Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:49 PM GMT

PDB ID	:	1CN1
Title	:	CRYSTAL STRUCTURE OF DEMETALLIZED CONCANAVALIN A. THE METAL-BINDING REGION
Authors	:	Shoham, M.; Yonath, A.; Sussman, J.L.; Moult, J.; Traub, W.; Gilboa(Kalb), A.J.
Deposited on	:	1981-12-21
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

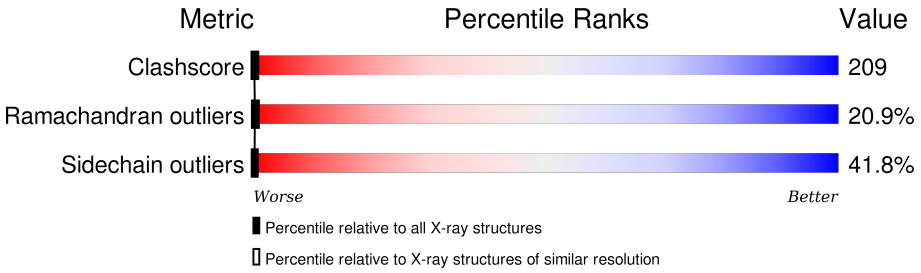
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	237	5% 31% 43% 21%
1	B	237	. 28% 44% 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3612 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1806	1139	300	365	2			
1	B	237	Total	C	N	O	S	0	0	0
			1806	1139	300	365	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	ALA	-	INSERTION	UNP P02866
A	?	-	ALA	DELETION	UNP P02866
B	186	ALA	-	INSERTION	UNP P02866
B	?	-	ALA	DELETION	UNP P02866

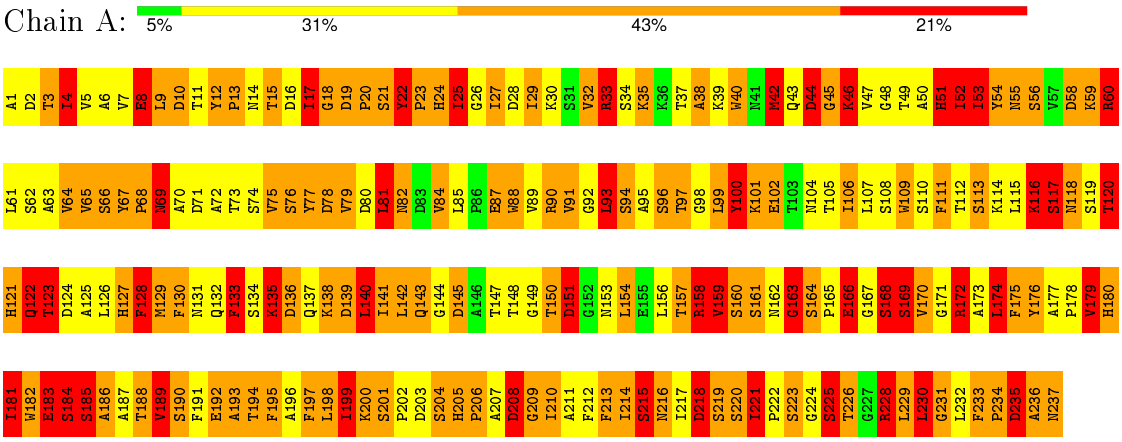
3 Residue-property plots (i)

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

Note EDS was not executed.

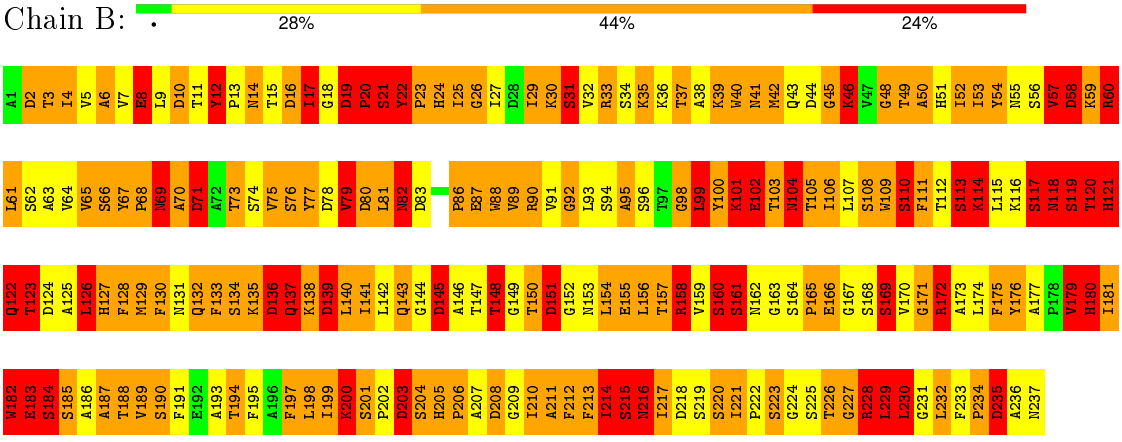
- Molecule 1: CONCANAVALIN A

Chain A:



- Molecule 1: CONCANAVALIN A

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.30Å 91.20Å 61.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3612	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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	A	2.22	56/1848 (3.0%)	2.21	91/2519 (3.6%)
1	B	2.16	45/1848 (2.4%)	2.31	102/2519 (4.0%)
All	All	2.19	101/3696 (2.7%)	2.26	193/5038 (3.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	TRP	NE1-CE2	-12.83	1.20	1.37
1	B	40	TRP	NE1-CE2	-11.25	1.23	1.37
1	A	20	PRO	N-CD	9.89	1.61	1.47
1	A	109	TRP	NE1-CE2	-9.69	1.25	1.37
1	A	87	GLU	CD-OE2	8.82	1.35	1.25
1	A	183	GLU	CD-OE1	-8.58	1.16	1.25
1	A	176	TYR	CE1-CZ	8.38	1.49	1.38
1	A	23	PRO	N-CD	7.88	1.58	1.47
1	A	56	SER	CA-CB	7.67	1.64	1.52
1	A	33	ARG	NE-CZ	7.60	1.43	1.33
1	B	206	PRO	N-CD	7.43	1.58	1.47
1	B	22	TYR	CE2-CZ	-7.42	1.28	1.38
1	B	163	GLY	CA-C	-7.35	1.40	1.51
1	A	24	HIS	CB-CG	7.33	1.63	1.50
1	A	178	PRO	N-CD	7.20	1.57	1.47
1	B	234	PRO	N-CD	7.20	1.57	1.47
1	B	133	PHE	CB-CG	7.17	1.63	1.51
1	B	197	PHE	CB-CG	7.17	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TRP	NE1-CE2	-6.95	1.28	1.37
1	A	24	HIS	C-O	6.90	1.36	1.23
1	A	228	ARG	C-O	6.90	1.36	1.23
1	B	121	HIS	C-O	6.90	1.36	1.23
1	B	144	GLY	N-CA	6.86	1.56	1.46
1	A	163	GLY	C-O	6.85	1.34	1.23
1	B	209	GLY	C-O	6.85	1.34	1.23
1	A	88	TRP	NE1-CE2	-6.65	1.28	1.37
1	B	223	SER	CB-OG	6.56	1.50	1.42
1	A	175	PHE	CE1-CZ	6.37	1.49	1.37
1	A	40	TRP	CB-CG	6.36	1.61	1.50
1	A	229	LEU	C-O	6.32	1.35	1.23
1	A	161	SER	CB-OG	6.31	1.50	1.42
1	A	195	PHE	CB-CG	6.27	1.62	1.51
1	B	190	SER	CA-CB	-6.21	1.43	1.52
1	A	90	ARG	CD-NE	6.19	1.56	1.46
1	B	175	PHE	CE1-CZ	6.19	1.49	1.37
1	B	110	SER	CB-OG	-6.16	1.34	1.42
1	B	24	HIS	CB-CG	6.12	1.61	1.50
1	B	230	LEU	C-O	6.12	1.34	1.23
1	A	81	LEU	N-CA	6.11	1.58	1.46
