



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:29 PM UTC

PDB ID : 1RVF / pdb_00001rvf
Title : FAB COMPLEXED WITH INTACT HUMAN RHINOVIRUS
Authors : Smith, T.J.
Deposited on : 1996-09-05
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

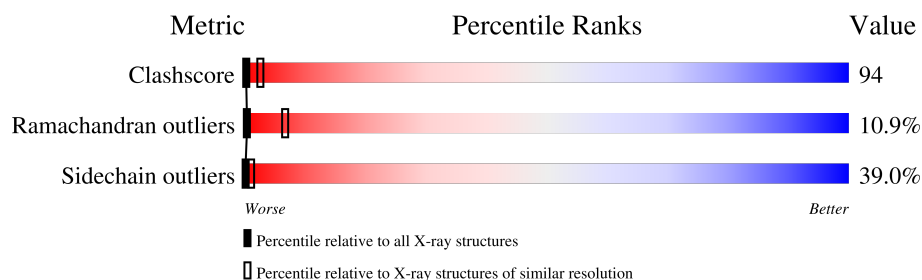
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	15% 40% 31% 7% 6%
2	2	262	11% 44% 34% 7% .
3	3	236	13% 50% 30% 6%
4	4	68	9% 26% 18% 6% 41%
5	L	110	8% 41% 39% 12%
6	H	119	12% 42% 40% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8019 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 HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	110	Total	C	N	O	S	0	0	0
			834	524	139	166	5			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	14	PHE	SER	conflict	UNP X79906
L	15	PRO	LEU	conflict	UNP X79906
L	18	LYS	ARG	conflict	UNP X79906
L	21	ILE	MET	conflict	UNP X79906
L	24	SER	THR	conflict	UNP X79906
L	26	THR	SER	conflict	UNP X79906
L	?	-	SER	deletion	UNP X79906
L	?	-	SER	deletion	UNP X79906
L	31	ASN	SER	conflict	UNP X79906
L	33	MET	LEU	conflict	UNP X79906
L	36	PHE	TYR	conflict	UNP X79906
L	42	THR	SER	conflict	UNP X79906
L	51	SER	THR	conflict	UNP X79906
L	77	ARG	SER	conflict	UNP X79906
L	89	GLN	HIS	conflict	UNP X79906
L	91	ARG	TYR	conflict	UNP X79906
L	92	SER	HIS	conflict	UNP X79906
L	93	SER	ARG	conflict	UNP X79906
L	94	TYR	PHE	conflict	UNP X79906
L	96	ILE	HIS	conflict	UNP X79906
L	100	SER	GLY	conflict	UNP X79906

- Molecule 6 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	119	Total	C	N	O	S	0	0	0
			917	579	153	181	4			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	2	GLY	ILE	conflict	UNP S38950
H	9	ALA	PRO	conflict	UNP S38950
H	16	SER	ALA	conflict	UNP S38950
H	28	ALA	THR	conflict	UNP S38950
H	30	SER	THR	conflict	UNP S38950
H	31	SER	ASP	conflict	UNP S38950
H	32	PHE	TYR	conflict	UNP S38950
H	33	TRP	TYR	conflict	UNP S38950
H	34	VAL	ILE	conflict	UNP S38950
H	35	ASN	HIS	conflict	UNP S38950

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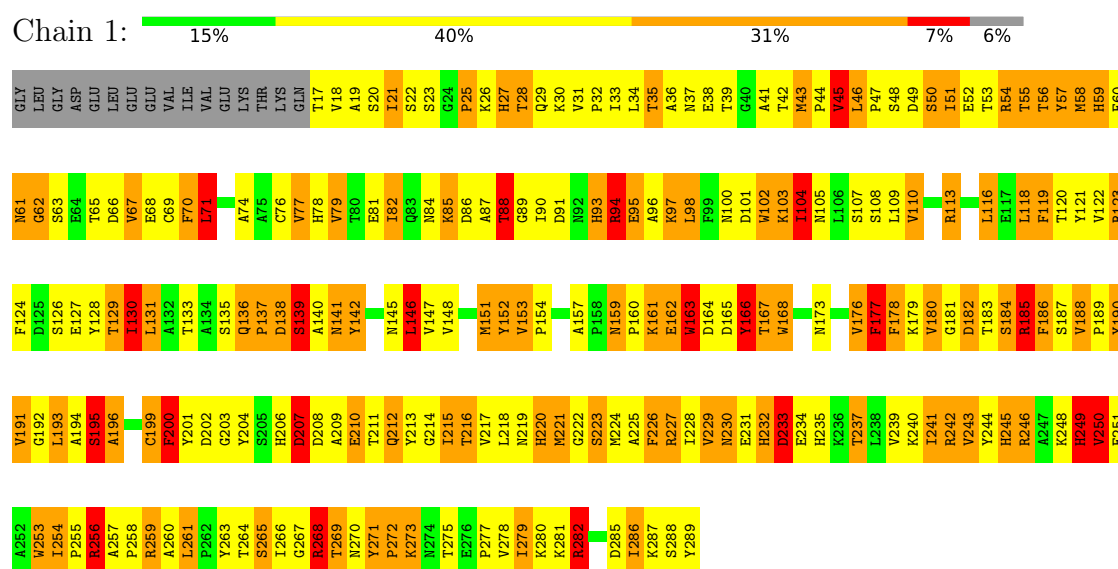
Chain	Residue	Modelled	Actual	Comment	Reference
H	43	GLN	GLU	conflict	UNP S38950
H	50	GLN	TRP	conflict	UNP S38950
H	54	ASP	SER	conflict	UNP S38950
H	56	ASP	ASN	conflict	UNP S38950
H	57	ASN	THR	conflict	UNP S38950
H	61	GLY	GLU	conflict	UNP S38950
H	71	ALA	VAL	conflict	UNP S38950
H	73	LYS	THR	conflict	UNP S38950
H	76	THR	SER	conflict	UNP S38950
H	82A	TYR	SER	conflict	UNP S38950
H	95	SER	GLY	conflict	UNP S38950
H	97	ASN	-	insertion	UNP S38950
H	98	TYR	-	insertion	UNP S38950
H	99	PRO	LYS	conflict	UNP S38950
H	100I	TYR	PHE	conflict	UNP S38950

3 Residue-property plots

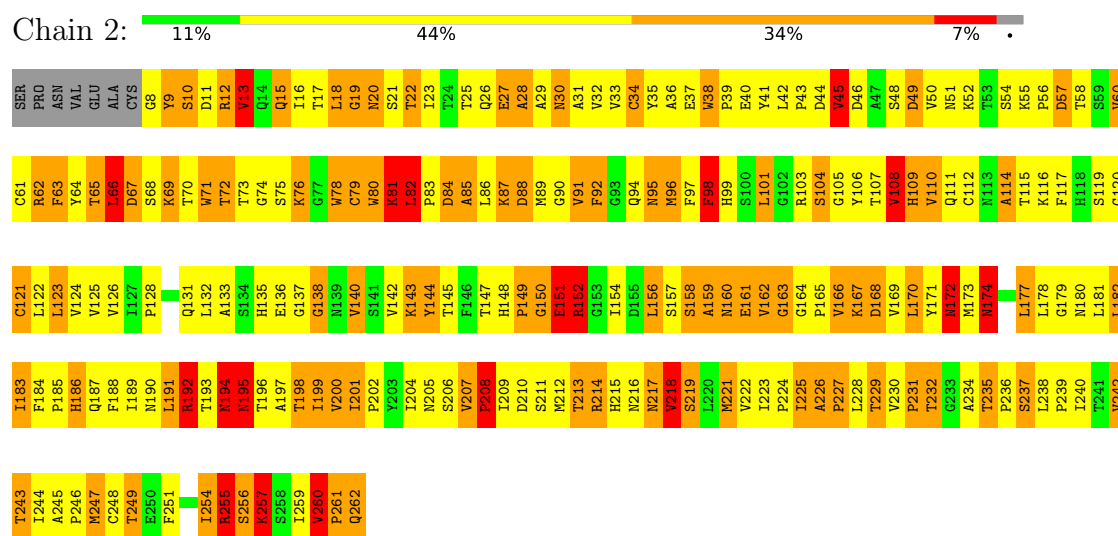
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

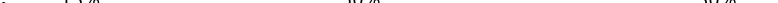
• Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN

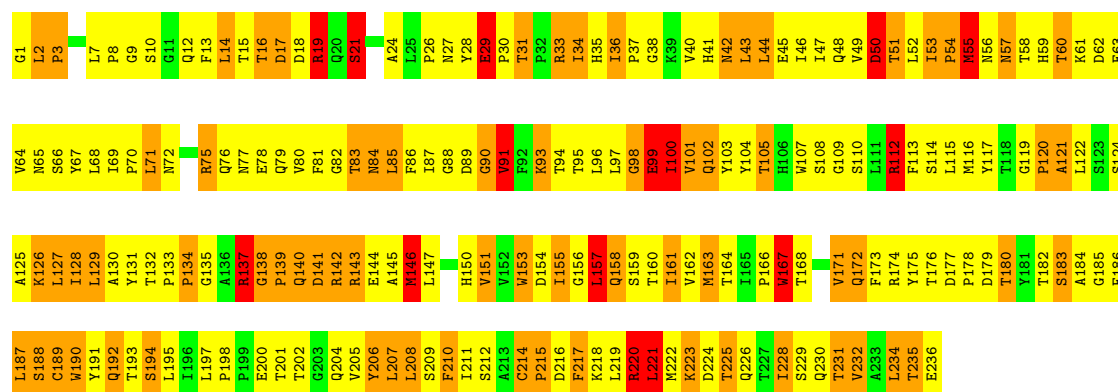


• Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN

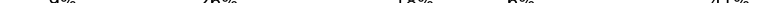


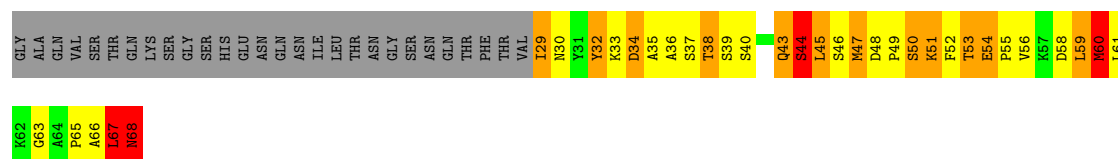
• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN

Chain 3:  13% 50% 30% 6%

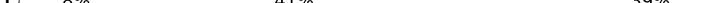


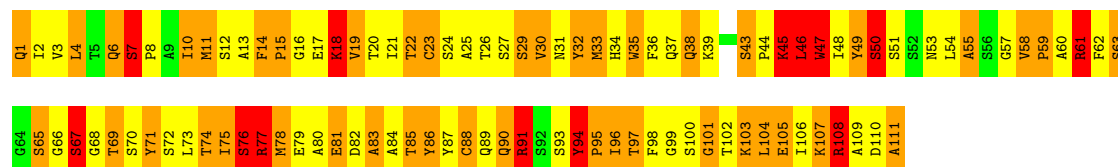
- Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN

Chain 4: 

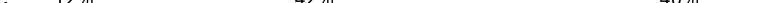


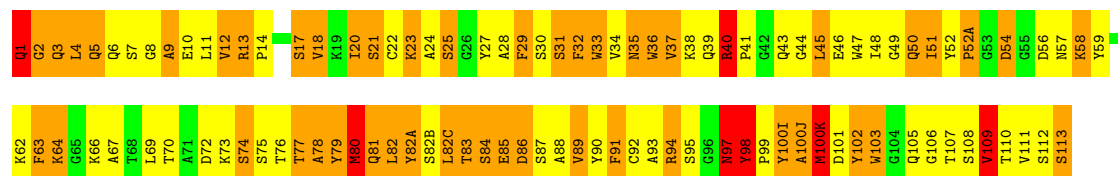
- Molecule 5: FAB 17-IA

Chain L:  8% 41% 39% 12%



- Molecule 6: FAB 17-IA

Chain H:  12% 42% 40% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	372.00Å 372.00Å 372.00Å 108.40° 108.40° 108.40°	Depositor
Resolution (Å)	10.00 – 4.00	Depositor
% Data completeness (in resolution range)	64.5 (10.00-4.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.21	5/2228 (0.2%)	1.66	52/3031 (1.7%)
2	2	1.27	9/2001 (0.4%)	1.64	36/2735 (1.3%)
3	3	1.37	13/1898 (0.7%)	1.72	36/2597 (1.4%)
4	4	1.34	3/302 (1.0%)	1.95	10/406 (2.5%)
5	L	1.29	6/854 (0.7%)	1.81	22/1157 (1.9%)
6	H	1.33	9/941 (1.0%)	1.83	25/1272 (2.0%)
All	All	1.29	45/8224 (0.5%)	1.72	181/11198 (1.6%)

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
6	H	0	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	111	ALA	CA-C	11.38	1.76	1.52
3	3	139	PRO	CA-C	-7.88	1.42	1.52
2	2	8	GLY	N-CA	7.80	1.58	1.45
6	H	113	SER	CA-C	7.66	1.69	1.52
4	4	29	ILE	N-CA	7.63	1.60	1.46
6	H	113	SER	C-OXT	7.47	1.38	1.23
6	H	78	ALA	C-N	-7.26	1.27	1.33
3	3	100	ILE	N-CA	6.86	1.54	1.46
5	L	111	ALA	C-OXT	6.46	1.36	1.23
3	3	134	PRO	CA-C	6.21	1.58	1.52
3	3	120	PRO	CA-C	-6.10	1.45	1.52
4	4	68	ASN	C-OXT	6.08	1.35	1.23
5	L	111	ALA	C-O	6.02	1.35	1.23
2	2	150	GLY	N-CA	5.83	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	76	SER	N-CA	5.80	1.53	1.46
3	3	1	GLY	N-CA	5.79	1.54	1.45
3	3	135	GLY	N-CA	5.76	1.53	1.45
6	H	33	TRP	NE1-CE2	-5.62	1.31	1.37
2	2	38	TRP	NE1-CE2	-5.61	1.31	1.37
6	H	36	TRP	NE1-CE2	-5.58	1.31	1.37
5	L	35	TRP	NE1-CE2	-5.53	1.31	1.37
6	H	47	TRP	NE1-CE2	-5.52	1.31	1.37
1	1	253	TRP	NE1-CE2	-5.51	1.31	1.37
3	3	107	TRP	NE1-CE2	-5.50	1.31	1.37
3	3	139	PRO	C-N	-5.46	1.26	1.33
3	3	153	TRP	NE1-CE2	-5.46	1.31	1.37
1	1	102	TRP	NE1-CE2	-5.44	1.31	1.37
1	1	168	TRP	NE1-CE2	-5.44	1.31	1.37
6	H	79	TYR	CA-C	-5.42	1.48	1.53
2	2	80	TRP	NE1-CE2	-5.38	1.31	1.37
3	3	190	TRP	NE1-CE2	-5.37	1.31	1.37
2	2	239	PRO	C-N	-5.36	1.26	1.33
6	H	103	TRP	NE1-CE2	-5.35	1.31	1.37
6	H	113	SER	C-O	5.33	1.34	1.23
5	L	47	TRP	NE1-CE2	-5.31	1.31	1.37
2	2	239	PRO	CA-C	-5.30	1.45	1.52
2	2	10	SER	N-CA	5.29	1.52	1.45
2	2	78	TRP	NE1-CE2	-5.28	1.31	1.37
2	2	71	TRP	NE1-CE2	-5.21	1.31	1.37
3	3	167	TRP	NE1-CE2	-5.16	1.31	1.37
3	3	112	ARG	C-N	-5.13	1.26	1.33
1	1	200	PHE	C-N	-5.04	1.27	1.33
1	1	146	LEU	C-N	-5.03	1.27	1.33
4	4	68	ASN	CA-C	5.03	1.63	1.52
3	3	99	GLU	CA-C	5.01	1.59	1.52

