1:1:46:LEU:HA	1:1:65:LEU:O	2.16	0.45
1:1:64:ARG:NH2	1:1:136:LEU:CG	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:TRP:CZ3	2:2:169:TYR:CE1	3.04	0.45
1:1:96:VAL:HG13	1:1:96:VAL:O	2.15	0.45
1:1:130:GLU:CG	1:1:239:ARG:HH11	2.29	0.45
2:2:195:ASN:N	2:2:199:ASN:HB2	2.26	0.45
3:3:214:ALA:HB1	3:3:218:PHE:HB2	1.92	0.45
3:3:226:PRO:HB2	3:3:227:THR:H	0.96	0.45
1:1:6:GLU:OE1	2:2:198:THR:CB	2.65	0.45
1:1:34:ALA:O	1:1:38:ASP:CB	2.60	0.45
1:1:97:ARG:HH11	2:2:172:ARG:HB3	1.74	0.45
1:1:142:ALA:HA	1:1:178:VAL:CB	2.46	0.45
2:2:102:ARG:O	2:2:260:ARG:N	2.36	0.45
3:3:124:LYS:CB	3:3:194:THR:HG23	2.47	0.45
3:3:202:THR:CB	3:3:203:PRO:CD	2.61	0.45
1:1:144:VAL:HG22	1:1:176:TRP:CE3	2.51	0.45
2:2:102:ARG:NH2	2:2:262:GLU:OE1	2.49	0.45
1:1:78:PRO:O	1:1:84:PRO:HB2	2.08	0.45
1:1:98:SER:O	1:1:109:MET:CB	2.64	0.45
1:1:204:ASN:C	1:1:204:ASN:HD22	2.20	0.45
2:2:9:ASN:HB3	2:2:27:GLN:O	2.15	0.45
2:2:107:LYS:HB3	2:2:255:VAL:CG1	2.46	0.45
2:2:265:ILE:CG1	2:2:266:ALA:N	2.79	0.45
3:3:138:THR:C	3:3:139:THR:HG22	2.36	0.45
1:1:72:PRO:CB	1:1:113:ASP:CB	2.94	0.45
1:1:201:ALA:C	2:2:178:THR:HG22	2.37	0.45
1:1:203:PHE:O	1:1:205:GLY:N	2.47	0.45
2:2:101:ARG:CB	2:2:217:TRP:CZ2	2.95	0.45
3:3:53:PHE:CD1	3:3:211:LEU:HD23	2.51	0.45
2:2:114:VAL:HG13	2:2:202:VAL:HG13	1.99	0.45
3:3:98:VAL:HG13	3:3:99:ALA:N	2.32	0.45
3:3:107:GLY:HA3	3:3:217:ASP:O	2.17	0.45
3:3:155:LEU:HD12	3:3:156:ASN:N	2.31	0.45
1:1:108:LEU:HD21	2:2:175:PHE:HD2	1.75	0.45
1:1:146:ARG:CA	1:1:227:TRP:HE3	2.30	0.45
1:1:259:PRO:CA	1:1:260:THR:N	2.68	0.45
2:2:185:GLN:O	2:2:187:THR:N	2.41	0.45
3:3:36:TYR:HD1	3:3:36:TYR:H	1.65	0.45
3:3:67:PHE:CZ	3:3:125:PHE:CD2	3.03	0.45
3:3:115:PHE:CZ	3:3:153:LEU:HD21	2.52	0.45
1:1:142:ALA:CB	1:1:231:ASN:CB	2.80	0.45
2:2:201:THR:CG2	2:2:202:VAL:N	2.79	0.45
3:3:81:TYR:O	3:3:188:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:37:TYR:OH	1:1:119:PHE:O	2.28	0.44
1:1:64:ARG:HH22	1:1:136:LEU:CG	2.31	0.44
1:1:70:LEU:HD21	1:1:226:LEU:HB3	1.98	0.44
1:1:79:ASP:HA	1:1:84:PRO:HA	1.99	0.44
1:1:110:THR:O	1:1:110:THR:OG1	2.34	0.44
1:1:152:ALA:CB	3:3:224:ILE:HD13	2.47	0.44
2:2:150:PRO:O	2:2:151:PHE:CE1	2.68	0.44
2:2:210:ASN:ND2	2:2:211:VAL:N	2.64	0.44
1:1:62:ASP:O	1:1:63:TYR:CG	2.69	0.44
1:1:130:GLU:CG	1:1:239:ARG:HD2	2.47	0.44
1:1:263:LYS:CD	1:1:264:ILE:HA	2.42	0.44
2:2:71:THR:C	2:2:73:SER:N	2.71	0.44