1	B	8	GLU	CD-OE2	6.10	1.32	1.25
1	B	48	GLY	CA-C	-6.02	1.42	1.51
1	B	33	ARG	NE-CZ	5.97	1.40	1.33
1	B	172	ARG	CZ-NH1	5.97	1.40	1.33
1	B	171	GLY	CA-C	5.96	1.61	1.51
1	A	111	PHE	CE1-CZ	-5.90	1.26	1.37
1	A	192	GLU	CD-OE2	-5.87	1.19	1.25
1	A	182	TRP	CB-CG	5.84	1.60	1.50
1	A	22	TYR	CD2-CE2	5.83	1.48	1.39
1	A	1	ALA	N-CA	5.79	1.57	1.46
1	A	109	TRP	CD1-NE1	5.77	1.47	1.38
1	A	231	GLY	CA-C	5.76	1.61	1.51
1	B	102	GLU	CD-OE1	5.75	1.31	1.25
1	A	130	PHE	CB-CG	5.72	1.61	1.51
1	A	24	HIS	CG-CD2	-5.65	1.26	1.35
1	A	113	SER	CB-OG	-5.59	1.34	1.42
1	B	50	ALA	C-N	-5.55	1.21	1.34
1	B	114	LYS	C-N	-5.55	1.21	1.34
1	A	233	PHE	CB-CG	5.54	1.60	1.51
1	A	8	GLU	C-O	5.54	1.33	1.23
1	A	21	SER	CB-OG	5.54	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	SER	C-O	5.54	1.33	1.23
1	B	23	PRO	N-CA	5.53	1.56	1.47
1	B	100	TYR	CE1-CZ	5.51	1.45	1.38
1	A	182	TRP	CE3-CZ3	5.48	1.47	1.38
1	A	140	LEU	N-CA	5.47	1.57	1.46
1	B	130	PHE	N-CA	5.47	1.57	1.46
1	B	168	SER	CA-CB	5.42	1.61	1.52
1	A	183	GLU	CD-OE2	5.41	1.31	1.25
1	A	51	HIS	CE1-NE2	5.38	1.45	1.32
1	A	24	HIS	C-N	-5.37	1.21	1.34
1	B	92	GLY	N-CA	5.35	1.54	1.46
1	B	121	HIS	ND1-CE1	5.34	1.48	1.34
1	A	4	ILE	C-O	5.34	1.33	1.23
1	A	100	TYR	N-CA	5.31	1.56	1.46
1	A	185	SER	CB-OG	-5.30	1.35	1.42
1	B	184	SER	CB-OG	-5.30	1.35	1.42
1	B	204	SER	CB-OG	-5.30	1.35	1.42
1	A	65	VAL	CA-CB	-5.30	1.43	1.54
1	B	148	THR	C-N	5.29	1.42	1.33
1	A	168	SER	CB-OG	5.28	1.49	1.42
1	B	108	SER	CB-OG	5.28	1.49	1.42
1	B	175	PHE	CG-CD1	-5.28	1.30	1.38
1	A	54	TYR	CE2-CZ	5.24	1.45	1.38
1	B	12	TYR	CG-CD1	-5.22	1.32	1.39
1	A	159	VAL	C-N	-5.19	1.22	1.34
1	A	182	TRP	NE1-CE2	-5.17	1.30	1.37
1	A	109	TRP	CD2-CE3	5.17	1.48	1.40
1	A	193	ALA	N-CA	5.15	1.56	1.46
1	B	230	LEU	N-CA	5.15	1.56	1.46
1	A	172	ARG	NE-CZ	5.14	1.39	1.33
1	A	228	ARG	NE-CZ	5.14	1.39	1.33
1	B	228	ARG	CZ-NH1	5.14	1.39	1.33
1	A	225	SER	C-O	5.14	1.33	1.23
1	A	67	TYR	C-N	5.12	1.44	1.34
1	B	166	GLU	CD-OE2	5.06	1.31	1.25
1	B	12	TYR	CE1-CZ	-5.05	1.31	1.38
1	B	100	TYR	CG-CD2	5.04	1.45	1.39
1	A	122	GLN	CD-OE1	5.02	1.34	1.24
1	B	103	THR	C-N	-5.01	1.22	1.34
1	A	197	PHE	CA-CB	-5.01	1.43	1.53
1	B	183	GLU	CA-CB	-5.01	1.43	1.53

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	B	57	VAL	C-N-CA	12.23	152.27	121.70
1	A	160	SER	C-N-CA	11.18	149.66	121.70
1	A	78	ASP	CB-CG-OD1	11.07	128.26	118.30
1	B	12	TYR	CB-CG-CD2	-10.75	114.55	121.00
1	B	136	ASP	CB-CG-OD1	10.56	127.81	118.30
1	A	33	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	117	SER	C-N-CA	10.37	147.61	121.70
1	B	118	ASN	C-N-CA	10.27	147.38	121.70
1	B	228	ARG	NE-CZ-NH1	-9.89	115.36	120.30
1	B	104	ASN	C-N-CA	9.84	146.29	121.70
1	A	203	ASP	C-N-CA	9.83	146.28	121.70
1	A	190	SER	C-N-CA	9.83	146.27	121.70
1	A	195	PHE	CB-CG-CD2	-9.71	114.00	120.80
1	A	17	ILE	C-N-CA	9.36	141.96	122.30
1	A	135	LYS	C-N-CA	9.35	145.07	121.70
1	B	203	ASP	CB-CG-OD2	9.33	126.70	118.30
1	A	68	PRO	C-N-CA	9.07	144.37	121.70