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	94	TYR	O-C-N	-12.74	106.67	121.32
1	1	271	TYR	O-C-N	12.50	130.60	121.85
2	2	261	PRO	O-C-N	11.80	138.56	122.64
4	4	67	LEU	O-C-N	11.10	137.49	123.28
6	H	97	ASN	N-CA-C	-11.02	99.82	113.38
6	H	97	ASN	O-C-N	10.59	136.29	122.42
5	L	7	SER	O-C-N	-10.01	109.81	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	225	THR	O-C-N	9.95	135.03	123.29
5	L	32	TYR	O-C-N	8.97	134.80	123.14
2	2	82	LEU	O-C-N	-8.86	111.13	121.32
6	H	98	TYR	O-C-N	-8.76	111.25	121.32
1	1	221	MET	N-CA-C	-8.74	100.00	113.02
3	3	54	PRO	CB-CA-C	-8.73	101.46	112.89
6	H	109	VAL	O-C-N	8.59	132.30	123.20
6	H	79	TYR	O-C-N	8.34	129.36	123.11
6	H	89	VAL	O-C-N	8.33	132.06	123.07
6	H	85	GLU	N-CA-C	-8.21	103.78	113.88
3	3	235	THR	O-C-N	8.21	132.79	123.27
6	H	1	GLN	O-C-N	8.09	135.94	123.00
6	H	52(A)	PRO	O-C-N	8.05	131.90	122.23
2	2	67	ASP	O-C-N	8.00	132.37	123.33
5	L	88	CYS	N-CA-C	-7.99	100.58	110.41
6	H	79	TYR	CB-CA-C	-7.96	102.85	114.87
6	H	91	PHE	CA-CB-CG	7.91	121.71	113.80
3	3	29	GLU	O-C-N	7.80	130.80	121.60
1	1	162	GLU	O-C-N	7.77	132.28	123.27
3	3	139	PRO	N-CA-C	-7.70	98.96	111.21
3	3	134	PRO	CB-CA-C	-7.53	103.35	111.56
1	1	277	PRO	O-C-N	7.43	132.22	123.01
5	L	45	LYS	O-C-N	7.36	132.24	123.33
3	3	225	THR	CA-C-N	7.34	130.44	120.38
3	3	225	THR	C-N-CA	7.34	130.44	120.38
4	4	32	TYR	O-C-N	7.34	132.53	123.21
3	3	29	GLU	CA-C-N	7.21	127.13	120.21
3	3	29	GLU	C-N-CA	7.21	127.13	120.21
1	1	223	SER	O-C-N	7.15	132.96	122.81
3	3	3	PRO	O-C-N	7.14	131.22	123.01
1	1	219	ASN	N-CA-C	7.05	121.10	107.71
1	1	110	VAL	CB-CA-C	-6.91	101.96	112.05
6	H	72	ASP	O-C-N	6.82	132.13	123.12
1	1	250	VAL	CB-CA-C	-6.80	102.10	111.49
1	1	104	ILE	O-C-N	6.77	129.99	122.75
3	3	72	ASN	O-C-N	6.74	131.23	123.27
2	2	260	VAL	O-C-N	6.68	128.71	121.10
5	L	14	PHE	O-C-N	-6.59	115.44	121.30
2	2	163	GLY	N-CA-C	-6.54	106.04	115.27
3	3	134	PRO	N-CA-C	6.54	120.76	110.50
1	1	250	VAL	O-C-N	6.52	131.01	122.47
2	2	226	ALA	CA-C-N	6.51	126.47	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	226	ALA	C-N-CA	6.51	126.47	119.76
4	4	67	LEU	CA-C-N	6.48	133.37	121.70
4	4	67	LEU	C-N-CA	6.48	133.37	121.70
1	1	220	HIS	CA-CB-CG	6.43	120.23	113.80
2	2	159	ALA	O-C-N	6.42	131.10	123.33
5	L	32	TYR	CA-CB-CG	-6.42	102.34	113.90
1	1	220	HIS	O-C-N	6.40	131.55	123.23
2	2	227	PRO	N-CA-C	6.37	121.08	111.14
5	L	32	TYR	CB-CA-C	6.33	119.86	110.62
4	4	60	MET	O-C-N	6.31	130.58	123.19
2	2	201	ILE	N-CA-C	6.31	114.92	107.73
1	1	139	SER	O-C-N	6.28	130.94	122.59
2	2	235	THR	O-C-N	6.27	128.53	121.32
1	1	28	THR	O-C-N	6.20	130.44	122.68
2	2	168	ASP	O-C-N	6.20	130.92	123.36
1	1	128	TYR	CA-CB-CG	6.18	125.03	113.90
1	1	176	VAL	CB-CA-C	-6.15	101.21	111.29
2	2	162	VAL	O-C-N	6.06	130.33	122.94
1	1	28	THR	N-CA-C	6.05	115.99	108.19
4	4	44	SER	O-C-N	5.98	128.55	122.09
1	1	221	MET	O-C-N	5.96	129.71	122.20
1	1	181	GLY	N-CA-C	-5.96	107.73	115.59
5	L	108	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	1	206	HIS	O-C-N	5.94	129.85	123.56
5	L	59	PRO	O-C-N	5.92	130.63	122.64
2	2	161	GLU	CA-C-N	-5.92	114.97	122.37
2	2	161	GLU	C-N-CA	-5.92	114.97	122.37
2	2	168	ASP	N-CA-C	5.91	119.15	108.69
1	1	220	HIS	N-CA-CB	5.88	121.06	110.83
1	1	185	ARG	NE-CZ-NH2	5.88	124.49	119.20
3	3	206	TYR	O-C-N	5.87	129.95	123.25
3	3	215	PRO	O-C-N	5.86	129.78	122.22
1	1	250	VAL	N-CA-C	5.85	117.58	109.45
4	4	65	PRO	O-C-N	5.84	130.53	122.64
3	3	229	SER	O-C-N	5.83	128.65	123.41
1	1	166	TYR	N-CA-C	-5.81	106.33	113.41
1	1	177	PHE	CB-CA-C	-5.76	101.14	110.77
2	2	143	LYS	O-C-N	5.75	129.71	123.10
3	3	137	ARG	NE-CZ-NH2	5.75	124.37	119.20
6	H	63	PHE	CA-CB-CG	-5.73	108.07	113.80
2	2	214	ARG	NE-CZ-NH2	5.69	124.32	119.20
6	H	108	SER	CA-C-N	-5.67	115.56	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	108	SER	C-N-CA	-5.67	115.56	123.10
2	2	239	PRO	O-C-N	5.67	129.91	123.00
3	3	120	PRO	O-C-N	5.60	129.45	123.01
3	3	33	ARG	NE-CZ-NH2	5.58	124.22	119.20
5	L	94	TYR	CA-CB-CG	-5.57	103.87	113.90
3	3	226	GLN	CB-CA-C	-5.55	101.25	110.68
6	H	79	TYR	N-CA-CB	5.54	115.16	109.51
3	3	60	THR	N-CA-C	-5.52	104.90	111.69
2	2	192	ARG	NE-CZ-NH2	5.52	124.16	119.20
3	3	192	GLN	O-C-N	5.51	127.82	122.09
1	1	63	SER	N-CA-C	-5.49	105.31	112.23
6	H	85	GLU	O-C-N	5.47	129.70	122.36
1	1	268	ARG	NE-CZ-NH2	5.45	124.11	119.20
6	H	13	ARG	NE-CZ-NH2	5.45	124.10	119.20
3	3	155	ILE	O-C-N	5.44	128.92	122.83
1	1	227	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	1	28	THR	CB-CA-C	-5.43	102.64	114.10
3	3	50	ASP	O-C-N	5.41	129.98	123.16
1	1	57	TYR	CA-CB-CG	-5.40	104.18	113.90
3	3	85	LEU	O-C-N	5.40	130.86	122.87
3	3	112	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	1	93	HIS	CA-CB-CG	-5.40	108.40	113.80
2	2	62	ARG	NE-CZ-NH2	5.38	124.05	119.20
2	2	235	THR	CA-C-N	5.38	126.57	119.84
2	2	235	THR	C-N-CA	5.38	126.57	119.84
3	3	75	ARG	NE-CZ-NH2	5.37	124.04	119.20
2	2	168	ASP	CA-CB-CG	-5.37	107.23	112.60
3	3	202	THR	N-CA-C	5.36	116.28	108.14
1	1	242	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	3	220	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	1	54	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	1	282	ARG	NE-CZ-NH2	5.34	124.00	119.20
6	H	54	ASP	CA-CB-CG	5.34	117.94	112.60
6	H	40	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	3	19	ARG	N-CA-C	5.33	116.96	110.41
5	L	110	ASP	CB-CA-C	5.33	118.54	109.75
1	1	233	ASP	O-C-N	-5.32	115.51	122.59
5	L	61	ARG	NE-CZ-NH2	5.32	123.99	119.20
6	H	98	TYR	CA-CB-CG	-5.32	104.33	113.90
4	4	36	ALA	N-CA-C	-5.32	105.15	111.69
6	H	94	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	2	12	ARG	NE-CZ-NH2	5.31	123.98	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	130	ILE	CB-CA-C	-5.29	102.44	110.95
1	1	219	ASN	CB-CA-C	-5.28	104.00	111.76
2	2	81	LYS	N-CA-C	-5.28	103.52	110.43
5	L	86	TYR	O-C-N	5.28	130.09	123.23
1	1	113	ARG	NE-CZ-NH2	5.27	123.94	119.20
5	L	70	SER	O-C-N	5.26	129.48	123.27
2	2	67	ASP	N-CA-C	5.25	117.24	108.99
3	3	21	SER	CA-C-N	5.25	125.54	119.92
3	3	21	SER	C-N-CA	5.25	125.54	119.92
2	2	255	ARG	NE-CZ-NH2	5.25	123.92	119.20
5	L	91	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	1	94	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	1	246	ARG	NE-CZ-NH2	5.24	123.92	119.20
5	L	49	TYR	O-C-N	5.24	128.92	122.84
2	2	152	ARG	NE-CZ-NH2	5.24	123.91	119.20
2	2	208	PRO	O-C-N	5.23	129.70	122.64
1	1	271	TYR	CA-C-N	5.17	125.33	119.90
1	1	271	TYR	C-N-CA	5.17	125.33	119.90
1	1	29	GLN	N-CA-C	-5.17	107.52	113.88
5	L	18	LYS	N-CA-CB	5.17	117.87	110.06
1	1	123	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	2	255	ARG	O-C-N	5.16	129.45	122.59
1	1	256	ARG	NE-CZ-NH2	5.15	123.84	119.20
2	2	103	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	2	98	PHE	CA-CB-CG	-5.13	108.67	113.80
1	1	249	HIS	CA-CB-CG	-5.13	108.67	113.80
6	H	86	ASP	N-CA-C	-5.13	106.97	113.18
3	3	134	PRO	O-C-N	-5.13	117.59	123.03
3	3	174	ARG	NE-CZ-NH2	5.13	123.81	119.20
5	L	59	PRO	CA-C-N	5.12	127.65	120.28
5	L	59	PRO	C-N-CA	5.12	127.65	120.28
1	1	259	ARG	NE-CZ-NH2	5.12	123.81	119.20
4	4	36	ALA	O-C-N	5.12	128.88	122.23
1	1	192	GLY	N-CA-C	-5.10	105.23	112.37
2	2	194	ASN	N-CA-C	5.10	115.02	108.34
5	L	15	PRO	CB-CA-C	5.09	118.03	111.56
5	L	61	ARG	O-C-N	5.09	127.52	122.12
3	3	224	ASP	CA-C-N	-5.09	115.98	123.00
3	3	224	ASP	C-N-CA	-5.09	115.98	123.00
1	1	138	ASP	O-C-N	5.07	129.33	122.59
4	4	68	ASN	N-CA-CB	-5.07	101.88	110.50
6	H	1	GLN	CA-C-N	5.06	131.33	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1	GLN	C-N-CA	5.06	131.33	121.41
1	1	98	LEU	O-C-N	5.06	128.14	122.22
1	1	86	ASP	O-C-N	5.05	128.94	123.13
2	2	92	PHE	O-C-N	5.04	127.48	122.08
2	2	219	SER	O-C-N	5.04	129.44	123.24
1	1	272	PRO	CB-CA-C	-5.03	105.37	111.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	H	102	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2107	391	0
2	2	1952	0	1927	326	0
3	3	1849	0	1833	352	0
4	4	297	0	294	43	0
5	L	834	0	814	317	0
6	H	917	0	870	243	0
All	All	8019	0	7845	1490	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 94.