2:2:165:THR:CB	2:2:176:PHE:HA	2.48	0.44
2:2:210:ASN:HD21	2:2:220:HIS:HE1	1.52	0.44
3:3:7:VAL:CG2	3:3:11:LYS:HZ3	2.22	0.44
3:3:124:LYS:CE	3:3:152:ASP:OD1	2.64	0.44
4:4:22:ASN:N	4:4:22:ASN:ND2	2.64	0.44
4:4:27:ASN:C	4:4:29:TYR:N	2.69	0.44
1:1:68:LEU:HD11	1:1:70:LEU:HD12	1.99	0.44
2:2:194:LEU:CA	2:2:199:ASN:HD22	2.26	0.44
2:2:266:ALA:O	2:2:267:GLN:C	2.55	0.44
1:1:141:VAL:CG2	1:1:232:THR:CB	2.80	0.44
1:1:153:PRO:C	1:1:155:ASP:N	2.71	0.44
1:1:228:ILE:HG21	1:1:228:ILE:HD13	1.75	0.44
3:3:70:THR:HG21	3:3:205:ASN:HA	2.00	0.44
1:1:56:PHE:O	1:1:57:ASN:HB2	2.18	0.44
1:1:152:ALA:O	1:1:154:ALA:N	2.51	0.44
1:1:154:ALA:O	1:1:227:TRP:CZ2	2.71	0.44
2:2:188:VAL:HG23	2:2:188:VAL:O	2.16	0.44
3:3:90:MET:O	3:3:96:ALA:HB3	2.15	0.44
3:3:136:LYS:HG3	3:3:136:LYS:O	2.17	0.44
1:1:144:VAL:HG22	1:1:176:TRP:HE3	1.82	0.44
1:1:166:SER:O	1:1:167:LEU:C	2.55	0.44
3:3:51:PRO:HB2	3:3:211:LEU:CB	2.39	0.44
3:3:214:ALA:HB1	3:3:218:PHE:CD1	2.45	0.44
3:3:100:ARG:HA	3:3:174:THR:HG21	1.99	0.44
3:3:138:THR:H	3:3:142:GLN:NE2	2.16	0.44
1:1:157:THR:O	1:1:157:THR:HG22	2.18	0.44
2:2:125:SER:HB3	2:2:230:LEU:HD23	1.97	0.44
2:2:161:GLN:HE21	2:2:161:GLN:HB3	1.68	0.44
1:1:6:GLU:H	1:1:6:GLU:HG2	1.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:118:CYS:O	1:1:251:THR:HG23	2.18	0.44
1:1:129:LEU:HB2	1:1:223:PHE:CZ	2.53	0.44
1:1:141:VAL:HG13	1:1:232:THR:N	2.30	0.44
2:2:119:SER:OG	2:2:122:HIS:ND1	2.51	0.44
3:3:48:CYS:SG	3:3:98:VAL:CG1	3.06	0.44
3:3:112:LEU:HD23	3:3:211:LEU:HD12	1.94	0.44
1:1:100:GLY:HA3	1:1:109:MET:SD	2.56	0.43
1:1:125:TYR:N	1:1:198:LEU:O	2.38	0.43
2:2:131:ALA:HB2	2:2:189:TYR:CE1	2.52	0.43
3:3:67:PHE:O	3:3:68:SER:O	2.36	0.43
1:1:128:ASP:HB2	4:4:31:ASN:OD1	2.17	0.43
1:1:152:ALA:O	1:1:153:PRO:C	2.55	0.43
2:2:11:SER:O	2:2:14:VAL:CG1	2.66	0.43
2:2:67:LEU:HG	2:2:82:ILE:HD11	1.99	0.43
2:2:113:GLN:CG	2:2:203:ASP:OD1	2.51	0.43
1:1:202:TRP:HD1	2:2:134:PHE:O	2.01	0.43
2:2:41:HIS:ND1	2:2:41:HIS:N	2.66	0.43
3:3:7:VAL:O	3:3:11:LYS:CE	2.66	0.43
3:3:14:PHE:HE1	3:3:15:TYR:O	2.02	0.43
1:1:63:TYR:HB3	1:1:76:PHE:HZ	1.78	0.43
1:1:141:VAL:O	1:1:178:VAL:CB	2.66	0.43
1:1:193:SER:O	1:1:195:LEU:N	2.52	0.43
3:3:174:THR:O	3:3:175:SER:CB	2.53	0.43
1:1:19:PHE:N	1:1:19:PHE:CD1	2.86	0.43
1:1:129:LEU:HD11	1:1:240:TYR:CE1	2.52	0.43
3:3:48:CYS:SG	3:3:95:LEU:HD12	2.58	0.43