1	B	235	ASP	C-N-CA	8.96	144.11	121.70
1	A	88	TRP	CD1-CG-CD2	-8.76	99.30	106.30
1	B	60	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	12	TYR	CB-CG-CD1	8.56	126.14	121.00
1	B	80	ASP	C-N-CA	8.56	143.11	121.70
1	A	66	SER	C-N-CA	8.48	142.89	121.70
1	B	176	TYR	CB-CG-CD2	-8.44	115.94	121.00
1	B	21	SER	O-C-N	-8.39	109.27	122.70
1	A	60	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	58	ASP	C-N-CA	8.32	142.51	121.70
1	B	206	PRO	C-N-CA	8.05	141.83	121.70
1	B	26	GLY	C-N-CA	8.01	141.71	121.70
1	A	230	LEU	O-C-N	-7.94	109.70	123.20
1	B	33	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	128	PHE	CB-CG-CD2	-7.76	115.36	120.80
1	B	150	THR	O-C-N	-7.69	110.40	122.70
1	B	46	LYS	C-N-CA	7.63	140.79	121.70
1	B	145	ASP	CB-CG-OD1	7.62	125.15	118.30
1	A	88	TRP	CE2-CD2-CG	7.46	113.27	107.30
1	A	109	TRP	O-C-N	7.38	134.50	122.70
1	B	68	PRO	C-N-CA	7.36	140.11	121.70
1	B	20	PRO	C-N-CA	7.36	140.09	121.70
1	B	54	TYR	CB-CG-CD2	7.33	125.40	121.00
1	A	182	TRP	CG-CD2-CE3	-7.30	127.33	133.90
1	A	236	ALA	O-C-N	7.30	134.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	ASP	CB-CG-OD2	7.29	124.86	118.30
1	B	54	TYR	CB-CG-CD1	-7.21	116.68	121.00
1	A	221	ILE	O-C-N	7.14	134.67	121.10
1	B	2	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	109	TRP	NE1-CE2-CZ2	-7.06	122.64	130.40
1	B	17	ILE	O-C-N	-7.03	111.24	123.20
1	B	228	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	B	218	ASP	C-N-CA	7.01	139.23	121.70
1	B	148	THR	C-N-CA	-7.00	107.59	122.30
1	B	197	PHE	CB-CG-CD1	-7.00	115.90	120.80
1	B	182	TRP	C-N-CA	6.99	139.17	121.70
1	A	20	PRO	N-CD-CG	-6.98	92.72	103.20
1	A	174	LEU	C-N-CA	6.98	139.14	121.70
1	A	124	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	218	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	215	SER	C-N-CA	6.88	138.90	121.70
1	A	205	HIS	O-C-N	6.84	134.09	121.10
1	A	120	THR	O-C-N	6.81	133.60	122.70
1	A	206	PRO	N-CD-CG	-6.79	93.02	103.20
1	B	99	LEU	O-C-N	-6.79	111.84	122.70
1	A	184	SER	C-N-CA	6.78	138.66	121.70
1	B	79	VAL	O-C-N	-6.77	111.87	122.70
1	B	206	PRO	N-CD-CG	-6.76	93.06	103.20
1	B	133	PHE	CG-CD2-CE2	-6.72	113.41	120.80
1	A	178	PRO	N-CD-CG	-6.72	93.12	103.20
1	B	22	TYR	CB-CG-CD2	-6.66	117.01	121.00
1	A	88	TRP	CG-CD2-CE3	-6.65	127.91	133.90
1	B	96	SER	C-N-CA	6.62	138.26	121.70
1	B	33	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	B	82	ASN	O-C-N	6.61	133.27	122.70
1	A	151	ASP	C-N-CA	6.60	136.15	122.30
1	B	33	ARG	NH1-CZ-NH2	6.57	126.63	119.40
1	A	234	PRO	N-CD-CG	-6.56	93.36	103.20
1	A	235	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	208	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	124	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	102	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	B	155	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	B	22	TYR	CG-CD2-CE2	-6.42	116.16	121.30