All (1490) 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)
5:L:111:ALA:C	5:L:111:ALA:CA	1.76	1.53
5:L:7:SER:CB	5:L:22:THR:HG23	1.50	1.39
6:H:99:PRO:HG2	6:H:100(I):TYR:CE1	1.59	1.35
5:L:6:GLN:HG3	5:L:101:GLY:N	1.40	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:94:TYR:O	5:L:96:ILE:N	1.62	1.31
4:4:44:SER:O	4:4:45:LEU:HD23	1.40	1.18
5:L:54:LEU:HD12	5:L:58:VAL:HG23	1.25	1.16
6:H:51:ILE:HG22	6:H:69:LEU:HD13	1.17	1.14
3:3:151:VAL:CG2	3:3:163:MET:HG3	1.76	1.14
4:4:35:ALA:O	4:4:38:THR:HG23	1.44	1.12
1:1:193:LEU:H	1:1:193:LEU:CD1	1.60	1.11
5:L:67:SER:HA	5:L:71:TYR:CZ	1.85	1.10
5:L:19:VAL:HG23	5:L:75:ILE:HB	1.33	1.10
3:3:214:CYS:SG	3:3:215:PRO:HD2	1.92	1.09
1:1:107:SER:HB2	1:1:266:ILE:HG23	1.11	1.08
5:L:12:SER:HA	5:L:105:GLU:HB3	1.12	1.08
2:2:30:ASN:ND2	4:4:58:ASP:HB2	1.68	1.08
6:H:52:TYR:HD1	6:H:52(A):PRO:HD2	1.19	1.08
1:1:45:VAL:CG2	3:3:162:VAL:HG11	1.85	1.07
5:L:6:GLN:CG	5:L:101:GLY:H	1.66	1.07
6:H:27:TYR:CE1	6:H:94:ARG:HD2	1.88	1.07
1:1:70:PHE:O	1:1:70:PHE:CD2	2.07	1.07
3:3:151:VAL:HG21	3:3:163:MET:HG3	1.09	1.07
5:L:33:MET:HG2	5:L:71:TYR:CG	1.90	1.07
5:L:94:TYR:CE2	6:H:58:LYS:HD3	1.88	1.07
5:L:91:ARG:HG2	5:L:91:ARG:HH11	1.14	1.06
5:L:54:LEU:CD1	5:L:58:VAL:HG23	1.85	1.06
1:1:21:ILE:H	1:1:21:ILE:CD1	1.67	1.05
2:2:23:ILE:HD12	2:2:63:PHE:CE2	1.90	1.05
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.32	1.05
5:L:7:SER:HB2	5:L:22:THR:HG23	1.36	1.05
5:L:78:MET:SD	5:L:79:GLU:O	2.15	1.05
1:1:193:LEU:HD12	1:1:193:LEU:N	1.64	1.05
3:3:151:VAL:HG21	3:3:163:MET:CG	1.86	1.05
1:1:45:VAL:HG21	3:3:162:VAL:CG1	1.87	1.05
5:L:44:PRO:CG	6:H:45:LEU:HD11	1.87	1.04
2:2:63:PHE:CD1	2:2:245:ALA:HB2	1.91	1.04
3:3:179:ASP:HB3	3:3:182:THR:CG2	1.88	1.03
5:L:18:LYS:HD2	5:L:76:SER:HA	1.37	1.03
6:H:69:LEU:HD23	6:H:80:MET:HB2	1.39	1.03
6:H:99:PRO:CG	6:H:100(I):TYR:CE1	2.41	1.03
3:3:19:ARG:HE	3:3:19:ARG:HA	1.14	1.02
3:3:19:ARG:HA	3:3:19:ARG:NE	1.68	1.02
5:L:21:ILE:HD12	5:L:73:LEU:HD22	1.40	1.02
1:1:21:ILE:H	1:1:21:ILE:HD13	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:104:LEU:HD12	5:L:105:GLU:N	1.75	1.01
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.42	1.01
2:2:123:LEU:HG	2:2:123:LEU:O	1.61	1.00
5:L:12:SER:CA	5:L:105:GLU:HB3	1.92	1.00
4:4:32:TYR:HB2	4:4:37:SER:HB3	1.43	1.00
1:1:68:GLU:O	1:1:68:GLU:HG3	1.60	1.00
5:L:7:SER:CB	5:L:22:THR:CG2	2.40	1.00
5:L:18:LYS:CD	5:L:76:SER:HA	1.91	0.99
3:3:218:LYS:O	3:3:219:LEU:HD12	1.61	0.99
5:L:6:GLN:HG3	5:L:101:GLY:H	0.83	0.99
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.43	0.99
1:1:190:TYR:OH	1:1:194:ALA:O	1.79	0.99
5:L:43:SER:O	5:L:45:LYS:HD3	1.62	0.99
5:L:104:LEU:HD12	5:L:105:GLU:H	1.23	0.98
6:H:100(J):ALA:HB1	6:H:100(K):MET:HE3	1.44	0.98
6:H:40:ARG:HB2	6:H:43:GLN:HG3	1.43	0.97
3:3:68:LEU:O	3:3:70:PRO:HD3	1.65	0.96
3:3:126:LYS:O	3:3:192:GLN:HB3	1.63	0.96
3:3:85:LEU:O	3:3:184:ALA:HB3	1.66	0.95
1:1:43:MET:HE3	1:1:44:PRO:HD2	1.45	0.95
1:1:193:LEU:H	1:1:193:LEU:HD12	0.79	0.95
3:3:214:CYS:SG	3:3:215:PRO:CD	2.54	0.95
1:1:107:SER:HB2	1:1:266:ILE:CG2	1.97	0.94
6:H:105:GLN:HG2	6:H:106:GLY:N	1.81	0.94
5:L:33:MET:HG2	5:L:71:TYR:CB	1.98	0.94
5:L:46:LEU:HD23	6:H:101:ASP:HA	1.49	0.94
6:H:99:PRO:HG2	6:H:100(I):TYR:HE1	1.23	0.94
5:L:11:MET:HE1	5:L:104:LEU:HA	1.50	0.94
5:L:30:VAL:CG2	5:L:90:GLN:HG3	1.98	0.94
5:L:62:PHE:CD1	5:L:75:ILE:HG12	2.01	0.94
2:2:30:ASN:HD21	4:4:58:ASP:HB2	1.29	0.94
2:2:83:PRO:HG2	2:2:216:ASN:HA	1.50	0.93
1:1:248:LYS:O	1:1:249:HIS:HB2	1.68	0.93
2:2:104:SER:OG	2:2:249:THR:HG23	1.67	0.93
4:4:35:ALA:O	4:4:38:THR:CG2	2.15	0.93
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.49	0.93
3:3:126:LYS:HE2	3:3:154:ASP:HB2	1.50	0.93
5:L:14:PHE:CA	5:L:107:LYS:HB2	1.98	0.93
3:3:2:LEU:HG	3:3:2:LEU:O	1.67	0.93
6:H:37:VAL:HB	6:H:46:GLU:O	1.68	0.93
5:L:7:SER:N	5:L:22:THR:O	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:27:GLU:O	2:2:28:ALA:O	1.85	0.93
5:L:108:ARG:HG3	5:L:109:ALA:N	1.83	0.93
3:3:153:TRP:CE3	3:3:161:ILE:HG21	2.03	0.92
1:1:21:ILE:HD13	1:1:21:ILE:N	1.78	0.92
5:L:10:ILE:HG13	5:L:103:LYS:O	1.68	0.92
1:1:107:SER:CB	1:1:266:ILE:HG23	1.99	0.92
4:4:44:SER:O	4:4:45:LEU:CD2	2.18	0.91
6:H:35:ASN:HD21	6:H:95:SER:HB2	1.35	0.91
2:2:29:ALA:HA	4:4:67:LEU:HD23	1.51	0.91
2:2:98:PHE:CE1	2:2:257:LYS:HB2	2.05	0.91
5:L:2:ILE:HG22	5:L:25:ALA:HB1	1.53	0.91
6:H:39:GLN:HA	6:H:44:GLY:O	1.70	0.91
2:2:190:ASN:O	2:2:192:ARG:N	2.04	0.91
1:1:41:ALA:HB3	4:4:60:MET:HE1	1.53	0.90
1:1:46:LEU:HD21	3:3:215:PRO:CG	2.02	0.90
2:2:207:VAL:HG12	2:2:208:PRO:HD2	1.53	0.90
6:H:40:ARG:HB2	6:H:43:GLN:CG	2.00	0.90
1:1:87:ALA:O	1:1:90:ILE:HG12	1.72	0.90
2:2:12:ARG:HA	2:2:27:GLU:O	1.72	0.90
5:L:44:PRO:HG3	6:H:45:LEU:HD11	1.50	0.90
6:H:97:ASN:HD21	6:H:101:ASP:CB	1.85	0.90
5:L:78:MET:HE2	5:L:82:ASP:HB2	1.51	0.90
3:3:157:LEU:HD23	3:3:157:LEU:O	1.72	0.90
6:H:97:ASN:HD21	6:H:101:ASP:CG	1.79	0.90
2:2:183:ILE:CG1	3:3:96:LEU:HD22	2.02	0.89
5:L:7:SER:OG	5:L:22:THR:OG1	1.88	0.89
5:L:62:PHE:HA	5:L:74:THR:O	1.71	0.89
1:1:124:PHE:O	1:1:190:TYR:HB2	1.71	0.89
3:3:173:PHE:HE2	3:3:220:ARG:NH1	1.68	0.89
6:H:36:TRP:CD1	6:H:69:LEU:HD21	2.07	0.89
1:1:65:THR:OG1	3:3:42:ASN:ND2	2.04	0.89
3:3:97:LEU:O	3:3:101:VAL:HB	1.72	0.89
5:L:13:ALA:CB	5:L:78:MET:HG2	2.03	0.88
5:L:75:ILE:O	5:L:77:ARG:N	2.05	0.88
3:3:173:PHE:HE2	3:3:220:ARG:HH11	1.20	0.88
5:L:7:SER:OG	5:L:22:THR:CG2	2.21	0.88
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.55	0.88
1:1:279:ILE:HB	3:3:62:ASP:OD1	1.73	0.88
3:3:105:THR:C	3:3:176:THR:HG23	1.98	0.88
1:1:207:ASP:HA	2:2:144:TYR:CE2	2.08	0.88
5:L:91:ARG:HG2	5:L:91:ARG:NH1	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:85:ALA:HA	2:2:150:GLY:HA2	1.55	0.88
1:1:160:PRO:HB3	1:1:168:TRP:NE1	1.89	0.88
2:2:108:VAL:HG12	2:2:244:ILE:HG12	1.55	0.88
2:2:187:GLN:NE2	2:2:198:THR:H	1.71	0.88
5:L:89:GLN:HG3	5:L:98:PHE:CD2	2.09	0.87
5:L:94:TYR:HE2	6:H:58:LYS:HD3	1.38	0.87
3:3:173:PHE:CE2	3:3:220:ARG:NH1	2.43	0.87
5:L:77:ARG:NE	5:L:79:GLU:OE2	2.07	0.87
3:3:115:LEU:CD2	3:3:129:LEU:HD11	2.04	0.87
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.57	0.87
6:H:52:TYR:CD1	6:H:52(A):PRO:HD2	2.10	0.87
5:L:7:SER:HB3	5:L:22:THR:HG23	1.55	0.86
3:3:85:LEU:O	3:3:184:ALA:CB	2.23	0.86
1:1:260:ALA:HB1	1:1:278:VAL:HG21	1.55	0.86
1:1:186:PHE:CD1	3:3:24:ALA:HB2	2.10	0.86
2:2:234:ALA:O	2:2:236:PRO:HD3	1.76	0.86
5:L:12:SER:HA	5:L:105:GLU:CB	2.03	0.85
5:L:33:MET:HE2	5:L:88:CYS:HB2	1.55	0.85
5:L:14:PHE:HA	5:L:107:LYS:HB2	1.57	0.85
5:L:77:ARG:HG2	5:L:77:ARG:HH11	1.42	0.85
6:H:2:GLY:HA2	6:H:25:SER:O	1.76	0.85
4:4:59:LEU:HG	4:4:60:MET:N	1.89	0.85
3:3:18:ASP:O	4:4:39:SER:HB2	1.77	0.85
5:L:2:ILE:HD12	5:L:93:SER:HB2	1.59	0.85
1:1:45:VAL:HG21	3:3:162:VAL:HG11	0.94	0.85
1:1:77:VAL:C	1:1:109:LEU:HD12	2.01	0.84
5:L:15:PRO:HA	5:L:78:MET:O	1.76	0.84
1:1:70:PHE:CG	3:3:43:LEU:HD11	2.11	0.84
1:1:289:TYR:OH	3:3:139:PRO:O	1.95	0.84
3:3:18:ASP:OD1	4:4:40:SER:HB3	1.75	0.84
5:L:7:SER:OG	5:L:22:THR:HG23	1.77	0.84
6:H:12:VAL:CG1	6:H:18:VAL:HG13	2.07	0.84
1:1:153:VAL:HG13	1:1:157:ALA:HB3	1.57	0.84
5:L:6:GLN:OE1	5:L:87:TYR:HA	1.77	0.84
5:L:21:ILE:HG12	5:L:102:THR:HG21	1.60	0.84
1:1:282:ARG:HB2	3:3:57:ASN:HB2	1.59	0.84
1:1:135:SER:C	1:1:137:PRO:HD3	2.03	0.84
2:2:84:ASP:OD1	2:2:85:ALA:N	2.10	0.84
1:1:110:VAL:HG22	3:3:230:GLN:OE1	1.77	0.83
1:1:70:PHE:O	1:1:70:PHE:CG	2.30	0.83
5:L:67:SER:HA	5:L:71:TYR:CE1	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:178:PHE:CD2	1:1:184:SER:HB3	2.12	0.83
3:3:14:LEU:HD12	3:3:15:THR:N	1.92	0.83
3:3:214:CYS:CB	3:3:215:PRO:HD2	2.08	0.83
6:H:81:GLN:NE2	6:H:82(A):TYR:CE1	2.46	0.83
6:H:23:LYS:HD3	6:H:77:THR:HG22	1.60	0.83
2:2:71:TRP:CE2	2:2:228:LEU:HB2	2.13	0.83
5:L:54:LEU:HD11	5:L:62:PHE:HB2	1.61	0.83
2:2:187:GLN:HE21	2:2:198:THR:H	1.24	0.83
5:L:30:VAL:O	5:L:71:TYR:OH	1.96	0.83
5:L:29:SER:HA	5:L:68:GLY:O	1.78	0.82
3:3:157:LEU:HD23	3:3:157:LEU:C	2.04	0.82
3:3:14:LEU:HD12	3:3:16:THR:H	1.44	0.82
3:3:110:SER:O	3:3:214:CYS:HB2	1.79	0.82
5:L:4:LEU:HD12	5:L:88:CYS:SG	2.19	0.82
2:2:10:SER:O	2:2:13:VAL:HG23	1.80	0.82
3:3:142:ARG:O	3:3:143:ARG:C	2.22	0.82
1:1:88:THR:O	1:1:88:THR:CG2	2.26	0.82
3:3:146:MET:HG2	3:3:146:MET:O	1.77	0.82
5:L:48:ILE:HD11	5:L:54:LEU:HD13	1.62	0.82
1:1:201:TYR:H	2:2:131:GLN:HE22	1.28	0.81
3:3:157:LEU:C	3:3:157:LEU:CD2	2.53	0.81
4:4:32:TYR:CB	4:4:37:SER:HB3	2.09	0.81
1:1:166:TYR:CD1	1:1:167:THR:N	2.48	0.81
5:L:55:ALA:HB3	5:L:58:VAL:HG11	1.63	0.81
3:3:19:ARG:NE	3:3:19:ARG:CA	2.42	0.81
2:2:81:LYS:HE2	2:2:132:LEU:HD11	1.63	0.81
1:1:77:VAL:O	1:1:109:LEU:HD12	1.81	0.81
2:2:255:ARG:O	2:2:257:LYS:N	2.13	0.81
6:H:20:ILE:CG2	6:H:107:THR:HG21	2.11	0.81
1:1:253:TRP:NE1	3:3:36:ILE:HG13	1.95	0.80
1:1:259:ARG:NH1	2:2:174:ASN:O	2.14	0.80
6:H:101:ASP:CG	6:H:102:TYR:H	1.87	0.80
1:1:281:LYS:HG2	1:1:282:ARG:N	1.95	0.80
2:2:217:ASN:O	2:2:218:VAL:HG12	1.81	0.80
3:3:172:GLN:O	3:3:173:PHE:CD1	2.35	0.80
3:3:141:ASP:HA	3:3:190:TRP:CZ3	2.17	0.80
2:2:184:PHE:HB3	2:2:185:PRO:HD2	1.64	0.80
3:3:198:PRO:O	3:3:201:THR:HG22	1.81	0.80
5:L:30:VAL:CG2	5:L:90:GLN:CG	2.59	0.80
5:L:13:ALA:HB1	5:L:78:MET:HG2	1.64	0.80
3:3:18:ASP:CG	4:4:40:SER:HB3	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:LYS:HG2	4:4:63:GLY:O	1.81	0.79
2:2:38:TRP:CG	2:2:39:PRO:HD2	2.17	0.79
6:H:18:VAL:HG22	6:H:82(C):LEU:HD11	1.62	0.79
6:H:20:ILE:HG22	6:H:107:THR:HG21	1.63	0.79
6:H:37:VAL:HA	6:H:46:GLU:O	1.81	0.79
1:1:74:ALA:HB3	3:3:15:THR:HB	1.63	0.79
5:L:13:ALA:N	5:L:105:GLU:O	2.15	0.79
1:1:148:VAL:HG11	1:1:241:ILE:HD11	1.64	0.79
1:1:178:PHE:HD2	1:1:184:SER:HB3	1.45	0.79
2:2:195:ASN:HD22	2:2:196:THR:N	1.80	0.79
5:L:2:ILE:CG2	5:L:25:ALA:HB1	2.14	0.78
6:H:97:ASN:HD21	6:H:101:ASP:HB3	1.46	0.78
6:H:40:ARG:HA	6:H:88:ALA:HB1	1.65	0.78
1:1:141:ASN:N	1:1:141:ASN:OD1	2.15	0.78
1:1:201:TYR:CE2	1:1:203:GLY:HA3	2.19	0.78
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.66	0.78
3:3:65:ASN:HA	3:3:68:LEU:HD12	1.66	0.78
5:L:19:VAL:CG2	5:L:75:ILE:HB	2.12	0.78
6:H:97:ASN:ND2	6:H:101:ASP:CG	2.42	0.78
1:1:161:LYS:HE2	1:1:161:LYS:HA	1.66	0.78
6:H:17:SER:HB3	6:H:82(A):TYR:HA	1.64	0.78
1:1:204:TYR:HD2	1:1:211:THR:HG23	1.49	0.77
2:2:254:ILE:O	2:2:255:ARG:HB3	1.83	0.77
5:L:1:GLN:HA	5:L:1:GLN:OE1	1.83	0.77
2:2:83:PRO:CG	2:2:216:ASN:HA	2.14	0.77
2:2:232:THR:O	2:2:232:THR:HG22	1.83	0.77
3:3:126:LYS:HE2	3:3:154:ASP:CB	2.14	0.77
1:1:26:LYS:O	1:1:27:HIS:HB2	1.84	0.77
1:1:282:ARG:HD3	1:1:285:ASP:O	1.85	0.77
3:3:105:THR:O	3:3:176:THR:HG23	1.85	0.77
2:2:217:ASN:C	2:2:218:VAL:HG12	2.10	0.77
1:1:65:THR:O	3:3:42:ASN:ND2	2.18	0.76
3:3:157:LEU:HD22	3:3:158:GLN:OE1	1.84	0.76
5:L:43:SER:O	5:L:45:LYS:CD	2.32	0.76
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.20	0.76
1:1:110:VAL:HG22	3:3:230:GLN:CD	2.10	0.76
2:2:150:GLY:O	2:2:152:ARG:N	2.19	0.76
5:L:30:VAL:HG23	5:L:90:GLN:HG3	1.65	0.76
1:1:46:LEU:HD21	3:3:215:PRO:HG3	1.66	0.76
4:4:68:ASN:N	4:4:68:ASN:OD1	2.18	0.76
6:H:100(I):TYR:CD1	6:H:100(I):TYR:N	2.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:65:ASN:C	3:3:67:TYR:H	1.94	0.75
6:H:52:TYR:HD1	6:H:52(A):PRO:CD	1.97	0.75
1:1:88:THR:O	1:1:88:THR:HG22	1.85	0.75
2:2:116:LYS:HA	3:3:121:ALA:HB3	1.68	0.75
5:L:7:SER:HG	5:L:22:THR:HG1	1.27	0.75
3:3:46:ILE:O	3:3:49:VAL:HG23	1.85	0.75
2:2:166:VAL:HG12	2:2:173:MET:HB3	1.67	0.75
5:L:36:PHE:HE2	6:H:103:TRP:NE1	1.83	0.75
5:L:77:ARG:HH11	5:L:77:ARG:CG	1.98	0.75
5:L:33:MET:HE3	5:L:89:GLN:H	1.51	0.75
5:L:14:PHE:N	5:L:107:LYS:HB2	2.02	0.75
5:L:89:GLN:HG2	5:L:98:PHE:HA	1.68	0.75
6:H:101:ASP:CG	6:H:102:TYR:N	2.45	0.74
3:3:214:CYS:CB	3:3:215:PRO:CD	2.65	0.74
6:H:4:LEU:HG	6:H:102:TYR:CD2	2.22	0.74
3:3:126:LYS:O	3:3:192:GLN:CB	2.35	0.74
6:H:12:VAL:CG1	6:H:18:VAL:CG1	2.65	0.74
1:1:161:LYS:HE2	1:1:161:LYS:CA	2.16	0.74
5:L:13:ALA:CA	5:L:107:LYS:HG3	2.18	0.74
1:1:266:ILE:HD12	3:3:236:GLU:HG2	1.70	0.74
1:1:186:PHE:HD1	3:3:24:ALA:HB2	1.48	0.74
3:3:55:MET:HA	3:3:91:VAL:CG1	2.18	0.74
6:H:3:GLN:O	6:H:24:ALA:HA	1.88	0.73
3:3:102:GLN:HG2	3:3:225:THR:OG1	1.88	0.73
1:1:45:VAL:O	1:1:46:LEU:HD23	1.88	0.73
2:2:195:ASN:ND2	2:2:196:THR:HG23	2.03	0.73
3:3:115:LEU:HD22	3:3:129:LEU:HD11	1.71	0.73
3:3:141:ASP:HA	3:3:190:TRP:CH2	2.24	0.73
2:2:69:LYS:HG2	2:2:78:TRP:NE1	2.04	0.73
3:3:128:ILE:HG22	3:3:190:TRP:O	1.88	0.73
1:1:191:VAL:HG12	3:3:28:TYR:CZ	2.24	0.73
3:3:108:SER:O	3:3:218:LYS:N	2.20	0.73
5:L:7:SER:HB2	5:L:22:THR:CG2	2.15	0.73
5:L:94:TYR:C	5:L:96:ILE:N	2.47	0.73
6:H:33:TRP:HZ3	6:H:57:ASN:HA	1.52	0.73
1:1:130:ILE:HD13	1:1:243:VAL:HG13	1.71	0.72
5:L:62:PHE:HD1	5:L:75:ILE:HG12	1.50	0.72
1:1:67:VAL:HG22	3:3:41:HIS:O	1.90	0.72
3:3:124:SER:O	3:3:195:LEU:HD12	1.89	0.72
6:H:41:PRO:HD3	6:H:88:ALA:HA	1.71	0.72
1:1:282:ARG:HG3	3:3:57:ASN:ND2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:158:SER:OG	2:2:159:ALA:N	2.21	0.72