3:3:117:GLY:CA	3:3:206:SER:OG	2.66	0.43
1:1:108:LEU:HD12	1:1:112:GLN:HE22	0.26	0.43
1:1:146:ARG:CG	1:1:227:TRP:CZ3	3.01	0.43
3:3:125:PHE:O	3:3:151:TRP:N	2.32	0.43
4:4:32:SER:O	4:4:33:ILE:O	2.37	0.43
1:1:130:GLU:HG2	1:1:239:ARG:CG	2.48	0.43
1:1:203:PHE:CZ	1:1:219:PRO:CD	2.98	0.43
1:1:265:ASN:OD1	1:1:276:GLU:C	2.57	0.43
2:2:3:ASN:O	2:2:5:GLU:CG	2.67	0.43
3:3:8:ARG:CG	3:3:8:ARG:NH1	2.42	0.43
3:3:67:PHE:HZ	3:3:125:PHE:CD2	2.24	0.43
1:1:96:VAL:HG11	2:2:176:PHE:CE1	2.53	0.43
1:1:97:ARG:HG2	2:2:172:ARG:NH1	2.33	0.43
1:1:77:CYS:SG	1:1:85:GLN:HG2	2.52	0.43
1:1:104:ALA:HB1	1:1:105:ASN:H	1.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:122:PHE:CZ	1:1:243:MET:CE	3.02	0.43
1:1:130:GLU:HG2	1:1:239:ARG:HH11	1.84	0.43
2:2:54:ASP:HB3	2:2:55:LYS:HG2	2.00	0.43
2:2:114:VAL:C	2:2:115:GLN:HG3	2.36	0.43
2:2:168:ARG:NH1	2:2:173:THR:H	2.16	0.43
2:2:185:GLN:C	2:2:187:THR:N	2.71	0.43
3:3:94:MET:O	3:3:97:ALA:HB3	2.18	0.43
1:1:142:ALA:H	1:1:231:ASN:CG	2.22	0.43
1:1:153:PRO:C	1:1:155:ASP:H	2.22	0.43
2:2:82:ILE:HG21	2:2:225:LEU:HD23	2.01	0.43
3:3:69:ALA:O	3:3:70:THR:CB	2.63	0.43
4:4:54:ASN:HD22	4:4:54:ASN:HA	1.62	0.43
1:1:123:THR:C	1:1:124:PHE:CD1	2.91	0.42
1:1:154:ALA:HB3	1:1:225:ARG:NH1	2.32	0.42
1:1:160:LEU:O	1:1:161:ILE:C	2.57	0.42
2:2:116:CYS:HB3	2:2:194:LEU:HD11	1.99	0.42
2:2:230:LEU:HD23	2:2:231:SER:N	2.33	0.42
1:1:122:PHE:CZ	1:1:243:MET:HE1	2.54	0.42
1:1:149:PRO:O	1:1:152:ALA:HB3	2.19	0.42
1:1:191:TYR:HE1	1:1:193:SER:HB3	1.82	0.42
2:2:10:LEU:HG	2:2:11:SER:OG	2.19	0.42
2:2:101:ARG:HG3	2:2:101:ARG:H	1.67	0.42
1:1:68:LEU:HD11	1:1:70:LEU:HD13	2.00	0.42
1:1:146:ARG:CB	1:1:167:LEU:HG	2.42	0.42
1:1:190:PRO:HB2	1:1:191:TYR:H	1.36	0.42
1:1:213:LYS:HZ1	3:3:179:PRO:HG2	1.81	0.42
2:2:47:SER:HB2	3:3:167:SER:O	2.19	0.42
2:2:129:PHE:CZ	2:2:186:TRP:NE1	2.75	0.42
2:2:134:PHE:CE1	2:2:181:GLN:CD	2.93	0.42
3:3:52:THR:HG23	3:3:93:SER:HA	2.01	0.42
1:1:108:LEU:HD11	1:1:110:THR:HG23	1.99	0.42
3:3:202:THR:HA	3:3:203:PRO:HD3	1.48	0.42
4:4:35:LEU:HD13	4:4:35:LEU:HA	1.85	0.42
1:1:56:PHE:HD1	1:1:229:GLN:NE2	2.17	0.42
1:1:133:VAL:CG1	1:1:185:VAL:CG1	2.98	0.42
1:1:141:VAL:O	1:1:178:VAL:CA	2.67	0.42
2:2:81:ARG:NE	2:2:136:THR:HA	2.33	0.42
2:2:128:VAL:HG21	2:2:202:VAL:HG11	2.01	0.42
2:2:206:VAL:HG12	2:2:223:TRP:CZ2	2.54	0.42
3:3:44:LEU:O	3:3:47:LEU:N	2.53	0.42