1	A	175	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	B	169	SER	C-N-CA	6.40	137.70	121.70
1	A	195	PHE	CG-CD2-CE2	-6.39	113.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	VAL	O-C-N	6.38	132.90	122.70
1	A	55	ASN	C-N-CA	6.36	137.61	121.70
1	B	113	SER	O-C-N	6.33	132.83	122.70
1	B	212	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	A	38	ALA	O-C-N	6.27	132.73	122.70
1	B	23	PRO	O-C-N	6.26	132.71	122.70
1	A	151	ASP	CB-CG-OD1	6.23	123.90	118.30
1	B	101	LYS	O-C-N	6.22	132.66	122.70
1	A	209	GLY	C-N-CA	6.20	137.19	121.70
1	A	150	THR	C-N-CA	-6.18	106.26	121.70
1	A	145	ASP	O-C-N	-6.07	112.99	122.70
1	B	65	VAL	O-C-N	-6.06	113.00	122.70
1	A	44	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	139	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	175	PHE	CB-CG-CD2	-6.03	116.58	120.80
1	A	77	TYR	CB-CG-CD2	6.01	124.61	121.00
1	B	161	SER	N-CA-CB	-6.00	101.50	110.50
1	B	67	TYR	CB-CG-CD2	-5.99	117.40	121.00
1	A	168	SER	C-N-CA	-5.94	106.86	121.70
1	B	19	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	2	ASP	O-C-N	5.92	132.17	122.70
1	B	137	GLN	O-C-N	-5.92	113.23	122.70
1	A	24	HIS	C-N-CA	5.90	136.46	121.70
1	B	83	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	33	ARG	C-N-CA	5.87	136.37	121.70
1	B	213	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	A	229	LEU	C-N-CA	5.84	136.31	121.70
1	B	202	PRO	N-CD-CG	-5.84	94.44	103.20
1	B	172	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	86	PRO	N-CD-CG	-5.76	94.56	103.20
1	B	14	ASN	C-N-CA	5.73	136.02	121.70
1	A	97	THR	CA-C-N	5.69	127.58	116.20
1	B	20	PRO	O-C-N	5.68	131.80	122.70
1	A	8	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	B	89	VAL	O-C-N	5.66	131.76	122.70
1	A	23	PRO	N-CD-CG	-5.60	94.80	103.20
1	B	133	PHE	CD1-CE1-CZ	-5.58	113.41	120.10
1	B	139	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	203	ASP	CA-C-N	-5.55	104.99	117.20
1	B	78	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	136	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	213	PHE	C-N-CA	5.50	135.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	TRP	CD1-CG-CD2	-5.50	101.90	106.30
1	A	147	THR	C-N-CA	-5.49	107.97	121.70
1	A	228	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	88	TRP	CH2-CZ2-CE2	-5.48	111.92	117.40
1	B	58	ASP	OD1-CG-OD2	-5.47	112.90	123.30
1	B	165	PRO	C-N-CA	5.47	135.38	121.70
1	B	71	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	158	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	96	SER	C-N-CA	5.46	135.35	121.70
1	A	97	THR	O-C-N	-5.46	113.91	123.20
1	A	133	PHE	O-C-N	-5.45	113.98	122.70
1	A	223	SER	C-N-CA	5.45	133.74	122.30
1	B	228	ARG	CD-NE-CZ	5.43	131.20	123.60
1	A	220	SER	C-N-CA	-5.42	108.14	121.70
1	B	37	THR	C-N-CA	5.42	135.26	121.70
1	A	2	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	114	LYS	C-N-CA	5.40	135.20	121.70
1	B	111	PHE	CB-CG-CD2	5.36	124.55	120.80