2:2:183:ILE:HG12	3:3:96:LEU:HD22	1.70	0.72
6:H:82:LEU:HB2	6:H:82(C):LEU:HD21	1.72	0.72
1:1:118:LEU:HD12	1:1:118:LEU:O	1.89	0.72
5:L:83:ALA:HB2	5:L:106:ILE:HB	1.71	0.72
2:2:86:LEU:O	2:2:88:ASP:N	2.20	0.72
4:4:45:LEU:O	4:4:45:LEU:HG	1.89	0.72
6:H:7:SER:HB2	6:H:21:SER:H	1.54	0.72
6:H:40:ARG:C	6:H:43:GLN:HB2	2.14	0.72
4:4:43:GLN:HG3	4:4:45:LEU:HB3	1.70	0.72
4:4:49:PRO:HB2	4:4:53:THR:OG1	1.89	0.72
1:1:285:ASP:O	1:1:288:SER:HB2	1.90	0.72
5:L:13:ALA:C	5:L:107:LYS:HG3	2.14	0.72
1:1:245:HIS:ND1	1:1:245:HIS:C	2.48	0.71
5:L:76:SER:C	5:L:77:ARG:HG3	2.14	0.71
5:L:94:TYR:HE2	6:H:58:LYS:CD	2.02	0.71
6:H:22:CYS:HG	6:H:92:CYS:HG	1.34	0.71
1:1:152:TYR:O	1:1:154:PRO:HD3	1.91	0.71
2:2:62:ARG:O	2:2:245:ALA:HB1	1.90	0.71
5:L:4:LEU:HD12	5:L:99:GLY:HA2	1.71	0.71
2:2:94:GLN:O	2:2:97:PHE:N	2.23	0.71
2:2:111:GLN:HG2	2:2:196:THR:CG2	2.19	0.71
2:2:195:ASN:HD22	2:2:195:ASN:C	1.98	0.71
5:L:78:MET:CE	5:L:82:ASP:HB2	2.20	0.71
5:L:94:TYR:CE2	6:H:58:LYS:CD	2.72	0.71
6:H:38:LYS:CG	6:H:90:TYR:HE1	2.03	0.71
1:1:201:TYR:H	2:2:131:GLN:NE2	1.87	0.71
1:1:287:LYS:HE3	3:3:79:GLN:HB3	1.71	0.71
2:2:42:LEU:HD12	2:2:43:PRO:HD2	1.70	0.71
2:2:94:GLN:C	2:2:96:MET:N	2.46	0.71
6:H:4:LEU:HG	6:H:102:TYR:HD2	1.56	0.71
6:H:40:ARG:HB2	6:H:43:GLN:CB	2.21	0.71
1:1:268:ARG:HG3	1:1:268:ARG:HH11	1.53	0.71
5:L:4:LEU:CD1	5:L:88:CYS:SG	2.79	0.71
2:2:229:THR:HG22	2:2:229:THR:O	1.90	0.70
1:1:210:GLU:HA	1:1:210:GLU:OE1	1.84	0.70
2:2:81:LYS:HA	2:2:219:SER:HB3	1.72	0.70
5:L:33:MET:HG2	5:L:71:TYR:CD2	2.24	0.70
6:H:57:ASN:C	6:H:58:LYS:HG2	2.17	0.70
1:1:161:LYS:N	1:1:165:ASP:OD2	2.22	0.70
6:H:39:GLN:HB2	6:H:45:LEU:HD23	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:TRP:HB3	1:1:224:MET:HB3	1.72	0.70
5:L:54:LEU:HD11	5:L:62:PHE:CB	2.22	0.70
2:2:84:ASP:O	2:2:86:LEU:N	2.24	0.70
2:2:180:ASN:HA	3:3:51:THR:HG22	1.73	0.70
5:L:33:MET:HG2	5:L:71:TYR:HB2	1.73	0.70
2:2:29:ALA:HA	4:4:67:LEU:CD2	2.21	0.70
5:L:111:ALA:C	5:L:111:ALA:CB	2.64	0.70
6:H:6:GLN:HE22	6:H:91:PHE:HA	1.55	0.70
6:H:27:TYR:HD1	6:H:32:PHE:CE1	2.09	0.70
1:1:46:LEU:HD22	1:1:47:PRO:HD3	1.74	0.70
5:L:105:GLU:OE1	5:L:105:GLU:HA	1.89	0.70
6:H:99:PRO:HG2	6:H:100(I):TYR:CZ	2.25	0.70
5:L:36:PHE:HE2	6:H:103:TRP:HE1	1.38	0.70
2:2:67:ASP:CG	2:2:68:SER:N	2.50	0.70
3:3:117:TYR:CZ	3:3:119:GLY:HA3	2.27	0.70
6:H:75:SER:OG	6:H:77:THR:OG1	2.08	0.70
1:1:67:VAL:CG2	3:3:41:HIS:O	2.38	0.69
1:1:77:VAL:HG11	1:1:245:HIS:HB3	1.73	0.69
3:3:115:LEU:HD23	3:3:129:LEU:HD11	1.72	0.69
3:3:214:CYS:SG	3:3:215:PRO:HD3	2.32	0.69
5:L:21:ILE:HD12	5:L:73:LEU:CD2	2.19	0.69
5:L:37:GLN:HG2	5:L:38:GLN:N	2.07	0.69
5:L:75:ILE:C	5:L:77:ARG:H	1.99	0.69
2:2:86:LEU:C	2:2:88:ASP:H	1.99	0.69
6:H:37:VAL:CB	6:H:46:GLU:O	2.41	0.69
1:1:58:MET:CE	3:3:216:ASP:HA	2.21	0.69
5:L:78:MET:HE2	5:L:82:ASP:CB	2.22	0.69
6:H:37:VAL:CA	6:H:46:GLU:O	2.39	0.69
3:3:71:LEU:HD22	3:3:207:LEU:HD21	1.75	0.69
3:3:137:ARG:O	3:3:138:GLY:C	2.35	0.69
2:2:182:LEU:HD12	2:2:182:LEU:H	1.57	0.69
2:2:183:ILE:HG13	3:3:96:LEU:HD22	1.73	0.69
2:2:232:THR:O	2:2:232:THR:CG2	2.41	0.69
5:L:2:ILE:HG12	5:L:27:SER:HB2	1.74	0.69
5:L:26:THR:OG1	5:L:27:SER:N	2.25	0.69
6:H:97:ASN:N	6:H:97:ASN:OD1	2.25	0.69
2:2:18:LEU:O	2:2:19:GLY:C	2.35	0.69
6:H:5:GLN:O	6:H:23:LYS:HE3	1.92	0.69
1:1:207:ASP:HA	2:2:144:TYR:HE2	1.57	0.69
2:2:111:GLN:HG2	2:2:196:THR:HG22	1.74	0.69
2:2:137:GLY:O	2:2:140:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:44:PRO:CB	6:H:45:LEU:HD11	2.22	0.69
2:2:10:SER:OG	2:2:12:ARG:HB2	1.93	0.69
3:3:16:THR:CG2	3:3:16:THR:O	2.40	0.69
2:2:122:LEU:HD11	2:2:240:ILE:HD11	1.76	0.68
2:2:126:VAL:HG23	2:2:199:ILE:HD12	1.75	0.68
6:H:62:LYS:HG3	6:H:63:PHE:CD1	2.28	0.68
3:3:140:GLN:O	3:3:141:ASP:HB3	1.91	0.68
3:3:86:PHE:C	3:3:88:GLY:H	2.00	0.68
3:3:153:TRP:CD2	3:3:161:ILE:HG21	2.28	0.68
5:L:91:ARG:HD2	5:L:96:ILE:HD13	1.75	0.68
6:H:51:ILE:CG2	6:H:69:LEU:HD13	2.09	0.68
1:1:259:ARG:NH2	1:1:270:ASN:O	2.25	0.68
3:3:179:ASP:CB	3:3:182:THR:HG22	2.21	0.68
5:L:77:ARG:HD3	5:L:77:ARG:O	1.94	0.68
1:1:78:HIS:HA	1:1:109:LEU:HD11	1.75	0.68
1:1:254:ILE:HD11	2:2:204:ILE:CG2	2.24	0.68
2:2:69:LYS:HG2	2:2:78:TRP:CD1	2.28	0.68
2:2:132:LEU:CD2	2:2:173:MET:HE2	2.24	0.68
5:L:62:PHE:O	5:L:63:SER:HB3	1.92	0.68
6:H:22:CYS:C	6:H:23:LYS:HD3	2.18	0.68
1:1:282:ARG:NH2	3:3:82:GLY:O	2.26	0.68
5:L:31:ASN:O	5:L:32:TYR:CD1	2.46	0.68
1:1:46:LEU:HD21	3:3:215:PRO:HG2	1.75	0.68
2:2:230:VAL:HB	2:2:231:PRO:CD	2.24	0.68
3:3:19:ARG:HD2	3:3:19:ARG:N	2.09	0.68
5:L:86:TYR:O	5:L:101:GLY:HA2	1.92	0.68
1:1:46:LEU:HD22	1:1:47:PRO:CD	2.23	0.68
3:3:218:LYS:C	3:3:219:LEU:HD12	2.18	0.68
5:L:14:PHE:CD2	5:L:107:LYS:HD3	2.28	0.68
3:3:117:TYR:CE1	3:3:119:GLY:HA3	2.29	0.68
3:3:193:THR:O	3:3:194:SER:HB3	1.92	0.68
1:1:190:TYR:CD1	1:1:190:TYR:C	2.71	0.67
3:3:42:ASN:O	3:3:44:LEU:N	2.27	0.67
3:3:71:LEU:HD22	3:3:207:LEU:CD2	2.24	0.67
3:3:142:ARG:O	3:3:145:ALA:N	2.27	0.67
1:1:194:ALA:C	1:1:196:ALA:H	2.03	0.67
3:3:14:LEU:HD11	3:3:16:THR:HB	1.75	0.67
4:4:34:ASP:HB2	4:4:37:SER:OG	1.94	0.67
5:L:13:ALA:O	5:L:78:MET:SD	2.53	0.67
1:1:25:PRO:HD3	1:1:52:GLU:OE2	1.94	0.67
1:1:282:ARG:NH1	1:1:288:SER:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:79:CYS:HB2	2:2:221:MET:HG3	1.75	0.67
3:3:231:THR:OG1	3:3:232:VAL:HG22	1.94	0.67
1:1:81:GLU:HB3	1:1:240:LYS:HG2	1.76	0.67
1:1:136:GLN:HB3	1:1:140:ALA:HB2	1.75	0.67
6:H:7:SER:CB	6:H:21:SER:H	2.08	0.67
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.09	0.67
5:L:23:CYS:HB2	5:L:88:CYS:SG	2.34	0.67
6:H:3:GLN:HG2	6:H:5:GLN:NE2	2.09	0.67
5:L:90:GLN:NE2	5:L:97:THR:HG23	2.10	0.67
1:1:131:LEU:HB2	1:1:183:THR:HG22	1.76	0.67
5:L:31:ASN:O	5:L:32:TYR:CG	2.48	0.67
6:H:35:ASN:ND2	6:H:95:SER:HB2	2.06	0.67
1:1:41:ALA:HB3	4:4:60:MET:CE	2.23	0.67
1:1:209:ALA:H	2:2:261:PRO:HB3	1.59	0.67
1:1:121:TYR:OH	2:2:205:ASN:HA	1.95	0.66
2:2:109:HIS:HA	2:2:197:ALA:O	1.94	0.66
3:3:18:ASP:OD2	4:4:40:SER:HB3	1.96	0.66
3:3:89:ASP:HA	3:3:93:LYS:CD	2.19	0.66
1:1:110:VAL:HG22	3:3:230:GLN:CG	2.25	0.66
1:1:159:ASN:C	1:1:167:THR:HG21	2.21	0.66
3:3:47:ILE:HG13	3:3:47:ILE:O	1.95	0.66
1:1:120:THR:O	1:1:199:CYS:HB2	1.95	0.66
1:1:147:VAL:O	1:1:229:VAL:HG22	1.94	0.66
2:2:21:SER:OG	2:2:63:PHE:HB2	1.95	0.66
2:2:94:GLN:C	2:2:96:MET:H	2.02	0.66
5:L:94:TYR:O	5:L:94:TYR:CD1	2.49	0.66
5:L:66:GLY:O	5:L:67:SER:HB3	1.96	0.66
1:1:208:ASP:N	2:2:261:PRO:HG3	2.10	0.66
2:2:10:SER:C	2:2:12:ARG:H	2.02	0.66
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.30	0.66
3:3:42:ASN:O	3:3:45:GLU:N	2.26	0.66
1:1:76:CYS:HB2	1:1:244:TYR:CE1	2.30	0.66
2:2:198:THR:O	2:2:199:ILE:HG12	1.96	0.66
1:1:208:ASP:CA	2:2:261:PRO:HG3	2.24	0.66
2:2:65:THR:O	2:2:65:THR:HG22	1.96	0.66
5:L:18:LYS:HD2	5:L:76:SER:CA	2.21	0.66
3:3:57:ASN:O	3:3:59:HIS:N	2.29	0.66
6:H:48:ILE:HA	6:H:63:PHE:CD2	2.30	0.66
1:1:19:ALA:HB2	1:1:57:TYR:O	1.95	0.65
5:L:62:PHE:HE1	5:L:75:ILE:CD1	2.09	0.65
2:2:205:ASN:OD1	2:2:207:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:83:THR:HG23	3:3:187:LEU:CD2	2.25	0.65
3:3:151:VAL:CG2	3:3:163:MET:CG	2.58	0.65
5:L:78:MET:HA	5:L:82:ASP:OD2	1.95	0.65
1:1:282:ARG:HH22	3:3:83:THR:HB	1.61	0.65
2:2:37:GLU:CG	3:3:37:PRO:HB3	2.26	0.65
2:2:171:TYR:O	2:2:173:MET:N	2.30	0.65
5:L:3:VAL:H	5:L:26:THR:HG23	1.60	0.65
6:H:62:LYS:HG2	6:H:63:PHE:CE1	2.31	0.65
2:2:27:GLU:OE1	2:2:27:GLU:HA	1.96	0.65
5:L:55:ALA:HB3	5:L:58:VAL:CG1	2.25	0.65
5:L:77:ARG:HB2	5:L:77:ARG:CZ	2.27	0.65
3:3:65:ASN:C	3:3:67:TYR:N	2.53	0.65
5:L:2:ILE:CD1	5:L:93:SER:HB2	2.26	0.65
5:L:31:ASN:HB3	5:L:32:TYR:CD2	2.31	0.65
6:H:35:ASN:N	6:H:35:ASN:HD22	1.94	0.65
1:1:78:HIS:HA	1:1:109:LEU:CD1	2.27	0.65
1:1:129:THR:HG21	3:3:13:PHE:CZ	2.31	0.65
1:1:160:PRO:HB3	1:1:168:TRP:HE1	1.60	0.65
2:2:68:SER:HA	2:2:240:ILE:O	1.96	0.65
6:H:12:VAL:HG21	6:H:82(C):LEU:HD13	1.78	0.65
1:1:201:TYR:H	1:1:215:ILE:HG22	1.61	0.65
6:H:80:MET:HE2	6:H:82:LEU:HG	1.79	0.65
1:1:110:VAL:N	3:3:230:GLN:OE1	2.30	0.65
2:2:166:VAL:HG12	2:2:173:MET:CB	2.27	0.65
5:L:10:ILE:HD11	5:L:105:GLU:HG2	1.78	0.65
5:L:16:GLY:HA2	5:L:77:ARG:NH1	2.12	0.65
5:L:54:LEU:O	5:L:55:ALA:O	2.14	0.65
1:1:43:MET:CE	1:1:44:PRO:HD2	2.23	0.64
1:1:84:ASN:ND2	1:1:232:HIS:HA	2.12	0.64
6:H:17:SER:HB3	6:H:82:LEU:O	1.97	0.64
5:L:65:SER:OG	5:L:66:GLY:N	2.28	0.64
2:2:95:ASN:HB3	2:2:251:PHE:CD2	2.32	0.64
2:2:44:ASP:O	2:2:45:VAL:C	2.40	0.64
2:2:171:TYR:O	2:2:172:ASN:C	2.41	0.64
3:3:153:TRP:CD1	3:3:153:TRP:C	2.76	0.64
5:L:18:LYS:HA	5:L:77:ARG:HA	1.78	0.64
6:H:87:SER:HA	6:H:109:VAL:O	1.97	0.64
1:1:77:VAL:C	1:1:109:LEU:CD1	2.70	0.64
3:3:101:VAL:CG2	3:3:219:LEU:HD21	2.27	0.64
4:4:49:PRO:O	4:4:51:LYS:N	2.30	0.64
5:L:31:ASN:C	5:L:32:TYR:CG	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:91:ARG:HH11	5:L:91:ARG:CG	2.01	0.64
6:H:12:VAL:HG13	6:H:18:VAL:HG11	1.78	0.64
1:1:44:PRO:HD3	4:4:54:GLU:OE2	1.96	0.64
1:1:97:LYS:HD2	6:H:52:TYR:HE2	1.62	0.64
1:1:161:LYS:HB2	1:1:162:GLU:OE1	1.98	0.64
2:2:170:LEU:HD13	2:2:170:LEU:O	1.98	0.64
2:2:123:LEU:HD12	2:2:188:PHE:CE1	2.32	0.64
2:2:18:LEU:O	2:2:20:ASN:N	2.31	0.63
3:3:14:LEU:CD1	3:3:16:THR:H	2.11	0.63
4:4:48:ASP:OD2	4:4:50:SER:HB2	1.98	0.63
1:1:109:LEU:HA	3:3:230:GLN:OE1	1.98	0.63
5:L:33:MET:CE	5:L:89:GLN:H	2.10	0.63
6:H:12:VAL:HG11	6:H:18:VAL:HG13	1.80	0.63
1:1:245:HIS:C	1:1:245:HIS:HD1	2.05	0.63
2:2:108:VAL:CG2	2:2:199:ILE:HB	2.28	0.63
5:L:11:MET:HE1	5:L:104:LEU:HD13	1.79	0.63
5:L:14:PHE:N	5:L:107:LYS:HG3	2.13	0.63
5:L:54:LEU:CD1	5:L:58:VAL:CG2	2.70	0.63
2:2:230:VAL:HG11	2:2:236:PRO:HA	1.80	0.63
4:4:49:PRO:O	4:4:50:SER:C	2.41	0.63
5:L:6:GLN:HB2	5:L:100:SER:OG	1.98	0.63
3:3:195:LEU:HD21	3:3:205:VAL:CG2	2.28	0.63
6:H:69:LEU:HA	6:H:80:MET:HB2	1.81	0.63
6:H:105:GLN:HG2	6:H:106:GLY:H	1.58	0.63
6:H:6:GLN:H	6:H:105:GLN:HE22	1.47	0.63
1:1:153:VAL:HG12	1:1:153:VAL:O	1.99	0.63
1:1:166:TYR:HD1	1:1:167:THR:H	1.44	0.63
3:3:98:GLY:O	3:3:100:ILE:N	2.32	0.63
3:3:177:ASP:CG	3:3:178:PRO:HD2	2.23	0.63
5:L:34:HIS:CD2	5:L:50:SER:H	2.17	0.63
1:1:261:LEU:HG	2:2:171:TYR:CE2	2.33	0.63
1:1:102:TRP:O	1:1:223:SER:HA	1.99	0.62
3:3:127:LEU:HA	3:3:192:GLN:H	1.63	0.62
6:H:22:CYS:O	6:H:77:THR:HA	1.99	0.62
3:3:14:LEU:HD12	3:3:14:LEU:C	2.24	0.62
5:L:84:ALA:O	5:L:104:LEU:N	2.32	0.62
1:1:44:PRO:O	1:1:45:VAL:O	2.17	0.62
6:H:50:GLN:H	6:H:69:LEU:HD12	1.65	0.62
6:H:63:PHE:O	6:H:64:LYS:C	2.37	0.62
6:H:80:MET:HG2	6:H:81:GLN:N	2.12	0.62
1:1:107:SER:HB3	1:1:113:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:20:SER:O	1:1:55:THR:HA	2.00	0.62
1:1:163:TRP:NE1	1:1:164:ASP:HB2	2.14	0.62
5:L:14:PHE:CD2	5:L:107:LYS:HB3	2.34	0.62
6:H:27:TYR:CD1	6:H:32:PHE:CE1	2.87	0.62
1:1:194:ALA:O	1:1:196:ALA:N	2.31	0.62
2:2:34:CYS:HB3	2:2:185:PRO:HG3	1.81	0.62
3:3:54:PRO:O	3:3:56:ASN:N	2.33	0.62
5:L:95:PRO:O	5:L:96:ILE:C	2.43	0.62
6:H:3:GLN:HA	6:H:102:TYR:CZ	2.34	0.62
1:1:42:THR:HG23	3:3:50:ASP:OD2	2.00	0.62
1:1:254:ILE:CD1	2:2:204:ILE:HG21	2.30	0.62
1:1:289:TYR:CE1	3:3:139:PRO:HD2	2.35	0.62
3:3:100:ILE:HG22	3:3:101:VAL:N	2.14	0.62
3:3:153:TRP:CE3	3:3:161:ILE:CG2	2.81	0.62
6:H:3:GLN:C	6:H:4:LEU:HD23	2.25	0.62
1:1:19:ALA:HB3	1:1:56:THR:OG1	2.00	0.62
2:2:66:LEU:HD12	2:2:89:MET:HE2	1.82	0.62
3:3:21:SER:O	4:4:37:SER:HA	2.00	0.62
3:3:124:SER:OG	3:3:125:ALA:N	2.32	0.62
3:3:214:CYS:HB3	3:3:216:ASP:OD1	2.00	0.62
1:1:67:VAL:HG22	3:3:41:HIS:C	2.24	0.62
2:2:83:PRO:O	2:2:96:MET:HE1	2.00	0.62
5:L:7:SER:OG	5:L:22:THR:CB	2.47	0.62
5:L:44:PRO:HG2	6:H:103:TRP:CH2	2.34	0.62
5:L:77:ARG:CG	5:L:77:ARG:NH1	2.62	0.62
5:L:47:TRP:O	5:L:55:ALA:CB	2.48	0.61
5:L:79:GLU:O	5:L:106:ILE:HD13	2.00	0.61
5:L:79:GLU:H	5:L:82:ASP:CG	2.08	0.61
6:H:22:CYS:O	6:H:77:THR:HG22	1.99	0.61
1:1:281:LYS:HG2	1:1:282:ARG:H	1.63	0.61
2:2:30:ASN:OD1	4:4:58:ASP:O	2.18	0.61
3:3:217:PHE:CE2	3:3:219:LEU:HD11	2.35	0.61
6:H:38:LYS:O	6:H:46:GLU:HB2	2.00	0.61
1:1:37:ASN:HB2	3:3:160:THR:OG1	2.01	0.61
2:2:95:ASN:O	2:2:99:HIS:ND1	2.32	0.61
2:2:260:VAL:HB	2:2:261:PRO:HD2	1.82	0.61
6:H:62:LYS:HG2	6:H:63:PHE:CZ	2.35	0.61
1:1:282:ARG:CG	3:3:57:ASN:ND2	2.64	0.61
2:2:110:VAL:HG11	2:2:124:VAL:CG2	2.30	0.61
2:2:230:VAL:CG1	2:2:236:PRO:HA	2.31	0.61
5:L:48:ILE:HA	5:L:53:ASN:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:33:TRP:CZ3	6:H:57:ASN:HA	2.36	0.61
6:H:38:LYS:HG3	6:H:90:TYR:CE1	2.35	0.61
5:L:14:PHE:O	5:L:15:PRO:C	2.42	0.61
2:2:76:LYS:HG3	2:2:169:VAL:HG11	1.83	0.61
1:1:195:SER:O	1:1:196:ALA:HB2	2.01	0.61
3:3:117:TYR:CE1	3:3:119:GLY:CA	2.84	0.61
5:L:62:PHE:CE1	5:L:75:ILE:HG12	2.35	0.61
2:2:110:VAL:HG23	2:2:242:VAL:HG22	1.83	0.61
2:2:229:THR:O	2:2:229:THR:CG2	2.48	0.61
5:L:7:SER:HB3	5:L:8:PRO:HD3	1.81	0.61
5:L:6:GLN:NE2	5:L:102:THR:H	1.99	0.60
5:L:73:LEU:HG	5:L:74:THR:N	2.14	0.60
1:1:204:TYR:CD2	1:1:211:THR:HG23	2.35	0.60
2:2:217:ASN:C	2:2:218:VAL:CG1	2.75	0.60
5:L:30:VAL:HG21	5:L:90:GLN:CG	2.31	0.60
5:L:82:ASP:O	5:L:104:LEU:HB3	2.01	0.60