1:1:96:VAL:HG23	1:1:112:GLN:NE2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:270:VAL:CG2	1:1:271:PRO:N	2.63	0.42
3:3:138:THR:HG23	3:3:142:GLN:HE21	1.85	0.42
1:1:53:GLU:O	1:1:54:THR:CB	2.66	0.42
1:1:130:GLU:CD	1:1:239:ARG:HH11	2.23	0.42
2:2:3:ASN:HB3	2:2:12:ASP:OD2	2.18	0.42
2:2:64:THR:O	2:2:65:ILE:CG2	2.67	0.42
2:2:183:GLN:HA	2:2:186:TRP:HB2	2.01	0.42
3:3:77:SER:OG	3:3:78:MET:CG	2.67	0.42
1:1:63:TYR:CE2	1:1:109:MET:SD	3.13	0.42
1:1:71:THR:C	1:1:73:LEU:H	2.23	0.42
1:1:76:PHE:O	1:1:93:TRP:CZ3	2.73	0.42
3:3:115:PHE:CE1	3:3:153:LEU:HD21	2.54	0.42
1:1:66:ASN:O	1:1:228:ILE:HG22	2.19	0.42
2:2:163:ALA:HA	2:2:164:PRO:HD2	1.78	0.42
1:1:122:PHE:HB3	1:1:245:VAL:HG22	1.95	0.41
2:2:206:VAL:HG11	2:2:223:TRP:CZ2	2.49	0.41
2:2:259:LEU:CG	2:2:260:ARG:N	2.78	0.41
3:3:78:MET:SD	3:3:192:GLN:HG2	2.60	0.41
1:1:208:ASP:N	2:2:219:GLN:NE2	2.49	0.41
3:3:115:PHE:CE2	3:3:153:LEU:CD2	3.02	0.41
1:1:122:PHE:O	1:1:200:ALA:HB3	2.19	0.41
1:1:173:PRO:HA	3:3:17:THR:CG2	2.50	0.41
2:2:70:TRP:CE2	2:2:233:LEU:CG	3.04	0.41
2:2:235:TYR:C	2:2:235:TYR:CD1	2.93	0.41
4:4:19:VAL:CG2	4:4:21:ILE:HG23	2.50	0.41
1:1:146:ARG:HH21	1:1:170:THR:CA	1.91	0.41
1:1:160:LEU:HD23	1:1:160:LEU:HA	1.89	0.41
2:2:7:MET:HA	2:2:120:GLN:CD	2.30	0.41
2:2:18:LYS:HG3	2:2:18:LYS:O	2.21	0.41
1:1:71:THR:CG2	1:1:71:THR:O	2.67	0.41
1:1:80:SER:O	1:1:82:SER:N	2.53	0.41
3:3:115:PHE:HA	3:3:208:ILE:HB	2.02	0.41
1:1:142:ALA:O	1:1:143:SER:CB	2.51	0.41
1:1:161:ILE:HB	3:3:228:LYS:NZ	2.35	0.41
1:1:258:THR:CB	1:1:259:PRO:HD2	2.38	0.41
2:2:64:THR:O	2:2:65:ILE:HG23	2.20	0.41
2:2:70:TRP:CE2	2:2:233:LEU:HG	2.56	0.41
2:2:107:LYS:HD3	2:2:255:VAL:CG1	2.50	0.41
2:2:251:PRO:HB2	2:2:254:PRO:HG3	2.02	0.41
3:3:115:PHE:CE2	3:3:117:GLY:CA	3.04	0.41
1:1:113:ASP:OD2	1:1:116:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:147:TRP:CE2	1:1:189:VAL:CG2	3.04	0.41
2:2:81:ARG:NH1	2:2:135:TYR:C	2.74	0.41
2:2:99:THR:CG2	2:2:256:PHE:CE2	2.89	0.41
2:2:132:PRO:CA	2:2:222:ASN:O	2.67	0.41
2:2:235:TYR:CD1	2:2:241:PRO:HG3	2.34	0.41
3:3:61:ASN:ND2	3:3:63:ARG:NH2	2.66	0.41
1:1:38:ASP:HA	1:1:240:TYR:O	2.21	0.41
1:1:63:TYR:CE1	1:1:109:MET:HE3	2.55	0.41
1:1:194:PRO:HG3	3:3:173:GLN:HE22	1.86	0.41
2:2:51:THR:O	2:2:51:THR:HG23	2.20	0.41
2:2:80:ILE:CG2	2:2:227:VAL:O	2.64	0.41
1:1:6:GLU:OE1	2:2:195:ASN:CB	2.68	0.41