1	A	77	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	84	VAL	C-N-CA	-5.36	108.31	121.70
1	B	176	TYR	CD1-CG-CD2	5.36	123.79	117.90
1	B	200	LYS	O-C-N	-5.35	114.14	122.70
1	B	120	THR	CA-C-N	-5.33	105.46	117.20
1	A	111	PHE	CD1-CE1-CZ	5.33	126.50	120.10
1	A	52	ILE	O-C-N	-5.29	114.24	122.70
1	B	70	ALA	O-C-N	5.29	131.16	122.70
1	B	158	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	161	SER	C-N-CA	5.28	134.91	121.70
1	A	169	SER	C-N-CA	5.28	134.91	121.70
1	B	124	ASP	OD1-CG-OD2	-5.27	113.28	123.30
1	B	214	ILE	O-C-N	5.27	131.14	122.70
1	A	128	PHE	O-C-N	-5.27	114.27	122.70
1	A	199	ILE	C-N-CA	5.26	134.85	121.70
1	A	166	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	228	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	93	LEU	O-C-N	5.23	131.07	122.70
1	B	128	PHE	CG-CD2-CE2	-5.23	115.05	120.80
1	A	46	LYS	O-C-N	5.22	131.05	122.70
1	A	68	PRO	N-CD-CG	-5.21	95.39	103.20
1	B	229	LEU	O-C-N	5.20	131.02	122.70
1	B	8	GLU	OE1-CD-OE2	-5.20	117.07	123.30
1	B	6	ALA	C-N-CA	5.19	134.67	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	TRP	CH2-CZ2-CE2	-5.18	112.22	117.40
1	A	158	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	94	SER	O-C-N	5.17	130.97	122.70
1	A	9	LEU	C-N-CA	5.17	134.62	121.70
1	B	160	SER	C-N-CA	5.16	134.61	121.70
1	A	109	TRP	CH2-CZ2-CE2	-5.16	112.24	117.40
1	B	223	SER	C-N-CA	-5.16	111.47	122.30
1	A	159	VAL	O-C-N	5.15	130.94	122.70
1	A	151	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	B	179	VAL	C-N-CA	-5.14	108.86	121.70
1	B	206	PRO	CA-C-N	-5.13	105.90	117.20
1	A	87	GLU	O-C-N	-5.11	114.53	122.70
1	A	109	TRP	NE1-CE2-CD2	5.10	112.40	107.30
1	B	107	LEU	O-C-N	-5.09	114.55	122.70
1	A	218	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	147	THR	CA-C-N	5.09	128.39	117.20
1	A	65	VAL	CA-CB-CG1	5.08	118.52	110.90
1	A	91	VAL	O-C-N	-5.08	114.57	123.20
1	B	184	SER	O-C-N	5.07	130.82	122.70
1	B	126	LEU	C-N-CA	-5.06	109.05	121.70
1	B	89	VAL	CA-CB-CG1	5.05	118.48	110.90
1	A	78	ASP	OD1-CG-OD2	-5.04	113.72	123.30
1	B	40	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	B	31	SER	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	57	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1735	794	5
1	B	1806	0	1740	721	23

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3612	0	3475	1483	23

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 209.

All (1483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:HIS:HB2	1:A:182:TRP:CZ3	1.17	1.69
1:A:180:HIS:CB	1:A:182:TRP:CZ3	1.95	1.46
1:A:222:PRO:CG	1:A:225:SER:HB3	1.43	1.45
1:A:115:LEU:HD22	1:A:180:HIS:NE2	1.39	1.35
1:A:222:PRO:HG2	1:A:225:SER:CB	1.53	1.35
1:B:6:ALA:CB	1:B:213:PHE:HA	1.57	1.33
1:A:180:HIS:HB2	1:A:182:TRP:CH2	1.65	1.32
1:A:29:ILE:HG12	1:A:35:LYS:CE	1.60	1.29
1:A:115:LEU:HD13	1:A:180:HIS:CE1	1.66	1.28
1:A:225:SER:HB2	1:A:231:GLY:CA	1.65	1.27
1:A:180:HIS:HB2	1:A:182:TRP:CE3	1.70	1.26