1:1:180:VAL:C	1:1:182:ASP:H	2.08	0.60
2:2:41:TYR:O	2:2:43:PRO:HD3	2.00	0.60
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.82	0.60
3:3:141:ASP:CA	3:3:190:TRP:CH2	2.85	0.60
5:L:33:MET:HB2	5:L:71:TYR:CD2	2.36	0.60
2:2:99:HIS:HD2	2:2:254:ILE:HA	1.66	0.60
5:L:6:GLN:OE1	5:L:87:TYR:CA	2.48	0.60
5:L:13:ALA:HA	5:L:17:GLU:OE1	2.00	0.60
5:L:21:ILE:HG22	5:L:22:THR:N	2.16	0.60
5:L:13:ALA:N	5:L:107:LYS:HG3	2.17	0.60
1:1:31:VAL:HG12	1:1:34:LEU:HB2	1.83	0.60
1:1:160:PRO:HB3	1:1:168:TRP:CE2	2.36	0.60
2:2:23:ILE:HD12	2:2:63:PHE:CZ	2.37	0.60
6:H:38:LYS:HG3	6:H:90:TYR:HE1	1.65	0.60
1:1:30:LYS:O	1:1:32:PRO:HD3	2.02	0.60
1:1:201:TYR:N	1:1:215:ILE:HG22	2.17	0.60
2:2:63:PHE:CD1	2:2:245:ALA:CB	2.79	0.60
3:3:167:TRP:O	3:3:167:TRP:CD1	2.54	0.60
1:1:66:ASP:OD2	4:4:43:GLN:HA	2.02	0.60
2:2:122:LEU:HD22	2:2:222:VAL:HG12	1.84	0.60
1:1:254:ILE:HD11	2:2:204:ILE:HG23	1.82	0.59
1:1:113:ARG:HD3	1:1:263:TYR:CE2	2.37	0.59
5:L:11:MET:SD	5:L:11:MET:N	2.75	0.59
6:H:40:ARG:HA	6:H:88:ALA:CB	2.32	0.59
1:1:261:LEU:HD12	1:1:271:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:30:ASN:HD21	4:4:58:ASP:CB	2.08	0.59
3:3:19:ARG:HE	3:3:19:ARG:CA	1.91	0.59
5:L:11:MET:CE	5:L:104:LEU:HD13	2.32	0.59
5:L:44:PRO:C	5:L:45:LYS:HD3	2.27	0.59
1:1:65:THR:C	3:3:42:ASN:ND2	2.60	0.59
2:2:71:TRP:HB3	2:2:238:LEU:O	2.03	0.59
1:1:94:ARG:C	1:1:96:ALA:H	2.09	0.59
1:1:248:LYS:O	1:1:249:HIS:CB	2.48	0.59
2:2:123:LEU:CD1	2:2:188:PHE:HE1	2.15	0.59
3:3:47:ILE:HG22	3:3:100:ILE:CD1	2.32	0.59
5:L:14:PHE:HB2	5:L:17:GLU:HG3	1.84	0.59
6:H:39:GLN:HG2	6:H:43:GLN:O	2.01	0.59
2:2:123:LEU:CD1	2:2:188:PHE:CE1	2.86	0.59
5:L:94:TYR:O	5:L:94:TYR:HD1	1.86	0.59
6:H:41:PRO:O	6:H:43:GLN:HG2	2.03	0.59
1:1:201:TYR:N	2:2:131:GLN:NE2	2.50	0.59
1:1:281:LYS:HE3	1:1:282:ARG:O	2.03	0.59
5:L:21:ILE:HG12	5:L:102:THR:CG2	2.31	0.59
6:H:27:TYR:CE1	6:H:32:PHE:CD1	2.91	0.59
1:1:69:CYS:C	1:1:71:LEU:H	2.10	0.59
1:1:265:SER:N	3:3:234:LEU:HD13	2.17	0.59
5:L:7:SER:HB2	5:L:22:THR:N	2.18	0.59
5:L:31:ASN:HB3	5:L:32:TYR:CE2	2.37	0.59
5:L:94:TYR:C	5:L:94:TYR:CD1	2.78	0.59
6:H:40:ARG:CA	6:H:88:ALA:HB1	2.31	0.59
2:2:10:SER:C	2:2:12:ARG:N	2.61	0.58
3:3:75:ARG:HB3	3:3:78:GLU:OE2	2.03	0.58
3:3:140:GLN:O	3:3:141:ASP:CB	2.50	0.58
1:1:113:ARG:O	1:1:113:ARG:HG2	2.03	0.58
2:2:116:LYS:CA	3:3:121:ALA:HB3	2.33	0.58
5:L:38:GLN:HG3	5:L:44:PRO:HA	1.85	0.58
1:1:200:PHE:N	1:1:200:PHE:CD1	2.71	0.58
2:2:160:ASN:HA	2:2:167:LYS:HZ2	1.68	0.58
2:2:228:LEU:HD12	2:2:229:THR:N	2.18	0.58
6:H:12:VAL:HG13	6:H:18:VAL:CG1	2.33	0.58
6:H:6:GLN:NE2	6:H:91:PHE:HA	2.18	0.58
1:1:207:ASP:OD1	2:2:213:THR:HB	2.04	0.58
1:1:286:ILE:HD11	3:3:81:PHE:HB3	1.84	0.58
2:2:49:ASP:OD1	2:2:51:ASN:HB2	2.03	0.58
3:3:164:THR:O	3:3:166:PRO:HD3	2.04	0.58
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:38:GLN:CG	5:L:44:PRO:HA	2.34	0.58
6:H:69:LEU:HD23	6:H:80:MET:CB	2.24	0.58
6:H:100(J):ALA:O	6:H:101:ASP:N	2.36	0.58
2:2:72:THR:C	2:2:74:GLY:H	2.08	0.58
5:L:82:ASP:O	5:L:84:ALA:N	2.34	0.58
1:1:68:GLU:O	1:1:68:GLU:CG	2.42	0.58
1:1:84:ASN:HD21	1:1:232:HIS:HA	1.66	0.58
3:3:185:GLY:C	3:3:186:PHE:CD1	2.82	0.58
5:L:3:VAL:N	5:L:26:THR:HG23	2.19	0.58
1:1:71:LEU:HD11	1:1:116:LEU:HD22	1.86	0.58
1:1:228:ILE:CD1	1:1:239:VAL:HG21	2.29	0.58
2:2:255:ARG:C	2:2:257:LYS:H	2.06	0.58
1:1:177:PHE:HD1	1:1:177:PHE:H	1.51	0.58
2:2:210:ASP:CG	2:2:211:SER:H	2.12	0.57
5:L:16:GLY:O	5:L:77:ARG:HB3	2.03	0.57
1:1:207:ASP:C	2:2:261:PRO:HG3	2.29	0.57
3:3:43:LEU:O	3:3:46:ILE:HG12	2.04	0.57
5:L:6:GLN:CG	5:L:101:GLY:N	2.35	0.57
5:L:6:GLN:HB3	5:L:102:THR:OG1	2.04	0.57
6:H:3:GLN:HG2	6:H:5:GLN:HE22	1.69	0.57
6:H:48:ILE:CG2	6:H:67:ALA:CB	2.82	0.57
3:3:180:THR:O	3:3:183:SER:HB3	2.03	0.57
6:H:2:GLY:HA2	6:H:25:SER:C	2.30	0.57
1:1:44:PRO:HG3	4:4:54:GLU:OE2	2.03	0.57
1:1:200:PHE:N	1:1:200:PHE:HD1	2.01	0.57
5:L:62:PHE:CE1	5:L:75:ILE:CD1	2.87	0.57
5:L:100:SER:OG	5:L:101:GLY:N	2.35	0.57
6:H:86:ASP:HA	6:H:90:TYR:OH	2.05	0.57
2:2:63:PHE:HD1	2:2:245:ALA:HB2	1.65	0.57
2:2:76:LYS:CG	2:2:169:VAL:HG11	2.35	0.57
2:2:116:LYS:HA	3:3:121:ALA:CB	2.34	0.57
3:3:83:THR:CG2	3:3:187:LEU:HD21	2.35	0.57
6:H:27:TYR:HE1	6:H:32:PHE:CD1	2.22	0.57
1:1:60:PHE:CD2	3:3:218:LYS:HG2	2.40	0.57
1:1:178:PHE:C	1:1:178:PHE:HD1	2.13	0.57
2:2:84:ASP:O	2:2:87:LYS:N	2.23	0.57
3:3:41:HIS:HB2	3:3:45:GLU:OE2	2.04	0.57
1:1:146:LEU:H	1:1:180:VAL:HG21	1.70	0.57
6:H:54:ASP:OD1	6:H:56:ASP:HB2	2.05	0.57
2:2:94:GLN:O	2:2:96:MET:N	2.38	0.57
2:2:214:ARG:O	2:2:215:HIS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:77:ARG:NH1	5:L:77:ARG:CB	2.67	0.57
6:H:6:GLN:HB2	6:H:105:GLN:NE2	2.19	0.57
1:1:36:ALA:O	1:1:39:THR:HG23	2.05	0.57
1:1:129:THR:HG22	1:1:244:TYR:HB2	1.86	0.57
1:1:138:ASP:OD1	1:1:138:ASP:N	2.37	0.57
5:L:54:LEU:HD13	5:L:58:VAL:HG23	1.82	0.57
5:L:57:GLY:O	5:L:59:PRO:HD3	2.05	0.57
1:1:286:ILE:HD11	3:3:81:PHE:CB	2.35	0.56
3:3:55:MET:HA	3:3:91:VAL:HG12	1.86	0.56
1:1:146:LEU:O	1:1:180:VAL:HG22	2.05	0.56
1:1:178:PHE:C	1:1:178:PHE:CD1	2.83	0.56
1:1:185:ARG:HH22	3:3:17:ASP:HB3	1.70	0.56
2:2:182:LEU:HD12	2:2:182:LEU:N	2.19	0.56
5:L:4:LEU:CD2	5:L:25:ALA:HB2	2.36	0.56
1:1:123:ARG:NH1	3:3:33:ARG:HB3	2.19	0.56
2:2:160:ASN:HA	2:2:167:LYS:NZ	2.20	0.56
2:2:181:LEU:C	2:2:183:ILE:H	2.14	0.56
2:2:190:ASN:C	2:2:192:ARG:H	2.13	0.56
3:3:216:ASP:O	3:3:217:PHE:C	2.48	0.56
5:L:2:ILE:HB	5:L:90:GLN:HE21	1.70	0.56
5:L:33:MET:CG	5:L:71:TYR:HB2	2.35	0.56
6:H:39:GLN:HB2	6:H:45:LEU:CD2	2.35	0.56
6:H:62:LYS:CG	6:H:63:PHE:CE1	2.88	0.56
6:H:94:ARG:O	6:H:100(K):MET:HA	2.04	0.56
1:1:110:VAL:HG22	3:3:230:GLN:HG2	1.86	0.56
2:2:121:CYS:HB2	2:2:190:ASN:HA	1.87	0.56
6:H:50:GLN:N	6:H:69:LEU:HD12	2.19	0.56
2:2:66:LEU:HD21	2:2:85:ALA:HB1	1.88	0.56
2:2:135:HIS:HE1	2:2:163:GLY:H	1.53	0.56
3:3:141:ASP:O	3:3:142:ARG:C	2.49	0.56
5:L:13:ALA:C	5:L:78:MET:HG2	2.30	0.56
5:L:80:ALA:C	5:L:82:ASP:H	2.14	0.56
6:H:27:TYR:CD1	6:H:94:ARG:HD2	2.37	0.56
1:1:67:VAL:C	1:1:69:CYS:H	2.14	0.56
1:1:228:ILE:HD11	1:1:239:VAL:CG2	2.29	0.56
2:2:110:VAL:HG11	2:2:124:VAL:HG21	1.87	0.56
5:L:73:LEU:HG	5:L:74:THR:H	1.69	0.56
2:2:101:LEU:HD12	2:2:209:ILE:HG12	1.88	0.56
2:2:190:ASN:C	2:2:192:ARG:N	2.63	0.56
3:3:28:TYR:CD1	3:3:28:TYR:C	2.83	0.56
1:1:289:TYR:CZ	3:3:139:PRO:O	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:41:HIS:CD2	4:4:46:SER:HB2	2.40	0.56
3:3:86:PHE:C	3:3:88:GLY:N	2.62	0.56
5:L:82:ASP:HB3	5:L:104:LEU:CD2	2.36	0.56
2:2:172:ASN:ND2	2:2:181:LEU:HD13	2.21	0.56
3:3:51:THR:O	3:3:210:PHE:HA	2.05	0.56
1:1:31:VAL:CG1	1:1:34:LEU:HB2	2.36	0.56
2:2:178:LEU:O	2:2:181:LEU:HB2	2.06	0.56
1:1:146:LEU:HA	1:1:230:ASN:HD21	1.70	0.55
3:3:128:ILE:O	3:3:189:CYS:HA	2.07	0.55
3:3:188:SER:O	3:3:189:CYS:HB2	2.05	0.55
5:L:77:ARG:HB2	5:L:77:ARG:NH1	2.21	0.55
2:2:156:LEU:HD21	2:2:173:MET:SD	2.46	0.55
3:3:2:LEU:HD12	3:3:2:LEU:C	2.31	0.55
6:H:10:GLU:OE1	6:H:10:GLU:HA	2.06	0.55
2:2:110:VAL:CG2	2:2:242:VAL:HG22	2.37	0.55
3:3:104:TYR:CD2	3:3:219:LEU:HD23	2.40	0.55
1:1:37:ASN:HB3	3:3:116:MET:HE3	1.89	0.55
1:1:74:ALA:HB3	3:3:15:THR:CB	2.35	0.55
1:1:104:ILE:HG13	1:1:222:GLY:O	2.06	0.55
2:2:44:ASP:O	2:2:46:ASP:N	2.39	0.55
2:2:182:LEU:H	2:2:182:LEU:CD1	2.19	0.55
3:3:200:GLU:HA	3:3:200:GLU:OE1	2.05	0.55
1:1:70:PHE:CZ	1:1:118:LEU:HD23	2.41	0.55
3:3:41:HIS:NE2	4:4:46:SER:HB2	2.22	0.55
3:3:141:ASP:N	3:3:190:TRP:CH2	2.74	0.55
3:3:175:TYR:CB	3:3:182:THR:HG21	2.29	0.55
6:H:36:TRP:CD1	6:H:69:LEU:CD2	2.85	0.55
2:2:105:GLY:O	2:2:247:MET:N	2.40	0.55
2:2:179:GLY:O	3:3:51:THR:HG22	2.07	0.55
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.72	0.55
5:L:6:GLN:HG2	5:L:100:SER:H	1.72	0.55
5:L:7:SER:O	5:L:8:PRO:C	2.45	0.55
5:L:47:TRP:O	5:L:58:VAL:HG11	2.07	0.55
1:1:39:THR:HG22	2:2:29:ALA:HB1	1.89	0.55
1:1:152:TYR:CD1	1:1:152:TYR:C	2.84	0.55
2:2:37:GLU:HG2	3:3:37:PRO:HB3	1.88	0.55
6:H:50:GLN:N	6:H:69:LEU:CD1	2.69	0.55
3:3:9:GLY:O	3:3:12:GLN:HG2	2.07	0.55
3:3:55:MET:HA	3:3:91:VAL:HG11	1.88	0.55
5:L:35:TRP:CH2	5:L:88:CYS:HB3	2.42	0.55
5:L:54:LEU:C	5:L:55:ALA:O	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:133:PRO:CB	3:3:134:PRO:HD2	2.37	0.55
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.55
1:1:199:CYS:C	1:1:200:PHE:HD1	2.14	0.54
1:1:265:SER:OG	1:1:268:ARG:HG3	2.08	0.54
1:1:282:ARG:HB2	3:3:57:ASN:CB	2.34	0.54
5:L:10:ILE:HD12	5:L:103:LYS:HB3	1.89	0.54
1:1:217:VAL:HG23	1:1:218:LEU:N	2.22	0.54
2:2:34:CYS:HB3	2:2:185:PRO:CG	2.37	0.54
1:1:146:LEU:O	1:1:180:VAL:CG2	2.55	0.54
2:2:144:TYR:CE1	2:2:148:HIS:CD2	2.95	0.54
2:2:171:TYR:C	2:2:173:MET:N	2.65	0.54
6:H:40:ARG:HB2	6:H:43:GLN:HB2	1.89	0.54
1:1:147:VAL:O	1:1:229:VAL:CG2	2.55	0.54
3:3:63:GLU:C	3:3:65:ASN:N	2.61	0.54
6:H:27:TYR:HE1	6:H:32:PHE:HD1	1.54	0.54
1:1:123:ARG:O	1:1:250:VAL:HA	2.07	0.54
1:1:141:ASN:O	1:1:142:TYR:HB3	2.07	0.54
1:1:254:ILE:CD1	2:2:204:ILE:CG2	2.85	0.54
2:2:126:VAL:HG21	2:2:199:ILE:HG21	1.89	0.54
3:3:129:LEU:O	3:3:130:ALA:HB2	2.07	0.54
6:H:40:ARG:CA	6:H:43:GLN:HB2	2.38	0.54
2:2:15:GLN:C	2:2:16:ILE:HG13	2.32	0.54
2:2:215:HIS:CD2	2:2:216:ASN:N	2.76	0.54
1:1:188:VAL:CG1	1:1:189:PRO:HD2	2.38	0.54
1:1:260:ALA:HB2	2:2:177:LEU:HD11	1.88	0.54
2:2:62:ARG:O	2:2:245:ALA:CB	2.56	0.54
2:2:128:PRO:HA	2:2:218:VAL:HB	1.88	0.54
6:H:99:PRO:CD	6:H:100(I):TYR:CE1	2.90	0.54
6:H:100(J):ALA:HB1	6:H:100(K):MET:CE	2.29	0.54
2:2:63:PHE:HA	2:2:245:ALA:HB2	1.90	0.54
3:3:195:LEU:HD21	3:3:205:VAL:HG21	1.89	0.54
1:1:177:PHE:CD1	1:1:177:PHE:N	2.75	0.54
1:1:151:MET:HE3	1:1:173:ASN:HD22	1.72	0.54
2:2:180:ASN:HA	3:3:51:THR:CG2	2.37	0.54
5:L:16:GLY:HA2	5:L:77:ARG:CZ	2.38	0.54
1:1:47:PRO:HA	3:3:164:THR:HG21	1.90	0.53
1:1:166:TYR:CE1	1:1:167:THR:HG23	2.43	0.53
2:2:62:ARG:HG3	2:2:63:PHE:N	2.22	0.53
5:L:30:VAL:HG21	5:L:90:GLN:HG3	1.83	0.53
6:H:14:PRO:HD3	6:H:112:SER:C	2.32	0.53
6:H:32:PHE:CD1	6:H:32:PHE:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:PRO:C	1:1:49:ASP:H	2.16	0.53
1:1:94:ARG:C	1:1:96:ALA:N	2.64	0.53
1:1:129:THR:OG1	1:1:185:ARG:CD	2.56	0.53
1:1:265:SER:HG	1:1:268:ARG:HG3	1.73	0.53
1:1:271:TYR:HB2	1:1:272:PRO:CD	2.34	0.53
2:2:255:ARG:HD3	2:2:255:ARG:N	2.22	0.53
3:3:126:LYS:HE2	3:3:154:ASP:CG	2.34	0.53
3:3:109:GLY:HA3	3:3:217:PHE:HA	1.89	0.53
6:H:35:ASN:ND2	6:H:35:ASN:N	2.54	0.53
2:2:34:CYS:C	2:2:36:ALA:H	2.17	0.53
2:2:71:TRP:O	2:2:237:SER:HA	2.08	0.53
1:1:21:ILE:H	1:1:21:ILE:HD12	1.63	0.53
1:1:124:PHE:CD1	1:1:124:PHE:C	2.86	0.53
2:2:85:ALA:HA	2:2:150:GLY:CA	2.36	0.53
6:H:70:THR:HG23	6:H:79:TYR:HB2	1.91	0.53
1:1:201:TYR:CE2	1:1:203:GLY:CA	2.91	0.53
2:2:37:GLU:HG3	3:3:37:PRO:HB3	1.89	0.53
2:2:99:HIS:ND1	2:2:251:PHE:HB3	2.23	0.53
3:3:16:THR:O	3:3:16:THR:HG22	2.07	0.53
3:3:42:ASN:O	3:3:43:LEU:C	2.52	0.53
3:3:76:GLN:O	3:3:77:ASN:HB2	2.09	0.53
6:H:5:GLN:O	6:H:22:CYS:HA	2.08	0.53
2:2:61:CYS:SG	2:2:249:THR:OG1	2.67	0.53
2:2:150:GLY:O	2:2:151:GLU:C	2.52	0.53
2:2:150:GLY:C	2:2:152:ARG:N	2.62	0.53
5:L:13:ALA:CB	5:L:78:MET:CG	2.83	0.53
6:H:62:LYS:HG3	6:H:63:PHE:N	2.22	0.53
2:2:181:LEU:O	2:2:183:ILE:N	2.42	0.53
2:2:225:ILE:CG2	3:3:208:LEU:HD21	2.39	0.53
3:3:51:THR:O	3:3:210:PHE:HB3	2.09	0.53
5:L:38:GLN:HE21	5:L:44:PRO:CD	2.22	0.53
1:1:102:TRP:CZ3	1:1:104:ILE:HG23	2.44	0.53
2:2:34:CYS:SG	2:2:202:PRO:HD2	2.49	0.53
3:3:54:PRO:C	3:3:56:ASN:H	2.17	0.53
3:3:175:TYR:CD2	3:3:182:THR:HG21	2.44	0.53
6:H:40:ARG:HB3	6:H:41:PRO:HD2	1.91	0.53
1:1:136:GLN:C	1:1:138:ASP:H	2.17	0.53
2:2:76:LYS:HG2	2:2:169:VAL:CG1	2.39	0.52
5:L:58:VAL:HG23	5:L:58:VAL:O	2.08	0.52
1:1:253:TRP:CD1	3:3:36:ILE:HG13	2.43	0.52
2:2:225:ILE:HG21	3:3:208:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:13:ALA:HB3	5:L:78:MET:HG2	1.86	0.52
6:H:35:ASN:HD22	6:H:35:ASN:H	1.57	0.52
3:3:128:ILE:CG2	3:3:190:TRP:O	2.57	0.52
3:3:143:ARG:O	3:3:144:GLU:C	2.53	0.52
3:3:53:ILE:CD1	3:3:113:PHE:HE1	2.22	0.52
3:3:101:VAL:HG22	3:3:219:LEU:HD21	1.91	0.52
3:3:173:PHE:CE2	3:3:220:ARG:HD3	2.44	0.52
5:L:48:ILE:CD1	5:L:54:LEU:HD13	2.37	0.52
6:H:51:ILE:HD12	6:H:52:TYR:H	1.72	0.52
1:1:254:ILE:HG23	2:2:35:TYR:CZ	2.45	0.52
3:3:26:PRO:C	3:3:28:TYR:H	2.16	0.52
3:3:90:GLY:O	3:3:91:VAL:C	2.52	0.52
3:3:113:PHE:HE2	3:3:129:LEU:HD21	1.75	0.52
3:3:126:LYS:HG2	3:3:154:ASP:HA	1.91	0.52
1:1:248:LYS:O	1:1:248:LYS:HG3	2.10	0.52
2:2:187:GLN:HE21	2:2:198:THR:N	2.01	0.52
3:3:63:GLU:O	3:3:66:SER:OG	2.24	0.52
3:3:101:VAL:HG23	3:3:219:LEU:HD21	1.91	0.52
6:H:32:PHE:HB3	6:H:95:SER:O	2.09	0.52
1:1:67:VAL:HG23	3:3:41:HIS:O	2.09	0.52
1:1:163:TRP:CD1	1:1:164:ASP:N	2.78	0.52
1:1:188:VAL:HG12	1:1:189:PRO:HD2	1.92	0.52
2:2:110:VAL:HG12	2:2:189:ILE:HD11	1.91	0.52
6:H:29:PHE:CE2	6:H:76:THR:HA	2.45	0.52
1:1:41:ALA:CB	4:4:60:MET:CE	2.87	0.52
3:3:2:LEU:HD12	3:3:3:PRO:N	2.24	0.52
5:L:25:ALA:O	5:L:69:THR:HG22	2.08	0.52
5:L:107:LYS:HB3	5:L:107:LYS:HZ2	1.74	0.52
1:1:256:ARG:NH2	2:2:128:PRO:O	2.43	0.52
3:3:113:PHE:CE2	3:3:129:LEU:HD21	2.45	0.52