1:1:6:GLU:HG3	2:2:198:THR:HG21	2.02	0.41
1:1:108:LEU:HD11	1:1:110:THR:HG22	1.88	0.41
1:1:113:ASP:OD2	1:1:240:TYR:OH	2.38	0.41
1:1:185:VAL:HG12	1:1:185:VAL:O	2.15	0.41
3:3:70:THR:C	3:3:72:SER:N	2.72	0.41
3:3:112:LEU:HD12	3:3:158:SER:OG	2.21	0.41
3:3:124:LYS:HB3	3:3:194:THR:HG23	2.02	0.41
2:2:6:GLU:OE2	2:2:13:ARG:HD3	2.20	0.41
3:3:70:THR:HG21	3:3:205:ASN:CA	2.51	0.41
3:3:139:THR:OG1	3:3:141:ASP:HB2	2.20	0.41
1:1:71:THR:HB	1:1:222:ASP:HA	2.02	0.40
3:3:48:CYS:SG	3:3:98:VAL:HG11	2.61	0.40
3:3:143:ALA:HB2	3:3:191:TRP:HZ2	1.83	0.40
3:3:192:GLN:HE21	3:3:192:GLN:HB3	1.72	0.40
4:4:23:ASN:ND2	4:4:30:GLN:NE2	2.65	0.40
1:1:167:LEU:HD13	1:1:167:LEU:HA	1.63	0.40
2:2:64:THR:C	2:2:65:ILE:HG23	2.41	0.40
2:2:125:SER:OG	2:2:230:LEU:CD2	2.69	0.40
4:4:26:SER:HB2	4:4:29:TYR:HD2	1.87	0.40
2:2:30:VAL:O	2:2:30:VAL:CG2	2.68	0.40
3:3:52:THR:CG2	3:3:93:SER:CA	2.99	0.40
3:3:165:PHE:CD2	3:3:167:SER:HB3	2.56	0.40
1:1:46:LEU:HB3	1:1:228:ILE:CG2	2.43	0.40
2:2:44:HIS:HA	2:2:45:PRO:HD3	1.81	0.40
2:2:104:TYR:HD1	2:2:104:TYR:C	2.25	0.40
2:2:165:THR:HA	2:2:176:PHE:HB2	2.03	0.40
3:3:74:PRO:CG	3:3:78:MET:SD	2.96	0.40
3:3:83:VAL:HG11	3:3:186:GLY:CA	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	270/276 (98%)	157 (58%)	48 (18%)	65 (24%)	0 0
2	2	265/267 (99%)	175 (66%)	43 (16%)	47 (18%)	0 2
3	3	230/232 (99%)	149 (65%)	46 (20%)	35 (15%)	0 3
4	4	27/45 (60%)	9 (33%)	10 (37%)	8 (30%)	0 0
All	All	792/820 (97%)	490 (62%)	147 (19%)	155 (20%)	0 2

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	18	ASP
1	1	51	ASN
1	1	57	ASN
1	1	70	LEU
1	1	81	SER
1	1	82	SER
1	1	86	LYS
1	1	89	ALA
1	1	91	VAL
1	1	94	ARG
1	1	95	TRP
1	1	106	PHE
1	1	107	PRO
1	1	111	LYS
1	1	120	SER
1	1	122	PHE
1	1	135	ALA
1	1	136	LEU
1	1	143	SER
1	1	178	VAL
1	1	183	SER
1	1	190	PRO

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Mol	Chain	Res	Type
1	1	212	THR
1	1	219	PRO
1	1	222	ASP
1	1	231	ASN
1	1	258	THR
1	1	263	LYS
1	1	264	ILE
1	1	267	ASP
1	1	270	VAL
1	1	272	ILE
1	1	274	GLU
2	2	4	THR
2	2	5	GLU
2	2	7	MET
2	2	11	SER
2	2	32	ARG
2	2	36	TYR
2	2	46	ALA
2	2	55	LYS
2	2	58	ALA
2	2	72	THR
2	2	86	HIS
2	2	132	PRO
2	2	151	PHE
2	2	156	GLU
2	2	163	ALA
2	2	165	THR
2	2	166	GLY
2	2	167	TYR
2	2	168	ARG
2	2	173	THR
2	2	175	PHE
2	2	186	TRP
2	2	196	LEU
2	2	237	THR
2	2	240	SER
2	2	265	ILE
3	3	21	THR
3	3	25	ILE
3	3	35	ASP
3	3	46	GLU