1:A:198:LEU:O	1:A:198:LEU:HD23	1.09	1.25
1:A:180:HIS:CB	1:A:182:TRP:CH2	2.17	1.23
1:B:88:TRP:CE2	1:B:182:TRP:HH2	1.61	1.19
1:B:6:ALA:HB2	1:B:213:PHE:HA	1.23	1.19
1:A:166:GLU:HG2	1:A:167:GLY:N	1.55	1.18
1:B:38:ALA:HB2	1:B:75:VAL:CG1	1.74	1.18
1:A:22:TYR:HB2	1:A:23:PRO:CD	1.76	1.16
1:B:22:TYR:HB2	1:B:23:PRO:CD	1.71	1.16
1:A:59:LYS:HE2	1:A:78:ASP:HB3	1.25	1.16
1:B:137:GLN:HB3	1:B:140:LEU:HB2	1.21	1.16
1:A:48:GLY:HA3	1:A:197:PHE:CE2	1.82	1.15
1:A:56:SER:HB2	1:A:188:THR:HA	1.20	1.15
1:A:29:ILE:CG1	1:A:35:LYS:HE3	1.76	1.15
1:A:45:GLY:H	1:A:200:LYS:HG3	1.06	1.14
1:B:88:TRP:CE2	1:B:182:TRP:CH2	2.35	1.14
1:B:141:ILE:O	1:B:173:ALA:HA	1.48	1.13
1:B:141:ILE:HG22	1:B:174:LEU:H	1.08	1.13
1:A:59:LYS:O	1:A:59:LYS:HG3	1.47	1.11
1:A:22:TYR:HE1	1:A:39:LYS:HA	1.07	1.10
1:A:106:ILE:HD13	1:A:154:LEU:HD13	1.18	1.10
1:A:53:ILE:HD12	1:A:53:ILE:N	1.64	1.10
1:B:91:VAL:HG23	1:B:214:ILE:HA	1.20	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HG2	1:B:131:ASN:HB3	1.15	1.10
1:B:210:ILE:HG22	1:B:211:ALA:H	1.15	1.10
1:B:4:ILE:HD12	1:B:4:ILE:C	1.70	1.09
1:B:22:TYR:HB2	1:B:23:PRO:HD2	1.12	1.09
1:B:32:VAL:HA	1:B:233:PHE:HE2	1.17	1.09
1:A:27:ILE:HG22	1:A:29:ILE:HD11	1.34	1.09
1:A:44:ASP:O	1:A:46:LYS:HD2	1.50	1.09
1:B:92:GLY:HA2	1:B:109:TRP:HH2	1.10	1.08
1:A:116:LYS:HD2	1:A:116:LYS:N	1.58	1.08
1:B:38:ALA:HB2	1:B:75:VAL:HG11	1.28	1.08
1:A:15:THR:HG22	1:A:21:SER:HA	1.18	1.08
1:B:207:ALA:HB1	1:B:208:ASP:HA	1.18	1.08
1:B:6:ALA:HB1	1:B:212:PHE:O	1.53	1.08
1:A:106:ILE:HD11	1:A:156:LEU:HG	1.31	1.08
1:B:38:ALA:CB	1:B:75:VAL:HG11	1.84	1.08
1:A:211:ALA:HB2	1:A:230:LEU:HD12	1.22	1.08
1:A:157:THR:OG1	1:A:169:SER:HB2	1.54	1.07
1:B:156:LEU:O	1:B:171:GLY:HA3	1.52	1.07
1:A:158:ARG:NH1	1:A:158:ARG:HG2	1.57	1.07
1:B:14:ASN:H	1:B:19:ASP:HB3	0.91	1.07
1:B:222:PRO:HG2	1:B:225:SER:OG	1.55	1.07
1:B:166:GLU:HG2	1:B:167:GLY:H	1.11	1.06
1:A:91:VAL:HG23	1:A:179:VAL:HG21	1.37	1.06
1:A:198:LEU:O	1:A:198:LEU:CD2	2.02	1.06
1:A:14:ASN:HB3	1:A:228:ARG:CZ	1.84	1.06
1:A:9:LEU:HD23	1:A:25:ILE:CG2	1.85	1.06
1:B:22:TYR:CB	1:B:23:PRO:HD2	1.84	1.06
1:A:9:LEU:HD23	1:A:25:ILE:HG22	1.39	1.05
1:B:207:ALA:CB	1:B:208:ASP:HA	1.80	1.05
1:A:174:LEU:N	1:A:174:LEU:HD23	1.67	1.05
1:B:92:GLY:HA2	1:B:109:TRP:CH2	1.91	1.04
1:B:14:ASN:N	1:B:19:ASP:HB3	1.73	1.04
1:B:137:GLN:HA	1:B:137:GLN:NE2	1.56	1.04
1:A:225:SER:CB	1:A:231:GLY:HA2	1.86	1.04
1:A:158:ARG:CG	1:A:158:ARG:HH11	1.69	1.04
1:A:51:HIS:C	1:A:52:ILE:HD13	1.76	1.04
1:B:9:LEU:HD22	1:B:25:ILE:HG22	1.40	1.03
1:B:56:SER:HB2	1:B:189:VAL:N	1.72	1.03
1:A:180:HIS:HD1	1:A:180:HIS:C	1.60	1.03
1:B:95:ALA:HB2	1:B:210:ILE:HG23	1.37	1.03
1:B:87:GLU:HG2	1:B:182:TRP:CD2	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD13	1:A:180:HIS:HE1	0.88	1.03
1:A:112:THR:HG23	1:A:127:HIS:HB2	1.07	1.03
1:B:88:TRP:CZ2	1:B:182:TRP:HH2	1.77	1.02
1:B:6:ALA:HB1	1:B:213:PHE:HA	1.41	1.02
1:B:141:ILE:HG22	1:B:174:LEU:N	1.74	1.02