3:3:115:LEU:HD23	3:3:129:LEU:CD1	2.39	0.52
1:1:214:GLY:O	1:1:217:VAL:HG22	2.09	0.52
5:L:7:SER:HB3	5:L:8:PRO:CD	2.40	0.52
6:H:3:GLN:HG3	6:H:102:TYR:OH	2.10	0.52
1:1:263:TYR:HB3	3:3:234:LEU:HD11	1.91	0.51
2:2:116:LYS:O	3:3:122:LEU:HB2	2.10	0.51
1:1:46:LEU:HD22	1:1:47:PRO:HD2	1.92	0.51
1:1:88:THR:O	1:1:88:THR:HG23	2.10	0.51
2:2:12:ARG:C	2:2:13:VAL:HG22	2.35	0.51
2:2:54:SER:C	2:2:55:LYS:HG3	2.34	0.51
2:2:76:LYS:HG2	2:2:169:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:82:LEU:O	2:2:83:PRO:C	2.50	0.51
3:3:117:TYR:CE1	3:3:119:GLY:N	2.79	0.51
6:H:22:CYS:O	6:H:23:LYS:HD3	2.11	0.51
1:1:151:MET:HE1	1:1:167:THR:O	2.10	0.51
1:1:208:ASP:HA	2:2:261:PRO:HG3	1.92	0.51
3:3:83:THR:HG23	3:3:187:LEU:HD21	1.90	0.51
5:L:15:PRO:HA	5:L:78:MET:HG3	1.91	0.51
5:L:86:TYR:CE2	5:L:104:LEU:HB2	2.45	0.51
1:1:199:CYS:HB3	1:1:200:PHE:HD1	1.75	0.51
3:3:76:GLN:C	3:3:78:GLU:H	2.16	0.51
5:L:11:MET:HE1	5:L:104:LEU:CD1	2.40	0.51
6:H:27:TYR:CZ	6:H:94:ARG:HD2	2.41	0.51
3:3:35:HIS:ND1	3:3:36:ILE:N	2.59	0.51
3:3:63:GLU:C	3:3:65:ASN:H	2.18	0.51
5:L:4:LEU:HD22	5:L:25:ALA:HB2	1.90	0.51
5:L:30:VAL:HG21	5:L:90:GLN:HB2	1.92	0.51
1:1:69:CYS:O	1:1:71:LEU:N	2.34	0.51
1:1:70:PHE:HZ	1:1:118:LEU:HD23	1.75	0.51
3:3:175:TYR:HD2	3:3:182:THR:HG21	1.76	0.51
6:H:6:GLN:NE2	6:H:106:GLY:HA2	2.25	0.51
1:1:77:VAL:O	1:1:77:VAL:HG23	2.11	0.51
2:2:111:GLN:HG2	2:2:196:THR:HG21	1.91	0.51
3:3:192:GLN:HA	3:3:192:GLN:NE2	2.26	0.51
5:L:6:GLN:CB	5:L:100:SER:OG	2.58	0.51
5:L:6:GLN:CB	5:L:101:GLY:H	2.23	0.51
5:L:54:LEU:HD21	5:L:63:SER:HA	1.91	0.51
1:1:166:TYR:HD1	1:1:166:TYR:H	1.59	0.51
5:L:33:MET:CG	5:L:71:TYR:CB	2.79	0.51
5:L:54:LEU:HD12	5:L:58:VAL:O	2.11	0.51
5:L:82:ASP:HB3	5:L:104:LEU:HD21	1.91	0.51
5:L:94:TYR:CE1	5:L:96:ILE:HG13	2.44	0.51
5:L:22:THR:HA	5:L:72:SER:HA	1.92	0.51
1:1:232:HIS:C	1:1:233:ASP:O	2.53	0.51
5:L:21:ILE:CG2	5:L:22:THR:N	2.73	0.51
5:L:59:PRO:O	5:L:62:PHE:HB2	2.10	0.51
6:H:98:TYR:O	6:H:99:PRO:C	2.50	0.51
2:2:23:ILE:O	2:2:23:ILE:HG22	2.11	0.50
2:2:33:VAL:HG22	2:2:200:VAL:HG21	1.92	0.50
2:2:64:TYR:O	2:2:243:THR:HG22	2.10	0.50
2:2:92:PHE:CD1	2:2:92:PHE:C	2.89	0.50
2:2:185:PRO:O	2:2:186:HIS:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:97:ASN:C	6:H:99:PRO:HD2	2.37	0.50
2:2:67:ASP:CG	2:2:68:SER:H	2.17	0.50
2:2:123:LEU:O	2:2:123:LEU:CG	2.41	0.50
5:L:30:VAL:HG21	5:L:90:GLN:CB	2.41	0.50
6:H:39:GLN:CB	6:H:45:LEU:HD23	2.39	0.50
6:H:79:TYR:O	6:H:80:MET:CB	2.59	0.50
1:1:136:GLN:HG2	1:1:235:HIS:CD2	2.47	0.50
1:1:190:TYR:HD1	1:1:190:TYR:O	1.94	0.50
5:L:14:PHE:CD2	5:L:107:LYS:CB	2.95	0.50
6:H:22:CYS:O	6:H:77:THR:CA	2.59	0.50
1:1:67:VAL:CG2	3:3:41:HIS:C	2.84	0.50
6:H:29:PHE:C	6:H:31:SER:H	2.19	0.50
6:H:29:PHE:CD2	6:H:76:THR:HG22	2.46	0.50
1:1:81:GLU:HB3	1:1:240:LYS:CG	2.40	0.50
1:1:231:GLU:O	1:1:232:HIS:C	2.54	0.50
3:3:50:ASP:HB2	3:3:210:PHE:HB3	1.93	0.50
3:3:82:GLY:O	3:3:83:THR:HB	2.11	0.50
5:L:6:GLN:OE1	5:L:88:CYS:N	2.40	0.50
5:L:14:PHE:CG	5:L:107:LYS:HB2	2.47	0.50
5:L:34:HIS:HD2	5:L:49:TYR:HA	1.76	0.50
5:L:65:SER:O	5:L:71:TYR:HB3	2.12	0.50
6:H:3:GLN:O	6:H:4:LEU:HD23	2.11	0.50
3:3:210:PHE:N	3:3:210:PHE:CD1	2.79	0.50
5:L:58:VAL:CG2	5:L:58:VAL:O	2.60	0.50
1:1:50:SER:O	1:1:51:ILE:CG2	2.60	0.50
1:1:122:VAL:CG1	1:1:124:PHE:CE2	2.95	0.50
1:1:176:VAL:HG23	1:1:176:VAL:O	2.12	0.50
2:2:79:CYS:SG	2:2:80:TRP:N	2.84	0.50
2:2:108:VAL:HG22	2:2:199:ILE:O	2.11	0.50
2:2:207:VAL:HG12	2:2:208:PRO:CD	2.35	0.50
6:H:12:VAL:O	6:H:111:VAL:HA	2.11	0.50
3:3:42:ASN:N	3:3:45:GLU:OE2	2.37	0.50
3:3:104:TYR:O	3:3:176:THR:HG21	2.12	0.50
5:L:3:VAL:HB	5:L:26:THR:CG2	2.41	0.50
5:L:47:TRP:O	5:L:55:ALA:HB3	2.12	0.50
6:H:82(C):LEU:HB3	6:H:111:VAL:HG21	1.94	0.50
2:2:99:HIS:HD2	2:2:254:ILE:CA	2.25	0.50
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.92	0.50
1:1:37:ASN:CB	3:3:116:MET:HE3	2.42	0.49
1:1:94:ARG:NH1	6:H:56:ASP:OD2	2.45	0.49
2:2:135:HIS:CB	2:2:160:ASN:ND2	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:184:PHE:HB3	2:2:185:PRO:CD	2.39	0.49
6:H:36:TRP:HA	6:H:91:PHE:O	2.12	0.49
1:1:102:TRP:O	1:1:223:SER:CA	2.60	0.49
1:1:199:CYS:HB3	1:1:200:PHE:CD1	2.45	0.49
2:2:65:THR:HA	2:2:243:THR:HG23	1.94	0.49
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.93	0.49
5:L:74:THR:CG2	5:L:75:ILE:N	2.75	0.49
6:H:82(C):LEU:HB3	6:H:111:VAL:CG2	2.42	0.49
3:3:47:ILE:HG22	3:3:100:ILE:HD12	1.94	0.49
6:H:33:TRP:CE3	6:H:50:GLN:NE2	2.80	0.49
1:1:119:PHE:HA	1:1:255:PRO:HA	1.95	0.49
1:1:273:LYS:HE2	2:2:136:GLU:C	2.38	0.49
5:L:47:TRP:CZ2	5:L:62:PHE:CE2	3.00	0.49
5:L:47:TRP:HZ2	5:L:62:PHE:CE2	2.31	0.49
1:1:46:LEU:CB	1:1:47:PRO:HD2	2.42	0.49
1:1:162:GLU:C	1:1:164:ASP:H	2.20	0.49
1:1:271:TYR:CB	1:1:272:PRO:CD	2.86	0.49
2:2:166:VAL:O	2:2:173:MET:HG2	2.12	0.49
3:3:120:PRO:O	3:3:121:ALA:C	2.55	0.49
1:1:180:VAL:C	1:1:182:ASP:N	2.70	0.49
1:1:194:ALA:C	1:1:196:ALA:N	2.71	0.49
3:3:126:LYS:CE	3:3:154:ASP:HB2	2.31	0.49
5:L:21:ILE:HB	5:L:73:LEU:HB3	1.95	0.49
1:1:201:TYR:O	1:1:201:TYR:CD2	2.66	0.49
3:3:195:LEU:HD21	3:3:205:VAL:HG22	1.93	0.49
5:L:49:TYR:CE1	5:L:55:ALA:HA	2.48	0.49
5:L:71:TYR:CD1	5:L:71:TYR:N	2.80	0.49
6:H:24:ALA:HB1	6:H:27:TYR:CE2	2.47	0.49
6:H:37:VAL:HG22	6:H:91:PHE:HD2	1.78	0.49
6:H:40:ARG:CB	6:H:43:GLN:HB2	2.42	0.49
1:1:165:ASP:HB3	1:1:167:THR:OG1	2.12	0.49
1:1:264:THR:O	1:1:265:SER:HB3	2.13	0.49
5:L:18:LYS:HG3	5:L:75:ILE:O	2.12	0.49
5:L:21:ILE:HG23	5:L:102:THR:OG1	2.12	0.49
5:L:30:VAL:O	5:L:71:TYR:CZ	2.66	0.49
5:L:36:PHE:CE2	6:H:103:TRP:NE1	2.69	0.49
5:L:83:ALA:HA	5:L:104:LEU:O	2.12	0.49
6:H:4:LEU:HD12	6:H:93:ALA:HA	1.94	0.49
6:H:8:GLY:O	6:H:9:ALA:C	2.55	0.49
6:H:38:LYS:HE3	6:H:85:GLU:O	2.13	0.49
1:1:97:LYS:HD2	6:H:52:TYR:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:121:TYR:CD2	2:2:206:SER:HB3	2.49	0.48
1:1:264:THR:OG1	1:1:270:ASN:HB2	2.13	0.48
3:3:54:PRO:HA	3:3:67:TYR:CD1	2.48	0.48
6:H:3:GLN:O	6:H:23:LYS:O	2.31	0.48
6:H:95:SER:HA	6:H:100(K):MET:HA	1.94	0.48
1:1:285:ASP:HB3	1:1:288:SER:H	1.78	0.48
3:3:47:ILE:HG21	3:3:100:ILE:HG21	1.96	0.48
5:L:47:TRP:C	5:L:48:ILE:HD12	2.38	0.48
3:3:177:ASP:OD1	3:3:178:PRO:HD2	2.13	0.48
5:L:38:GLN:HE21	5:L:44:PRO:HD3	1.77	0.48
6:H:1:GLN:O	6:H:2:GLY:O	2.31	0.48
1:1:20:SER:O	1:1:54:ARG:O	2.31	0.48
1:1:230:ASN:OD1	1:1:230:ASN:N	2.45	0.48
3:3:42:ASN:C	3:3:44:LEU:N	2.68	0.48
3:3:104:TYR:HD2	3:3:219:LEU:HD23	1.79	0.48
5:L:78:MET:SD	5:L:106:ILE:HD13	2.53	0.48
5:L:85:THR:HA	5:L:103:LYS:HA	1.96	0.48
1:1:261:LEU:HD12	1:1:271:TYR:CG	2.49	0.48
6:H:22:CYS:C	6:H:23:LYS:CD	2.87	0.48
6:H:51:ILE:HD12	6:H:52:TYR:N	2.29	0.48
1:1:94:ARG:O	1:1:96:ALA:N	2.47	0.48
1:1:136:GLN:N	1:1:137:PRO:HD3	2.27	0.48
3:3:47:ILE:HG22	3:3:100:ILE:HD13	1.95	0.48
3:3:52:LEU:HA	3:3:209:SER:O	2.13	0.48
5:L:7:SER:C	5:L:8:PRO:O	2.56	0.48
5:L:19:VAL:HG23	5:L:75:ILE:O	2.14	0.48
2:2:256:SER:O	2:2:257:LYS:O	2.31	0.48
5:L:50:SER:OG	6:H:99:PRO:O	2.30	0.48
1:1:21:ILE:HA	1:1:55:THR:HG23	1.95	0.48
2:2:30:ASN:ND2	2:2:31:ALA:H	2.11	0.48
3:3:16:THR:O	3:3:16:THR:HG23	2.14	0.48
5:L:44:PRO:CG	6:H:45:LEU:CD1	2.77	0.48
6:H:4:LEU:N	6:H:102:TYR:CE2	2.82	0.48
1:1:215:ILE:C	1:1:217:VAL:N	2.70	0.48
2:2:108:VAL:HG23	2:2:199:ILE:HB	1.95	0.48
5:L:54:LEU:HD13	5:L:58:VAL:CG2	2.41	0.48
1:1:87:ALA:O	1:1:89:GLY:N	2.47	0.48
1:1:163:TRP:CD1	1:1:163:TRP:C	2.83	0.48
2:2:120:GLY:O	2:2:191:LEU:HB2	2.13	0.48
3:3:131:TYR:HD1	3:3:186:PHE:O	1.96	0.48
5:L:15:PRO:HB3	5:L:79:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG21	6:H:82(C):LEU:CD1	2.44	0.48
2:2:183:ILE:O	2:2:183:ILE:CG2	2.61	0.47
6:H:83:THR:C	6:H:85:GLU:H	2.21	0.47
1:1:35:THR:OG1	1:1:36:ALA:N	2.47	0.47
1:1:152:TYR:C	1:1:152:TYR:HD1	2.22	0.47
1:1:166:TYR:HE1	1:1:167:THR:HG23	1.79	0.47
2:2:33:VAL:HA	2:2:200:VAL:HG23	1.97	0.47
2:2:122:LEU:HD22	2:2:222:VAL:CG1	2.44	0.47
3:3:26:PRO:O	3:3:28:TYR:N	2.47	0.47
3:3:65:ASN:O	3:3:67:TYR:N	2.47	0.47
6:H:11:LEU:HD12	6:H:110:THR:O	2.14	0.47
6:H:22:CYS:N	6:H:23:LYS:HE2	2.29	0.47
6:H:39:GLN:HG3	6:H:45:LEU:HD23	1.95	0.47
1:1:93:HIS:CD2	1:1:93:HIS:N	2.82	0.47
1:1:122:VAL:HG11	1:1:124:PHE:HE2	1.78	0.47
2:2:104:SER:OG	2:2:249:THR:CG2	2.51	0.47
2:2:126:VAL:CG2	2:2:199:ILE:HD12	2.43	0.47
2:2:135:HIS:CG	2:2:160:ASN:HD22	2.32	0.47
5:L:6:GLN:CG	5:L:100:SER:H	2.27	0.47
5:L:14:PHE:CG	5:L:107:LYS:CB	2.98	0.47
5:L:62:PHE:CE1	5:L:75:ILE:HD13	2.49	0.47
5:L:78:MET:SD	5:L:106:ILE:CD1	3.02	0.47
1:1:82:ILE:HD12	1:1:228:ILE:HG13	1.95	0.47
5:L:44:PRO:HD3	6:H:91:PHE:CZ	2.50	0.47
6:H:38:LYS:O	6:H:38:LYS:HG2	2.14	0.47
1:1:260:ALA:HB2	2:2:177:LEU:CD1	2.44	0.47
6:H:40:ARG:CB	6:H:43:GLN:CB	2.92	0.47
1:1:76:CYS:SG	1:1:77:VAL:N	2.87	0.47
2:2:261:PRO:O	2:2:262:GLN:HB3	2.13	0.47
1:1:70:PHE:CD2	3:3:43:LEU:HD11	2.49	0.47
1:1:78:HIS:N	1:1:109:LEU:CD1	2.78	0.47
1:1:162:GLU:C	1:1:164:ASP:N	2.71	0.47
1:1:251:GLU:HB3	1:1:253:TRP:CH2	2.50	0.47
2:2:25:THR:HG23	2:2:25:THR:O	2.14	0.47
2:2:34:CYS:C	2:2:36:ALA:N	2.72	0.47
2:2:107:THR:O	2:2:244:ILE:HG23	2.15	0.47
2:2:181:LEU:C	2:2:183:ILE:N	2.72	0.47
2:2:246:PRO:O	2:2:247:MET:HB3	2.15	0.47
3:3:142:ARG:O	3:3:143:ARG:O	2.32	0.47
5:L:13:ALA:HB3	5:L:78:MET:CG	2.45	0.47
5:L:33:MET:CE	5:L:89:GLN:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:89:GLN:NE2	6:H:100(K):MET:HE1	2.30	0.47
6:H:29:PHE:O	6:H:52(A):PRO:HG2	2.15	0.47
1:1:46:LEU:HB3	1:1:47:PRO:HD2	1.96	0.47
1:1:78:HIS:ND1	1:1:79:VAL:N	2.62	0.47
1:1:123:ARG:O	1:1:124:PHE:HB3	2.15	0.47
2:2:48:SER:O	2:2:49:ASP:C	2.56	0.47
2:2:84:ASP:O	2:2:85:ALA:C	2.58	0.47
3:3:7:LEU:HB3	3:3:8:PRO:HD2	1.97	0.47
3:3:53:ILE:HD11	3:3:113:PHE:CE1	2.49	0.47
5:L:85:THR:HG23	5:L:103:LYS:HG2	1.96	0.47
6:H:23:LYS:HA	6:H:76:THR:O	2.14	0.47
1:1:37:ASN:HB3	3:3:116:MET:CE	2.44	0.47
6:H:4:LEU:H	6:H:102:TYR:HE2	1.63	0.47
6:H:34:VAL:HG21	6:H:78:ALA:HB2	1.97	0.47
2:2:20:ASN:CG	2:2:20:ASN:O	2.57	0.47
2:2:91:VAL:HG12	2:2:95:ASN:HD21	1.80	0.47
3:3:130:ALA:HA	3:3:150:HIS:HA	1.97	0.47
3:3:153:TRP:CD2	3:3:161:ILE:CG2	2.96	0.47
5:L:31:ASN:C	5:L:32:TYR:CD2	2.93	0.47
6:H:40:ARG:O	6:H:43:GLN:HB2	2.15	0.47
1:1:116:LEU:C	1:1:118:LEU:H	2.23	0.46
2:2:33:VAL:O	4:4:55:PRO:HB3	2.15	0.46
1:1:58:MET:O	1:1:59:HIS:C	2.58	0.46
1:1:110:VAL:CG2	3:3:230:GLN:HG2	2.44	0.46
2:2:30:ASN:HD21	4:4:58:ASP:H	1.63	0.46
3:3:186:PHE:CD1	3:3:186:PHE:N	2.83	0.46
5:L:62:PHE:HE1	5:L:75:ILE:HD13	1.80	0.46
5:L:67:SER:CA	5:L:71:TYR:CE1	2.92	0.46
1:1:58:MET:C	1:1:59:HIS:CD2	2.93	0.46
1:1:102:TRP:CE3	1:1:104:ILE:HG23	2.51	0.46
1:1:204:TYR:CZ	1:1:213:TYR:HB2	2.50	0.46
2:2:225:ILE:HD13	2:2:225:ILE:HA	1.74	0.46
5:L:14:PHE:N	5:L:107:LYS:CB	2.75	0.46
5:L:108:ARG:CG	5:L:109:ALA:N	2.65	0.46
6:H:50:GLN:O	6:H:50:GLN:HG3	2.16	0.46
2:2:65:THR:OG1	2:2:243:THR:HG23	2.16	0.46
2:2:190:ASN:O	2:2:191:LEU:C	2.57	0.46
1:1:45:VAL:O	1:1:46:LEU:CD2	2.62	0.46
1:1:271:TYR:HA	1:1:272:PRO:HD3	1.58	0.46
2:2:150:GLY:C	2:2:152:ARG:H	2.23	0.46
3:3:53:ILE:HD11	3:3:113:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:13:ALA:O	5:L:78:MET:HG2	2.15	0.46
5:L:14:PHE:CE2	5:L:107:LYS:HB3	2.51	0.46
6:H:34:VAL:O	6:H:50:GLN:HA	2.15	0.46
6:H:35:ASN:O	6:H:92:CYS:HA	2.15	0.46
6:H:39:GLN:CG	6:H:45:LEU:HD23	2.45	0.46
1:1:19:ALA:HB3	1:1:56:THR:CB	2.45	0.46
3:3:71:LEU:CD2	3:3:207:LEU:HD21	2.44	0.46
3:3:141:ASP:O	3:3:142:ARG:O	2.33	0.46
4:4:44:SER:C	4:4:45:LEU:HD23	2.32	0.46
5:L:17:GLU:O	5:L:77:ARG:HA	2.16	0.46
6:H:38:LYS:HD2	6:H:90:TYR:CE1	2.51	0.46
1:1:285:ASP:HB3	1:1:287:LYS:H	1.80	0.46
5:L:43:SER:O	5:L:45:LYS:CE	2.63	0.46
1:1:50:SER:C	1:1:51:ILE:HG23	2.41	0.46
1:1:168:TRP:CZ3	1:1:227:ARG:HG2	2.51	0.46
2:2:123:LEU:HD13	2:2:188:PHE:HE1	1.80	0.46
3:3:13:PHE:CD1	3:3:13:PHE:C	2.91	0.46
3:3:57:ASN:ND2	3:3:57:ASN:H	2.13	0.46
3:3:71:LEU:HB3	3:3:195:LEU:HD22	1.98	0.46
5:L:18:LYS:HD3	5:L:76:SER:HA	1.88	0.46
1:1:69:CYS:C	1:1:71:LEU:N	2.71	0.46
1:1:166:TYR:CD1	1:1:166:TYR:C	2.93	0.46
2:2:137:GLY:O	2:2:138:GLY:O	2.34	0.46
3:3:36:ILE:HG22	3:3:37:PRO:HD2	1.96	0.46
3:3:171:VAL:HG22	3:3:173:PHE:H	1.80	0.46
5:L:89:GLN:OE1	6:H:100(K):MET:HE1	2.15	0.46
5:L:103:LYS:HD3	5:L:103:LYS:C	2.41	0.46
1:1:127:GLU:HB3	1:1:246:ARG:HB3	1.97	0.46
1:1:147:VAL:HG13	1:1:178:PHE:O	2.15	0.46
2:2:108:VAL:O	2:2:109:HIS:C	2.56	0.46
2:2:135:HIS:CB	2:2:160:ASN:HD22	2.28	0.46
3:3:221:LEU:C	3:3:221:LEU:CD2	2.89	0.46
5:L:47:TRP:HA	5:L:47:TRP:CE3	2.50	0.46
5:L:91:ARG:CZ	6:H:100(J):ALA:HA	2.47	0.46
1:1:146:LEU:H	1:1:146:LEU:HG	1.43	0.45
2:2:17:THR:OG1	2:2:22:THR:HG23	2.16	0.45
2:2:69:LYS:HG2	2:2:78:TRP:CE2	2.50	0.45
2:2:114:ALA:HB2	2:2:238:LEU:CD2	2.46	0.45
1:1:186:PHE:CD1	3:3:24:ALA:CB	2.92	0.45
3:3:40:VAL:HG12	3:3:41:HIS:N	2.32	0.45
3:3:173:PHE:CD2	3:3:220:ARG:NH1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:49:TYR:HE1	5:L:55:ALA:HA	1.80	0.45
1:1:204:TYR:CZ	2:2:144:TYR:HA	2.51	0.45
1:1:265:SER:HB2	3:3:235:THR:O	2.16	0.45
1:1:34:LEU:HD23	3:3:161:ILE:HA	1.99	0.45