3	3	53	PHE

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Mol	Chain	Res	Type
3	3	60	ASN
3	3	71	ASN
3	3	77	SER
3	3	78	MET
3	3	85	LEU
3	3	87	CYS
3	3	215	GLY
3	3	222	MET
3	3	228	LYS
4	4	14	SER
4	4	25	TYR
4	4	34	ASP
4	4	35	LEU
1	1	54	THR
1	1	63	TYR
1	1	87	THR
1	1	90	PRO
1	1	105	ASN
1	1	167	LEU
1	1	204	ASN
1	1	208	ASP
1	1	230	GLY
1	1	262	THR
1	1	269	PRO
1	1	275	LEU
2	2	6	GLU
2	2	42	GLY
2	2	143	GLY
2	2	154	ASP
2	2	162	GLY
2	2	172	ARG
2	2	183	GLN
2	2	242	ASP
2	2	262	GLU
3	3	59	THR
3	3	79	VAL
3	3	92	ASN
3	3	96	ALA
3	3	175	SER
3	3	182	THR
4	4	16	ASN
4	4	17	GLU

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Mol	Chain	Res	Type
4	4	33	ILE
1	1	48	PRO
1	1	53	GLU
1	1	61	ASN
1	1	77	CYS
1	1	160	LEU
1	1	166	SER
2	2	91	GLU
2	2	171	SER
2	2	214	SER
2	2	260	ARG
3	3	24	PRO
3	3	68	SER
3	3	70	THR
3	3	73	VAL
3	3	90	MET
3	3	168	PRO
3	3	226	PRO
4	4	23	ASN
1	1	49	GLY
1	1	58	TYR
1	1	84	PRO
1	1	242	LYS
1	1	247	CYS
1	1	253	PHE
2	2	45	PRO
2	2	148	SER
2	2	178	THR
2	2	213	PRO
3	3	94	MET
3	3	180	THR
1	1	88	LYS
1	1	161	ILE
1	1	261	THR
2	2	145	MET
2	2	169	TYR
3	3	76	THR
3	3	80	ASP
3	3	179	PRO
1	1	194	PRO
1	1	41	VAL
1	1	210	GLY

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Mol	Chain	Res	Type
2	2	174	GLY
3	3	224	ILE
1	1	43	ILE
1	1	271	PRO
3	3	231	PRO
2	2	147	PRO
3	3	230	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	236/237 (100%)	141 (60%)	95 (40%)	0 1
2	2	225/225 (100%)	155 (69%)	70 (31%)	0 2
3	3	198/204 (97%)	120 (61%)	78 (39%)	0 1
4	4	28/36 (78%)	16 (57%)	12 (43%)	0 0
All	All	687/702 (98%)	432 (63%)	255 (37%)	0 1

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	GLU
1	1	7	LYS
1	1	11	SER
1	1	13	ASP
1	1	20	VAL
1	1	26	LEU
1	1	29	ASN
1	1	31	THR
1	1	32	ARG
1	1	41	VAL
1	1	43	ILE
1	1	45	MET
1	1	47	ARG
1	1	50	GLN

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Mol	Chain	Res	Type
1	1	54	THR
1	1	57	ASN
1	1	59	GLN
1	1	60	GLU
1	1	68	LEU
1	1	69	LEU
1	1	70	LEU
1	1	73	LEU
1	1	77	CYS
1	1	79	ASP
1	1	80	SER
1	1	81	SER
1	1	82	SER
1	1	85	GLN
1	1	86	LYS
1	1	87	THR
1	1	91	VAL
1	1	92	GLN
1	1	93	TRP
1	1	94	ARG
1	1	95	TRP
1	1	97	ARG
1	1	101	VAL
1	1	102	ASN
1	1	105	ASN
1	1	108	LEU
1	1	112	GLN
1	1	114	TYR
1	1	116	PHE
1	1	119	PHE
1	1	120	SER
1	1	126	LYS
1	1	128	ASP
1	1	131	VAL
1	1	136	LEU
1	1	138	THR
1	1	140	THR
1	1	143	SER
1	1	145	LEU