1:A:115:LEU:CD1	1:A:180:HIS:HE1	1.72	1.02
1:B:137:GLN:HE21	1:B:137:GLN:CA	1.72	1.02
1:A:180:HIS:HB3	1:A:182:TRP:CH2	1.93	1.02
1:A:22:TYR:CB	1:A:23:PRO:HD2	1.84	1.01
1:B:173:ALA:C	1:B:174:LEU:HD23	1.80	1.01
1:B:7:VAL:HG22	1:B:212:PHE:HB3	1.42	1.01
1:A:4:ILE:HD12	1:A:232:LEU:HB3	1.40	1.01
1:B:56:SER:CB	1:B:188:THR:HA	1.90	1.01
1:B:121:HIS:C	1:B:122:GLN:HG3	1.79	1.01
1:A:92:GLY:HA3	1:A:174:LEU:HB3	1.37	1.01
1:A:52:ILE:HG12	1:A:193:ALA:HB3	1.40	1.00
1:A:87:GLU:CD	1:A:182:TRP:HB2	1.81	1.00
1:A:22:TYR:CE1	1:A:39:LYS:HA	1.97	1.00
1:B:159:VAL:HA	1:B:165:PRO:HA	1.41	1.00
1:B:53:ILE:HD11	1:B:62:SER:HB2	1.39	1.00
1:A:225:SER:CA	1:A:229:LEU:HB3	1.91	1.00
1:B:2:ASP:HA	1:B:216:ASN:HD21	1.25	1.00
1:A:54:TYR:HB3	1:A:191:PHE:CE2	1.96	1.00
1:B:61:LEU:HD22	1:B:81:LEU:HD13	1.43	1.00
1:B:158:ARG:HD3	1:B:166:GLU:OE2	1.60	1.00
1:B:226:THR:H	1:B:229:LEU:HD13	1.23	1.00
1:B:89:VAL:HG13	1:B:215:SER:O	1.63	0.99
1:B:4:ILE:O	1:B:4:ILE:HD12	1.63	0.99
1:A:115:LEU:C	1:A:116:LYS:HD2	1.83	0.98
1:A:122:GLN:HE22	1:B:132:GLN:HE22	1.04	0.98
1:A:67:TYR:O	1:A:70:ALA:HB3	1.62	0.98
1:A:115:LEU:CD1	1:A:180:HIS:CE1	2.46	0.97
1:A:106:ILE:HD13	1:A:154:LEU:CD1	1.93	0.97
1:A:106:ILE:HD11	1:A:156:LEU:CG	1.91	0.97
1:A:27:ILE:HG22	1:A:29:ILE:CD1	1.94	0.97
1:B:98:GLY:O	1:B:99:LEU:HD22	1.65	0.97
1:B:137:GLN:HA	1:B:137:GLN:HE21	0.80	0.97
1:A:29:ILE:HG12	1:A:35:LYS:HE3	0.98	0.97
1:B:7:VAL:CG2	1:B:212:PHE:HB3	1.94	0.97
1:A:56:SER:HB2	1:A:188:THR:CA	1.94	0.97
1:B:6:ALA:CB	1:B:213:PHE:CA	2.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:CD1	1:A:154:LEU:HD22	1.95	0.96
1:A:15:THR:CG2	1:A:21:SER:HA	1.94	0.96
1:A:66:SER:HA	1:A:72:ALA:HB2	1.46	0.96
1:A:225:SER:HB2	1:A:231:GLY:HA2	0.98	0.96
1:A:112:THR:CG2	1:A:127:HIS:HB2	1.93	0.96
1:A:172:ARG:HH11	1:A:232:LEU:HD22	1.29	0.96
1:A:115:LEU:CD2	1:A:180:HIS:NE2	2.29	0.96
1:A:137:GLN:HA	1:A:137:GLN:OE1	1.65	0.96
1:A:166:GLU:HG2	1:A:167:GLY:H	1.19	0.96
1:A:88:TRP:CD2	1:B:138:LYS:HD2	2.01	0.96
1:B:56:SER:HB3	1:B:188:THR:HA	1.46	0.95
1:B:23:PRO:HB2	1:B:40:TRP:HB3	1.45	0.95
1:A:122:GLN:HE22	1:B:132:GLN:NE2	1.65	0.95
1:A:91:VAL:CG2	1:A:179:VAL:HG21	1.96	0.95
1:A:62:SER:HB3	1:A:76:SER:HA	1.48	0.95
1:A:172:ARG:NH1	1:A:232:LEU:HD22	1.82	0.95
1:B:207:ALA:HB1	1:B:208:ASP:CA	1.97	0.95
1:A:42:MET:HG2	1:A:43:GLN:H	1.32	0.94
1:B:112:THR:HG23	1:B:127:HIS:HB2	1.48	0.94
1:B:101:LYS:HD2	1:B:101:LYS:N	1.80	0.94
1:A:112:THR:HG23	1:A:127:HIS:CB	1.96	0.94
1:A:116:LYS:HG2	1:A:117:SER:H	1.32	0.94
1:A:122:GLN:CG	1:B:131:ASN:HB3	1.97	0.94
1:B:180:HIS:CD2	1:B:182:TRP:CH2	2.54	0.94
1:A:50:ALA:HB3	1:A:195:PHE:CZ	2.03	0.94
1:B:180:HIS:CG	1:B:182:TRP:CZ3	2.56	0.94
1:A:17:ILE:HG13	1:A:17:ILE:O	1.65	0.94
1:A:115:LEU:HD12	1:A:189:VAL:HG22	1.49	0.94
1:B:137:GLN:CB	1:B:140:LEU:HB2	1.97	0.94
1:A:16:ASP:HB2	1:A:228:ARG:NH1	1.80	0.94
1:A:48:GLY:HA3	1:A:197:PHE:CZ	2.02	0.93
1:B:55:ASN:HB3	1:B:58:ASP:HB2	1.48	0.93