5:L:13:ALA:O	5:L:78:MET:CG	2.65	0.45
6:H:62:LYS:CG	6:H:63:PHE:CD1	2.99	0.45
1:1:136:GLN:OE1	1:1:237:THR:HG23	2.17	0.45
3:3:100:ILE:O	3:3:103:TYR:HB2	2.17	0.45
3:3:108:SER:HB2	3:3:173:PHE:HD1	1.80	0.45
1:1:74:ALA:HB3	3:3:15:THR:O	2.17	0.45
1:1:199:CYS:C	1:1:200:PHE:CD1	2.94	0.45
2:2:72:THR:C	2:2:74:GLY:N	2.72	0.45
2:2:169:VAL:HG23	2:2:170:LEU:N	2.32	0.45
5:L:19:VAL:O	5:L:74:THR:HA	2.17	0.45
6:H:4:LEU:HB2	6:H:102:TYR:HE2	1.81	0.45
6:H:38:LYS:CD	6:H:90:TYR:HE1	2.30	0.45
1:1:74:ALA:HB3	3:3:15:THR:CA	2.47	0.45
2:2:125:VAL:HG22	2:2:126:VAL:N	2.31	0.45
5:L:77:ARG:O	5:L:77:ARG:CD	2.64	0.45
1:1:193:LEU:CD1	1:1:193:LEU:N	2.39	0.45
2:2:132:LEU:HD21	2:2:173:MET:HE2	1.99	0.45
3:3:127:LEU:HA	3:3:192:GLN:HB2	1.99	0.45
5:L:82:ASP:O	5:L:104:LEU:HG	2.16	0.45
1:1:45:VAL:HG23	3:3:112:ARG:HD3	1.99	0.45
1:1:79:VAL:O	1:1:79:VAL:HG12	2.16	0.45
2:2:34:CYS:SG	2:2:201:ILE:HA	2.57	0.45
2:2:76:LYS:CG	2:2:169:VAL:CG1	2.94	0.45
3:3:70:PRO:HA	3:3:206:TYR:CD1	2.51	0.45
3:3:156:GLY:O	3:3:157:LEU:C	2.60	0.45
6:H:38:LYS:HD2	6:H:90:TYR:HE1	1.81	0.45
1:1:65:THR:C	3:3:42:ASN:HD21	2.25	0.45
1:1:264:THR:O	1:1:265:SER:CB	2.63	0.45
2:2:254:ILE:HG12	2:2:255:ARG:H	1.82	0.45
3:3:26:PRO:C	3:3:28:TYR:N	2.75	0.45
3:3:133:PRO:CB	3:3:134:PRO:CD	2.95	0.45
3:3:167:TRP:CD1	3:3:167:TRP:C	2.95	0.45
2:2:65:THR:O	2:2:66:LEU:O	2.34	0.44
2:2:108:VAL:O	2:2:110:VAL:N	2.50	0.44
2:2:226:ALA:HA	2:2:227:PRO:HD3	1.83	0.44
3:3:75:ARG:HB2	3:3:191:TYR:HE2	1.82	0.44
3:3:211:ILE:HG23	3:3:211:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:14:PHE:N	5:L:107:LYS:CG	2.80	0.44
5:L:62:PHE:CE1	5:L:75:ILE:CG1	3.00	0.44
6:H:6:GLN:H	6:H:105:GLN:NE2	2.11	0.44
6:H:33:TRP:CD2	6:H:52:TYR:HB2	2.51	0.44
6:H:97:ASN:O	6:H:99:PRO:CD	2.65	0.44
1:1:50:SER:O	1:1:51:ILE:HG23	2.17	0.44
1:1:129:THR:OG1	1:1:185:ARG:HD2	2.16	0.44
2:2:27:GLU:HG3	2:2:194:ASN:HA	1.99	0.44
2:2:33:VAL:HG22	2:2:200:VAL:CG2	2.47	0.44
3:3:175:TYR:HB2	3:3:182:THR:CG2	2.32	0.44
5:L:7:SER:HB2	5:L:22:THR:H	1.80	0.44
2:2:228:LEU:HD22	2:2:238:LEU:HB2	1.98	0.44
6:H:23:LYS:CD	6:H:77:THR:HG22	2.40	0.44
2:2:190:ASN:H	2:2:194:ASN:HB2	1.82	0.44
2:2:195:ASN:ND2	2:2:196:THR:N	2.58	0.44
1:1:279:ILE:HD12	1:1:279:ILE:HA	1.83	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
2:2:42:LEU:HD12	2:2:43:PRO:CD	2.43	0.44
2:2:122:LEU:HB2	2:2:189:ILE:HB	1.98	0.44
3:3:2:LEU:C	3:3:2:LEU:CD1	2.83	0.44
3:3:71:LEU:HD22	3:3:207:LEU:HD23	1.98	0.44
3:3:195:LEU:CD2	3:3:205:VAL:CG2	2.95	0.44
5:L:108:ARG:HG3	5:L:109:ALA:O	2.18	0.44
2:2:148:HIS:N	2:2:149:PRO:HD3	2.32	0.44
3:3:19:ARG:N	3:3:19:ARG:CD	2.64	0.44
5:L:39:LYS:HG2	5:L:84:ALA:HB2	1.99	0.44
6:H:69:LEU:HD23	6:H:69:LEU:HA	1.78	0.44
6:H:97:ASN:ND2	6:H:101:ASP:OD1	2.51	0.44
1:1:34:LEU:HD23	1:1:34:LEU:HA	1.81	0.44
1:1:35:THR:O	3:3:160:THR:HB	2.18	0.44
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.78	0.44
1:1:213:TYR:OH	2:2:131:GLN:HA	2.17	0.44
3:3:80:VAL:HG12	3:3:81:PHE:HD2	1.82	0.44
1:1:110:VAL:CG2	3:3:230:GLN:CG	2.95	0.44
1:1:166:TYR:C	1:1:168:TRP:N	2.76	0.44
1:1:178:PHE:HD2	1:1:184:SER:CB	2.24	0.44
1:1:208:ASP:O	1:1:211:THR:HG22	2.18	0.44
2:2:106:TYR:HD1	2:2:246:PRO:HA	1.83	0.44
5:L:75:ILE:C	5:L:77:ARG:N	2.66	0.44
6:H:41:PRO:C	6:H:43:GLN:N	2.76	0.44
1:1:209:ALA:HA	2:2:144:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:84:ASN:HA	3:3:186:PHE:HA	2.00	0.44
3:3:190:TRP:CD1	3:3:190:TRP:N	2.86	0.44
5:L:23:CYS:HB2	5:L:88:CYS:CB	2.48	0.44
6:H:98:TYR:C	6:H:100(I):TYR:N	2.74	0.44
1:1:85:LYS:C	1:1:232:HIS:HB3	2.43	0.43
1:1:195:SER:O	1:1:196:ALA:CB	2.65	0.43
1:1:232:HIS:O	1:1:233:ASP:O	2.35	0.43
5:L:18:LYS:HA	5:L:77:ARG:CA	2.45	0.43
6:H:22:CYS:CA	6:H:23:LYS:HE2	2.48	0.43
6:H:28:ALA:O	6:H:29:PHE:C	2.60	0.43
1:1:78:HIS:CA	1:1:109:LEU:CD1	2.95	0.43
1:1:135:SER:O	1:1:137:PRO:HD3	2.18	0.43
2:2:57:ASP:HB3	2:2:58:THR:H	1.59	0.43
2:2:199:ILE:HG22	2:2:201:ILE:HG13	2.00	0.43
3:3:205:VAL:C	3:3:206:TYR:CG	2.96	0.43
1:1:44:PRO:C	1:1:45:VAL:O	2.61	0.43
1:1:44:PRO:CD	4:4:54:GLU:OE2	2.66	0.43
2:2:84:ASP:C	2:2:86:LEU:N	2.76	0.43
3:3:75:ARG:O	3:3:194:SER:HB3	2.18	0.43
3:3:83:THR:CG2	3:3:187:LEU:CD2	2.93	0.43
3:3:175:TYR:HD2	3:3:182:THR:CG2	2.30	0.43
1:1:74:ALA:CB	3:3:15:THR:O	2.66	0.43
1:1:96:ALA:C	1:1:98:LEU:N	2.74	0.43
1:1:130:ILE:HB	1:1:178:PHE:HE2	1.82	0.43
2:2:207:VAL:CG1	2:2:208:PRO:HD2	2.36	0.43
3:3:153:TRP:CD1	3:3:154:ASP:N	2.87	0.43
3:3:188:SER:HB2	3:3:189:CYS:H	1.36	0.43
1:1:46:LEU:CB	1:1:47:PRO:CD	2.96	0.43
3:3:140:GLN:C	3:3:141:ASP:OD1	2.61	0.43
6:H:97:ASN:O	6:H:99:PRO:HD2	2.18	0.43
1:1:121:TYR:CE2	2:2:206:SER:HB3	2.53	0.43
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.43
5:L:7:SER:CB	5:L:22:THR:CB	2.96	0.43
6:H:7:SER:OG	6:H:8:GLY:N	2.51	0.43
6:H:75:SER:O	6:H:76:THR:C	2.61	0.43
2:2:71:TRP:NE1	2:2:228:LEU:HB2	2.30	0.43
2:2:94:GLN:O	2:2:95:ASN:C	2.61	0.43
3:3:47:ILE:CG2	3:3:100:ILE:HD13	2.49	0.43
5:L:89:GLN:HG3	5:L:98:PHE:CE2	2.51	0.43
5:L:107:LYS:CB	5:L:107:LYS:NZ	2.82	0.43
6:H:12:VAL:HG11	6:H:18:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:99:PRO:HD2	6:H:100(I):TYR:CE1	2.54	0.43
1:1:129:THR:OG1	1:1:185:ARG:HD3	2.18	0.43
1:1:209:ALA:N	2:2:261:PRO:HB3	2.30	0.43
1:1:281:LYS:CG	1:1:282:ARG:N	2.75	0.43
2:2:12:ARG:HH22	3:3:157:LEU:HG	1.83	0.43
5:L:35:TRP:HB2	5:L:48:ILE:HB	2.00	0.43
1:1:70:PHE:CD2	3:3:43:LEU:HD21	2.54	0.43
3:3:100:ILE:C	3:3:102:GLN:N	2.75	0.43
5:L:6:GLN:HG3	5:L:100:SER:C	2.30	0.43
6:H:12:VAL:HG11	6:H:18:VAL:CG1	2.40	0.43
6:H:52:TYR:CD1	6:H:52:TYR:C	2.96	0.43
1:1:53:THR:HB	1:1:54:ARG:H	1.70	0.43
1:1:129:THR:HG22	1:1:129:THR:O	2.17	0.43
1:1:254:ILE:HD13	2:2:204:ILE:HG21	2.01	0.43
2:2:124:VAL:O	2:2:186:HIS:HB2	2.19	0.43
2:2:247:MET:O	2:2:248:CYS:HB2	2.19	0.43
3:3:2:LEU:HD12	3:3:3:PRO:O	2.19	0.43
3:3:145:ALA:O	3:3:147:LEU:N	2.52	0.43
5:L:61:ARG:C	5:L:75:ILE:HA	2.44	0.43
6:H:62:LYS:HG3	6:H:63:PHE:CG	2.54	0.43
1:1:101:ASP:HA	1:1:225:ALA:HA	2.00	0.42
1:1:232:HIS:O	1:1:232:HIS:CG	2.71	0.42
5:L:3:VAL:H	5:L:26:THR:CG2	2.30	0.42
5:L:94:TYR:HE1	5:L:96:ILE:HG13	1.84	0.42
6:H:40:ARG:CB	6:H:41:PRO:HD2	2.48	0.42
1:1:77:VAL:O	1:1:78:HIS:HB2	2.19	0.42
1:1:95:GLU:C	6:H:98:TYR:OH	2.61	0.42
3:3:75:ARG:HB2	3:3:191:TYR:CE2	2.55	0.42
5:L:3:VAL:O	5:L:25:ALA:HA	2.19	0.42
6:H:49:GLY:O	6:H:50:GLN:HB3	2.18	0.42
1:1:159:ASN:HA	1:1:160:PRO:HD3	1.93	0.42
2:2:22:THR:HG22	2:2:23:ILE:H	1.83	0.42
3:3:54:PRO:HA	3:3:67:TYR:HD1	1.83	0.42
3:3:55:MET:SD	3:3:81:PHE:CD1	3.12	0.42
3:3:217:PHE:CE2	3:3:219:LEU:CD1	3.01	0.42
5:L:17:GLU:C	5:L:77:ARG:HA	2.45	0.42
5:L:38:GLN:HG2	5:L:44:PRO:HA	2.00	0.42
5:L:66:GLY:HA3	5:L:71:TYR:HA	2.01	0.42
5:L:89:GLN:CD	6:H:100(K):MET:HE1	2.43	0.42
6:H:17:SER:CB	6:H:82:LEU:O	2.64	0.42
6:H:91:PHE:CG	6:H:103:TRP:HZ3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:213:TYR:HB3	2:2:142:VAL:O	2.19	0.42
3:3:195:LEU:CD2	3:3:205:VAL:HG22	2.49	0.42
4:4:33:LYS:O	4:4:33:LYS:HG2	2.20	0.42
1:1:212:GLN:HE22	1:1:268:ARG:HE	1.66	0.42
2:2:82:LEU:C	2:2:84:ASP:N	2.76	0.42
2:2:215:HIS:HD2	2:2:216:ASN:H	1.68	0.42
3:3:13:PHE:O	3:3:13:PHE:CG	2.70	0.42
5:L:36:PHE:HE2	6:H:103:TRP:CE2	2.36	0.42
5:L:86:TYR:HE2	5:L:104:LEU:CB	2.33	0.42
1:1:282:ARG:NH2	3:3:83:THR:HB	2.33	0.42
1:1:287:LYS:CE	3:3:79:GLN:HB3	2.45	0.42
5:L:47:TRP:O	5:L:58:VAL:HG21	2.20	0.42
5:L:60:ALA:O	5:L:61:ARG:C	2.61	0.42
6:H:66:LYS:NZ	6:H:83:THR:HG22	2.35	0.42
1:1:165:ASP:HB2	1:1:168:TRP:CD1	2.55	0.42
1:1:194:ALA:HA	3:3:31:THR:HG21	2.02	0.42
1:1:269:THR:O	2:2:133:ALA:HB2	2.20	0.42
2:2:168:ASP:H	2:2:173:MET:HG3	1.85	0.42
2:2:170:LEU:O	2:2:170:LEU:CD1	2.66	0.42
2:2:189:ILE:HD13	2:2:189:ILE:HG21	1.79	0.42
6:H:74:SER:C	6:H:76:THR:H	2.28	0.42
1:1:165:ASP:HB2	1:1:168:TRP:HD1	1.84	0.42
1:1:226:PHE:CD1	1:1:226:PHE:N	2.88	0.42
2:2:27:GLU:C	2:2:28:ALA:O	2.60	0.42
2:2:81:LYS:HG3	2:2:219:SER:HB3	2.01	0.42
3:3:29:GLU:HA	3:3:30:PRO:HD3	1.54	0.42
6:H:99:PRO:CG	6:H:100(I):TYR:HE1	2.03	0.42
1:1:103:LYS:O	1:1:104:ILE:C	2.61	0.42
1:1:168:TRP:CH2	1:1:227:ARG:HB3	2.54	0.42
3:3:176:THR:OG1	3:3:177:ASP:N	2.52	0.42
1:1:136:GLN:HE21	1:1:136:GLN:HB2	1.61	0.42
2:2:55:LYS:C	2:2:57:ASP:H	2.27	0.42
2:2:256:SER:O	2:2:257:LYS:HB3	2.20	0.42
3:3:102:GLN:O	3:3:223:LYS:HE3	2.20	0.42
5:L:30:VAL:O	5:L:30:VAL:HG12	2.19	0.42
5:L:47:TRP:O	5:L:48:ILE:HD12	2.20	0.42
6:H:29:PHE:CD2	6:H:76:THR:HA	2.55	0.42
1:1:28:THR:HB	1:1:30:LYS:H	1.84	0.41
1:1:110:VAL:HG11	3:3:230:GLN:HB3	2.01	0.41
6:H:81:GLN:HG2	6:H:82:LEU:N	2.25	0.41
1:1:255:PRO:HG3	3:3:46:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:ARG:C	2:2:13:VAL:CG2	2.93	0.41
5:L:10:ILE:HG12	5:L:11:MET:N	2.35	0.41
6:H:35:ASN:HD21	6:H:95:SER:CB	2.19	0.41
6:H:70:THR:CG2	6:H:79:TYR:HB2	2.50	0.41
1:1:215:ILE:O	1:1:216:THR:C	2.64	0.41
2:2:217:ASN:O	2:2:218:VAL:CG1	2.61	0.41
3:3:197:LEU:HD23	3:3:197:LEU:HA	1.81	0.41
5:L:14:PHE:HD2	5:L:107:LYS:HD3	1.80	0.41
5:L:18:LYS:CD	5:L:76:SER:CA	2.81	0.41
6:H:14:PRO:HA	6:H:111:VAL:CG1	2.50	0.41
1:1:185:ARG:NH2	3:3:17:ASP:HB3	2.33	0.41
1:1:251:GLU:HB3	1:1:253:TRP:CZ3	2.55	0.41
1:1:285:ASP:HB3	1:1:287:LYS:N	2.35	0.41
2:2:44:ASP:C	2:2:46:ASP:N	2.77	0.41
3:3:14:LEU:CD1	3:3:14:LEU:C	2.94	0.41
3:3:54:PRO:C	3:3:56:ASN:N	2.76	0.41
4:4:59:LEU:HG	4:4:60:MET:H	1.79	0.41
5:L:12:SER:HA	5:L:105:GLU:C	2.45	0.41
1:1:136:GLN:O	1:1:138:ASP:N	2.53	0.41
1:1:268:ARG:HH11	1:1:268:ARG:CG	2.25	0.41
2:2:82:LEU:HB2	2:2:218:VAL:O	2.21	0.41
2:2:111:GLN:HA	2:2:196:THR:HG22	2.03	0.41
2:2:115:THR:C	2:2:117:PHE:H	2.28	0.41
2:2:181:LEU:HD12	2:2:181:LEU:HA	1.80	0.41
2:2:210:ASP:CG	2:2:211:SER:N	2.77	0.41
3:3:221:LEU:HD23	3:3:222:MET:N	2.36	0.41
6:H:91:PHE:CB	6:H:103:TRP:HZ3	2.33	0.41
1:1:285:ASP:CB	1:1:288:SER:H	2.33	0.41
2:2:26:GLN:O	2:2:27:GLU:OE1	2.38	0.41
2:2:171:TYR:O	2:2:174:ASN:N	2.54	0.41
2:2:183:ILE:HG13	3:3:96:LEU:CD2	2.48	0.41
5:L:95:PRO:O	5:L:96:ILE:O	2.38	0.41
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.41
2:2:12:ARG:HH22	3:3:157:LEU:CG	2.33	0.41
2:2:96:MET:O	2:2:96:MET:HG3	2.20	0.41
2:2:228:LEU:HD12	2:2:229:THR:H	1.85	0.41
3:3:43:LEU:O	3:3:47:ILE:HG23	2.20	0.41
3:3:125:ALA:HB2	3:3:195:LEU:CD1	2.51	0.41
5:L:16:GLY:O	5:L:77:ARG:CB	2.68	0.41
5:L:66:GLY:O	5:L:67:SER:CB	2.67	0.41
1:1:110:VAL:HA	1:1:113:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:TRP:O	1:1:227:ARG:NH1	2.41	0.41
1:1:195:SER:CB	3:3:34:ILE:HG12	2.51	0.41
1:1:202:ASP:OD1	1:1:202:ASP:C	2.64	0.41
1:1:253:TRP:CD1	3:3:36:ILE:CG1	3.03	0.41
1:1:253:TRP:CG	3:3:36:ILE:HD12	2.56	0.41
2:2:170:LEU:HA	2:2:170:LEU:HD22	1.77	0.41
2:2:228:LEU:CD2	2:2:238:LEU:HB2	2.51	0.41
5:L:46:LEU:CD2	6:H:101:ASP:HA	2.36	0.41
6:H:57:ASN:O	6:H:58:LYS:HG2	2.20	0.41
2:2:41:TYR:N	2:2:41:TYR:CD1	2.89	0.41
2:2:183:ILE:O	2:2:183:ILE:HG22	2.20	0.41
3:3:228:ILE:HD12	3:3:228:ILE:HA	1.79	0.41
5:L:48:ILE:HD11	5:L:54:LEU:CD1	2.41	0.41
6:H:38:LYS:CG	6:H:90:TYR:CE1	2.91	0.41
6:H:52:TYR:CD1	6:H:52(A):PRO:CD	2.88	0.41
6:H:100(I):TYR:C	6:H:100(J):ALA:O	2.62	0.41
1:1:267:GLY:C	1:1:268:ARG:HG2	2.46	0.40
2:2:63:PHE:CE1	2:2:245:ALA:CB	3.03	0.40
2:2:65:THR:OG1	2:2:243:THR:CG2	2.69	0.40
5:L:16:GLY:HA2	5:L:77:ARG:HB2	2.03	0.40
5:L:47:TRP:O	5:L:55:ALA:HB2	2.21	0.40
6:H:27:TYR:HD1	6:H:32:PHE:HE1	1.63	0.40
6:H:79:TYR:O	6:H:80:MET:HB3	2.21	0.40
1:1:31:VAL:HG12	1:1:31:VAL:O	2.20	0.40
1:1:257:ALA:HA	1:1:258:PRO:HD3	1.89	0.40
2:2:30:ASN:CG	4:4:58:ASP:HB2	2.40	0.40
3:3:53:ILE:HD13	3:3:53:ILE:HG21	1.84	0.40
3:3:115:LEU:HG	3:3:207:LEU:HD12	2.03	0.40
5:L:6:GLN:CG	5:L:100:SER:OG	2.69	0.40
5:L:61:ARG:NE	5:L:79:GLU:HG2	2.36	0.40
6:H:48:ILE:CG2	6:H:67:ALA:HB2	2.51	0.40
1:1:41:ALA:CB	4:4:60:MET:HE1	2.36	0.40
2:2:108:VAL:HA	2:2:243:THR:O	2.22	0.40
2:2:114:ALA:HB2	2:2:238:LEU:HD21	2.03	0.40
2:2:164:GLY:C	2:2:165:PRO:O	2.63	0.40
2:2:173:MET:O	2:2:174:ASN:HB3	2.21	0.40
1:1:136:GLN:N	1:1:137:PRO:CD	2.85	0.40
2:2:9:TYR:CD1	2:2:9:TYR:N	2.90	0.40
3:3:75:ARG:O	3:3:76:GLN:HB2	2.22	0.40
5:L:74:THR:HG22	5:L:75:ILE:N	2.37	0.40
5:L:86:TYR:HE2	5:L:104:LEU:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:2:GLY:HA3	6:H:27:TYR:HD2	1.85	0.40
6:H:4:LEU:HG	6:H:102:TYR:CE2	2.54	0.40
1:1:42:THR:HG23	3:3:50:ASP:CG	2.46	0.40
1:1:61:ASN:O	1:1:62:GLY:C	2.65	0.40
1:1:122:VAL:CG1	1:1:123:ARG:N	2.84	0.40
1:1:282:ARG:N	3:3:57:ASN:HB2	2.37	0.40
2:2:12:ARG:HD3	2:2:27:GLU:O	2.22	0.40
3:3:35:HIS:C	3:3:36:ILE:HG12	2.45	0.40
3:3:86:PHE:CD1	3:3:86:PHE:N	2.89	0.40
6:H:38:LYS:CE	6:H:85:GLU:O	2.69	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	271/289 (94%)	205 (76%)	44 (16%)	22 (8%)	1	11
2	2	253/262 (97%)	162 (64%)	56 (22%)	35 (14%)	0	3
3	3	234/236 (99%)	172 (74%)	38 (16%)	24 (10%)	0	7
4	4	38/68 (56%)	23 (60%)	11 (29%)	4 (10%)	0	7
5	L	108/110 (98%)	73 (68%)	19 (18%)	16 (15%)	0	3
6	H	117/119 (98%)	84 (72%)	23 (20%)	10 (8%)	0	11
All	All	1021/1084 (94%)	719 (70%)	191 (19%)	111 (11%)	0	7