1	1	150	THR
1	1	157	THR
1	1	161	ILE

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Mol	Chain	Res	Type
1	1	167	LEU
1	1	169	GLU
1	1	176	TRP
1	1	177	LEU
1	1	182	ASN
1	1	183	SER
1	1	185	VAL
1	1	186	SER
1	1	191	TYR
1	1	192	ASN
1	1	195	LEU
1	1	196	SER
1	1	202	TRP
1	1	203	PHE
1	1	204	ASN
1	1	206	TRP
1	1	207	SER
1	1	208	ASP
1	1	209	PHE
1	1	211	ASN
1	1	212	THR
1	1	213	LYS
1	1	214	ASP
1	1	215	PHE
1	1	223	PHE
1	1	226	LEU
1	1	229	GLN
1	1	231	ASN
1	1	233	SER
1	1	238	ILE
1	1	241	LYS
1	1	247	CYS
1	1	249	ARG
1	1	251	THR
1	1	256	TRP
1	1	258	THR
1	1	265	ASN
1	1	268	ASN
1	1	271	PRO
2	2	3	ASN
2	2	4	THR
2	2	7	MET

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Mol	Chain	Res	Type
2	2	14	VAL
2	2	16	SER
2	2	25	ASN
2	2	27	GLN
2	2	30	VAL
2	2	32	ARG
2	2	33	LEU
2	2	41	HIS
2	2	43	GLU
2	2	50	ASP
2	2	54	ASP
2	2	56	VAL
2	2	60	GLU
2	2	66	ASP
2	2	74	GLN
2	2	80	ILE
2	2	82	ILE
2	2	88	LEU
2	2	101	ARG
2	2	102	ARG
2	2	104	TYR
2	2	105	LEU
2	2	113	GLN
2	2	115	GLN
2	2	130	MET
2	2	136	THR
2	2	141	LYS
2	2	142	THR
2	2	145	MET
2	2	146	GLU
2	2	148	SER
2	2	149	ASP
2	2	153	MET
2	2	154	ASP
2	2	155	THR
2	2	156	GLU
2	2	159	SER
2	2	161	GLN
2	2	168	ARG
2	2	169	TYR
2	2	170	ASP
2	2	172	ARG

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Mol	Chain	Res	Type
2	2	179	ASN
2	2	181	GLN
2	2	183	GLN
2	2	186	TRP
2	2	188	VAL
2	2	193	ILE
2	2	194	LEU
2	2	195	ASN
2	2	197	ARG
2	2	201	THR
2	2	204	LEU
2	2	209	VAL
2	2	210	ASN
2	2	211	VAL
2	2	214	SER
2	2	222	ASN
2	2	230	LEU
2	2	233	LEU
2	2	235	TYR
2	2	239	SER
2	2	240	SER
2	2	253	ASN
2	2	256	PHE
2	2	259	LEU
2	2	260	ARG
3	3	7	VAL
3	3	8	ARG
3	3	9	GLU
3	3	14	PHE
3	3	16	SER
3	3	17	THR
3	3	18	ASN
3	3	20	ASP
3	3	23	VAL
3	3	25	ILE
3	3	26	TYR
3	3	29	THR
3	3	35	ASP
3	3	37	MET
3	3	45	LEU
3	3	46	GLU
3	3	47	LEU

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Mol	Chain	Res	Type
3	3	53	PHE
3	3	54	LEU
3	3	56	ASN
3	3	58	ASN
3	3	59	THR
3	3	60	ASN
3	3	61	ASN
3	3	63	ARG
3	3	66	TYR
3	3	73	VAL
3	3	76	THR
3	3	78	MET
3	3	81	TYR
3	3	82	GLN
3	3	83	VAL
3	3	85	LEU
3	3	89	CYS
3	3	92	ASN
3	3	95	LEU
3	3	100	ARG
3	3	104	GLN
3	3	108	SER
3	3	110	ASN
3	3	112	LEU
3	3	116	THR
3	3	121	VAL
3	3	126	LEU
3	3	127	ILE
3	3	130	THR
3	3	139	THR
3	3	142	GLN
3	3	144	MET
3	3	146	SER
3	3	148	TYR
3	3	153	LEU
3	3	155	LEU
3	3	156	ASN
3	3	161	PHE
3	3	172	ARG
3	3	173	GLN