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	27	HIS
1	1	45	VAL

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Mol	Chain	Res	Type
1	1	88	THR
1	1	142	TYR
1	1	195	SER
1	1	207	ASP
1	1	233	ASP
1	1	249	HIS
2	2	28	ALA
2	2	66	LEU
2	2	85	ALA
2	2	87	LYS
2	2	151	GLU
2	2	191	LEU
2	2	256	SER
3	3	27	ASN
3	3	43	LEU
3	3	58	THR
3	3	99	GLU
3	3	141	ASP
3	3	142	ARG
3	3	143	ARG
3	3	189	CYS
4	4	47	MET
4	4	50	SER
5	L	7	SER
5	L	10	ILE
5	L	55	ALA
5	L	63	SER
5	L	76	SER
5	L	96	ILE
6	H	2	GLY
6	H	80	MET
6	H	98	TYR
1	1	48	SER
1	1	196	ALA
2	2	13	VAL
2	2	19	GLY
2	2	57	ASP
2	2	90	GLY
2	2	95	ASN
2	2	138	GLY
2	2	160	ASN
2	2	172	ASN

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Mol	Chain	Res	Type
2	2	174	ASN
2	2	182	LEU
2	2	195	ASN
2	2	218	VAL
2	2	255	ARG
2	2	257	LYS
3	3	38	GLY
3	3	55	MET
3	3	90	GLY
3	3	91	VAL
3	3	146	MET
3	3	221	LEU
5	L	65	SER
5	L	77	ARG
5	L	83	ALA
6	H	9	ALA
6	H	29	PHE
6	H	30	SER
6	H	100(J)	ALA
1	1	62	GLY
1	1	70	PHE
1	1	71	LEU
2	2	45	VAL
2	2	109	HIS
2	2	112	CYS
2	2	149	PRO
2	2	231	PRO
3	3	83	THR
3	3	138	GLY
3	3	157	LEU
3	3	194	SER
3	3	217	PHE
4	4	43	GLN
5	L	46	LEU
5	L	67	SER
5	L	81	GLU
6	H	100(K)	MET
1	1	95	GLU
1	1	163	TRP
1	1	232	HIS
2	2	30	ASN
2	2	108	VAL

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Mol	Chain	Res	Type
2	2	186	HIS
3	3	121	ALA
4	4	66	ALA
5	L	50	SER
5	L	95	PRO
6	H	50	GLN
6	H	84	SER
1	1	139	SER
2	2	144	TYR
2	2	208	PRO
3	3	98	GLY
1	1	51	ILE
2	2	56	PRO
2	2	114	ALA
2	2	224	PRO
3	3	69	ILE
3	3	87	ILE
1	1	25	PRO
1	1	137	PRO
1	1	33	ILE
1	1	254	ILE
5	L	75	ILE
5	L	101	GLY
2	2	60	VAL
3	3	34	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	239/253 (94%)	143 (60%)	96 (40%)	0	0
2	2	223/229 (97%)	136 (61%)	87 (39%)	0	1
3	3	209/209 (100%)	140 (67%)	69 (33%)	0	2
4	4	33/57 (58%)	16 (48%)	17 (52%)	0	0
5	L	92/92 (100%)	52 (56%)	40 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	96/96 (100%)	57 (59%)	39 (41%)	0	0
All	All	892/936 (95%)	544 (61%)	348 (39%)	0	1

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	17	THR
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	35	THR
1	1	38	GLU
1	1	43	MET
1	1	45	VAL
1	1	46	LEU
1	1	50	SER
1	1	55	THR
1	1	56	THR
1	1	58	MET
1	1	59	HIS
1	1	61	ASN
1	1	67	VAL
1	1	71	LEU
1	1	77	VAL
1	1	79	VAL
1	1	82	ILE
1	1	85	LYS
1	1	88	THR
1	1	91	ASP
1	1	94	ARG
1	1	97	LYS
1	1	100	ASN
1	1	103	LYS
1	1	104	ILE
1	1	105	ASN
1	1	108	SER
1	1	116	LEU
1	1	118	LEU
1	1	119	PHE
1	1	126	SER
1	1	129	THR

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Mol	Chain	Res	Type
1	1	130	ILE
1	1	131	LEU
1	1	133	THR
1	1	136	GLN
1	1	139	SER
1	1	141	ASN
1	1	145	ASN
1	1	146	LEU
1	1	151	MET
1	1	152	TYR
1	1	153	VAL
1	1	159	ASN
1	1	161	LYS
1	1	163	TRP
1	1	166	TYR
1	1	167	THR
1	1	177	PHE
1	1	178	PHE
1	1	179	LYS
1	1	180	VAL
1	1	182	ASP
1	1	184	SER
1	1	185	ARG
1	1	186	PHE
1	1	187	SER
1	1	188	VAL
1	1	190	TYR
1	1	191	VAL
1	1	193	LEU
1	1	195	SER
1	1	199	CYS
1	1	200	PHE
1	1	207	ASP
1	1	210	GLU
1	1	212	GLN
1	1	215	ILE
1	1	216	THR
1	1	220	HIS
1	1	221	MET
1	1	226	PHE
1	1	229	VAL
1	1	230	ASN

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Mol	Chain	Res	Type
1	1	234	GLU
1	1	237	THR
1	1	241	ILE
1	1	242	ARG
1	1	243	VAL
1	1	245	HIS
1	1	250	VAL
1	1	256	ARG
1	1	261	LEU
1	1	265	SER
1	1	268	ARG
1	1	269	THR
1	1	273	LYS
1	1	275	THR
1	1	279	ILE
1	1	280	LYS
1	1	282	ARG
1	1	286	ILE
2	2	9	TYR
2	2	11	ASP
2	2	13	VAL
2	2	15	GLN
2	2	18	LEU
2	2	20	ASN
2	2	22	THR
2	2	27	GLU
2	2	32	VAL
2	2	34	CYS
2	2	40	GLU
2	2	45	VAL
2	2	49	ASP
2	2	50	VAL
2	2	52	LYS
2	2	60	VAL
2	2	63	PHE
2	2	65	THR
2	2	66	LEU
2	2	69	LYS
2	2	70	THR
2	2	72	THR
2	2	73	THR
2	2	75	SER

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Mol	Chain	Res	Type
2	2	76	LYS
2	2	79	CYS
2	2	81	LYS
2	2	82	LEU
2	2	84	ASP
2	2	88	ASP
2	2	91	VAL
2	2	96	MET
2	2	98	PHE
2	2	101	LEU
2	2	104	SER
2	2	108	VAL
2	2	110	VAL
2	2	119	SER
2	2	121	CYS
2	2	123	LEU
2	2	140	VAL
2	2	143	LYS
2	2	145	THR
2	2	147	THR
2	2	151	GLU
2	2	152	ARG
2	2	154	ILE
2	2	156	LEU
2	2	157	SER
2	2	158	SER
2	2	161	GLU
2	2	162	VAL
2	2	166	VAL
2	2	167	LYS
2	2	170	LEU
2	2	172	ASN
2	2	174	ASN
2	2	177	LEU
2	2	183	ILE
2	2	192	ARG
2	2	193	THR
2	2	194	ASN
2	2	195	ASN
2	2	198	THR
2	2	199	ILE
2	2	200	VAL

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Mol	Chain	Res	Type
2	2	207	VAL
2	2	212	MET
2	2	213	THR
2	2	217	ASN
2	2	218	VAL
2	2	221	MET
2	2	225	ILE
2	2	229	THR
2	2	232	THR
2	2	235	THR
2	2	237	SER
2	2	242	VAL
2	2	243	THR
2	2	247	MET
2	2	249	THR
2	2	254	ILE
2	2	255	ARG
2	2	257	LYS
2	2	259	ILE
2	2	260	VAL
2	2	262	GLN
3	3	2	LEU
3	3	10	SER
3	3	14	LEU
3	3	16	THR
3	3	17	ASP
3	3	19	ARG
3	3	21	SER
3	3	29	GLU
3	3	31	THR
3	3	36	ILE
3	3	42	ASN
3	3	44	LEU
3	3	48	GLN
3	3	50	ASP
3	3	51	THR
3	3	53	ILE
3	3	55	MET
3	3	57	ASN
3	3	60	THR
3	3	61	LYS
3	3	64	VAL

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Mol	Chain	Res	Type
3	3	71	LEU
3	3	84	ASN
3	3	91	VAL
3	3	93	LYS
3	3	94	THR
3	3	95	THR
3	3	99	GLU
3	3	100	ILE
3	3	101	VAL
3	3	102	GLN
3	3	105	THR
3	3	112	ARG
3	3	114	SER
3	3	126	LYS
3	3	127	LEU
3	3	128	ILE
3	3	129	LEU
3	3	132	THR
3	3	137	ARG
3	3	140	GLN
3	3	146	MET
3	3	151	VAL
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	161	ILE
3	3	163	MET
3	3	167	TRP
3	3	168	THR
3	3	171	VAL
3	3	172	GLN
3	3	180	THR
3	3	183	SER
3	3	187	LEU
3	3	188	SER
3	3	204	GLN
3	3	207	LEU
3	3	208	LEU
3	3	210	PHE
3	3	212	SER
3	3	214	CYS
3	3	220	ARG

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Mol	Chain	Res	Type
3	3	221	LEU
3	3	223	LYS
3	3	228	ILE
3	3	231	THR
3	3	232	VAL
3	3	234	LEU
4	4	29	ILE
4	4	30	ASN
4	4	34	ASP
4	4	38	THR
4	4	44	SER
4	4	45	LEU
4	4	47	MET
4	4	51	LYS
4	4	52	PHE
4	4	53	THR
4	4	54	GLU
4	4	56	VAL
4	4	59	LEU
4	4	60	MET
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN
5	L	1	GLN
5	L	4	LEU
5	L	6	GLN
5	L	7	SER
5	L	11	MET
5	L	18	LYS
5	L	19	VAL
5	L	20	THR
5	L	22	THR
5	L	23	CYS
5	L	24	SER
5	L	29	SER
5	L	30	VAL
5	L	33	MET
5	L	38	GLN
5	L	43	SER
5	L	45	LYS
5	L	46	LEU
5	L	47	TRP

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Mol	Chain	Res	Type
5	L	50	SER
5	L	51	SER
5	L	58	VAL
5	L	61	ARG
5	L	67	SER
5	L	69	THR
5	L	71	TYR
5	L	74	THR
5	L	77	ARG
5	L	78	MET
5	L	81	GLU
5	L	85	THR
5	L	90	GLN
5	L	91	ARG
5	L	94	TYR
5	L	97	THR
5	L	103	LYS
5	L	104	LEU
5	L	105	GLU
5	L	107	LYS
5	L	108	ARG
6	H	1	GLN
6	H	3	GLN
6	H	4	LEU
6	H	5	GLN
6	H	12	VAL
6	H	13	ARG
6	H	17	SER
6	H	18	VAL
6	H	20	ILE
6	H	21	SER
6	H	23	LYS
6	H	25	SER
6	H	31	SER
6	H	32	PHE
6	H	35	ASN
6	H	37	VAL
6	H	40	ARG
6	H	45	LEU
6	H	51	ILE
6	H	58	LYS
6	H	59	TYR

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Mol	Chain	Res	Type
6	H	64	LYS
6	H	73	LYS
6	H	74	SER
6	H	77	THR
6	H	80	MET
6	H	81	GLN
6	H	82	LEU
6	H	82(A)	TYR
6	H	82(B)	SER
6	H	82(C)	LEU
6	H	83	THR
6	H	84	SER
6	H	89	VAL
6	H	97	ASN
6	H	100(I)	TYR
6	H	100(K)	MET
6	H	109	VAL
6	H	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	29	GLN
1	1	59	HIS
1	1	84	ASN
1	1	100	ASN
1	1	145	ASN
1	1	173	ASN
1	1	212	GLN
1	1	235	HIS
1	1	274	ASN
2	2	14	GLN
2	2	15	GLN
2	2	30	ASN
2	2	95	ASN
2	2	111	GLN
2	2	118	HIS
2	2	131	GLN
2	2	174	ASN
2	2	186	HIS
2	2	187	GLN
2	2	195	ASN

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Mol	Chain	Res	Type
2	2	216	ASN
2	2	217	ASN
2	2	262	GLN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	65	ASN
3	3	77	ASN
3	3	102	GLN
3	3	106	HIS
3	3	192	GLN
5	L	34	HIS
5	L	38	GLN
5	L	90	GLN
6	H	5	GLN
6	H	6	GLN
6	H	35	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.