3	3	175	SER
3	3	184	VAL

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Mol	Chain	Res	Type
3	3	189	THR
3	3	191	TRP
3	3	192	GLN
3	3	194	THR
3	3	196	LEU
3	3	204	THR
3	3	206	SER
3	3	207	ASP
3	3	208	ILE
3	3	209	LEU
3	3	212	VAL
3	3	219	THR
3	3	220	LEU
3	3	221	ARG
3	3	222	MET
3	3	227	THR
3	3	229	TRP
3	3	230	VAL
3	3	232	GLN
4	4	12	ASN
4	4	13	GLU
4	4	16	ASN
4	4	17	GLU
4	4	20	ILE
4	4	21	ILE
4	4	22	ASN
4	4	31	ASN
4	4	35	LEU
4	4	36	SER
4	4	53	SER
4	4	54	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	57	ASN
1	1	59	GLN
1	1	66	ASN
1	1	112	GLN
1	1	174	HIS
1	1	182	ASN
1	1	192	ASN

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Mol	Chain	Res	Type
1	1	204	ASN
1	1	211	ASN
1	1	229	GLN
1	1	268	ASN
2	2	3	ASN
2	2	25	ASN
2	2	74	GLN
2	2	86	HIS
2	2	113	GLN
2	2	161	GLN
2	2	183	GLN
2	2	185	GLN
2	2	210	ASN
2	2	219	GLN
2	2	222	ASN
2	2	257	ASN
3	3	10	HIS
3	3	18	ASN
3	3	58	ASN
3	3	61	ASN
3	3	82	GLN
3	3	92	ASN
3	3	103	ASN
3	3	142	GLN
3	3	145	GLN
3	3	156	ASN
4	4	12	ASN
4	4	16	ASN
4	4	22	ASN
4	4	27	ASN
4	4	28	GLN
4	4	30	GLN
4	4	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	19
2	2	8
3	3	8
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	265:ASN	C	266:ALA	N	23.91
1	1	259:PRO	C	260:THR	N	2.69
1	1	105:ASN	C	106:PHE	N	1.95
1	2	260:ARG	C	261:HIS	N	1.88
1	2	143:GLY	C	144:THR	N	1.77
1	1	75:SER	C	76:PHE	N	1.75
1	1	251:THR	C	252:LEU	N	1.69
1	2	259:LEU	C	260:ARG	N	1.69
1	2	147:PRO	C	148:SER	N	1.65
1	1	26:LEU	C	27:PRO	N	1.64
1	1	66:ASN	C	67:CYS	N	1.64
1	1	238:ILE	C	239:ARG	N	1.63
1	1	9:LYS	C	10:VAL	N	1.20
1	1	28:GLU	C	29:ASN	N	1.20
1	3	37:MET	C	38:CYS	N	1.20
1	3	168:PRO	C	169:THR	N	1.19
1	3	180:THR	C	181:ILE	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	156:VAL	C	157:THR	N	1.17
1	1	12:ASN	C	13:ASP	N	1.16
1	1	271:PRO	C	272:ILE	N	1.16
1	2	223:TRP	C	224:THR	N	1.16
1	3	47:LEU	C	48:CYS	N	1.16
1	3	176:TYR	C	177:THR	N	1.16
1	1	273:LEU	C	274:GLU	N	1.15
1	2	213:PRO	C	214:SER	N	1.14
1	3	29:THR	C	30:ILE	N	1.14
1	1	153:PRO	C	154:ALA	N	1.13
1	1	159:GLN	C	160:LEU	N	1.13
1	2	2:GLN	C	3:ASN	N	1.13
1	1	14:ASP	C	15:ALA	N	1.11
1	1	69:LEU	C	70:LEU	N	1.08
1	2	3:ASN	C	4:THR	N	1.08
1	3	164:PRO	C	165:PHE	N	1.08
1	1	27:PRO	C	28:GLU	N	1.02
1	3	74:PRO	C	75:ALA	N	0.99
1	4	34:ASP	C	35:LEU	N	0.83

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.