1:B:7:VAL:HG21	1:B:52:ILE:HD11	1.48	0.93
1:B:101:LYS:N	1:B:101:LYS:CD	2.29	0.93
1:B:225:SER:HA	1:B:229:LEU:HD22	1.49	0.93
1:B:9:LEU:HD13	1:B:40:TRP:CH2	2.04	0.93
1:A:11:THR:HG23	1:A:209:GLY:HA2	1.51	0.93
1:A:52:ILE:N	1:A:52:ILE:HD13	1.84	0.92
1:A:55:ASN:HB2	1:A:58:ASP:HB2	1.49	0.92
1:A:106:ILE:HB	1:A:154:LEU:HB3	1.48	0.92
1:A:87:GLU:O	1:A:182:TRP:HE3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:HA	1:B:211:ALA:CB	2.00	0.91
1:B:92:GLY:HA3	1:B:174:LEU:HA	1.52	0.91
1:A:45:GLY:N	1:A:200:LYS:HG3	1.84	0.91
1:B:58:ASP:C	1:B:59:LYS:HG3	1.88	0.91
1:A:174:LEU:CD2	1:A:174:LEU:N	2.34	0.91
1:B:74:SER:O	1:B:75:VAL:HG13	1.71	0.91
1:B:122:GLN:HE21	1:B:122:GLN:N	1.68	0.91
1:B:25:ILE:O	1:B:25:ILE:HD13	1.69	0.91
1:A:106:ILE:HD11	1:A:156:LEU:CD2	2.00	0.90
1:B:25:ILE:HD12	1:B:25:ILE:H	1.36	0.90
1:B:111:PHE:CD2	1:B:112:THR:N	2.40	0.90
1:A:211:ALA:HB2	1:A:230:LEU:CD1	2.00	0.90
1:A:56:SER:CB	1:A:188:THR:HA	2.00	0.90
1:B:137:GLN:HG3	1:B:140:LEU:HD22	1.53	0.90
1:A:13:PRO:HB3	1:A:21:SER:C	1.91	0.90
1:B:95:ALA:CB	1:B:210:ILE:HA	2.02	0.89
1:B:32:VAL:HG22	1:B:233:PHE:HD2	1.33	0.89
1:B:91:VAL:HG23	1:B:214:ILE:CA	2.03	0.89
1:B:32:VAL:HG22	1:B:233:PHE:CD2	2.08	0.89
1:A:13:PRO:HB3	1:A:22:TYR:HA	1.55	0.89
1:A:229:LEU:CD2	1:A:235:ASP:HA	2.03	0.89
1:A:229:LEU:HD21	1:A:235:ASP:HA	1.54	0.89
1:A:137:GLN:HG3	1:A:140:LEU:HB2	1.55	0.88
1:B:201:SER:CB	1:B:206:PRO:HB3	2.02	0.88
1:A:172:ARG:HD2	1:A:213:PHE:CZ	2.08	0.88
1:A:66:SER:HA	1:A:72:ALA:CB	2.04	0.88
1:B:38:ALA:CB	1:B:75:VAL:CG1	2.47	0.88
1:B:121:HIS:O	1:B:122:GLN:HG3	1.72	0.88
1:B:139:ASP:O	1:B:176:TYR:HB2	1.73	0.88
1:A:105:THR:HG21	1:A:198:LEU:HD22	1.53	0.88
1:A:88:TRP:CH2	1:A:182:TRP:CH2	2.61	0.88
1:B:4:ILE:CD1	1:B:4:ILE:C	2.41	0.88
1:A:91:VAL:HG23	1:A:179:VAL:CG2	2.04	0.88
1:A:92:GLY:CA	1:A:174:LEU:HB3	2.03	0.88
1:A:158:ARG:HG2	1:A:158:ARG:HH11	0.76	0.88
1:A:4:ILE:CD1	1:A:232:LEU:HB3	2.04	0.88
1:A:45:GLY:HA2	1:A:200:LYS:HD2	1.55	0.88
1:B:166:GLU:HG2	1:B:167:GLY:N	1.82	0.88
1:A:224:GLY:HA3	1:A:229:LEU:HD23	1.55	0.87
1:A:22:TYR:HB2	1:A:23:PRO:HD2	0.92	0.87
1:A:229:LEU:HD21	1:A:235:ASP:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASN:HB2	1:B:58:ASP:CB	2.04	0.87
1:B:141:ILE:HG21	1:B:174:LEU:HB2	1.54	0.87
1:A:32:VAL:HG22	1:A:233:PHE:CD2	2.09	0.87
1:B:32:VAL:HA	1:B:233:PHE:CE2	2.08	0.87
1:A:118:ASN:HA	1:A:185:SER:HB2	1.55	0.87
1:A:135:LYS:HA	1:A:148:THR:O	1.74	0.87
1:B:104:ASN:HB3	1:B:210:ILE:HD11	1.56	0.87
1:A:118:ASN:CA	1:A:185:SER:HB2	2.04	0.86
1:A:87:GLU:OE2	1:A:182:TRP:HB2	1.74	0.86
1:A:225:SER:N	1:A:229:LEU:HB3	1.89	0.86
1:A:13:PRO:HB3	1:A:22:TYR:N	1.89	0.86
1:A:225:SER:HA	1:A:229:LEU:O	1.75	0.86
1:A:143:GLN:C	1:A:143:GLN:NE2	2.28	0.86
1:A:58:ASP:O	1:A:59:LYS:HG2	1.76	0.86
1:B:111:PHE:HD2	1:B:112:THR:N	1.72	0.86
1:B:222:PRO:HG3	1:B:232:LEU:C	1.97	0.86
1:A:180:HIS:ND1	1:A:180:HIS:C	2.20	0.85
1:B:56:SER:CB	1:B:189:VAL:H	1.88	0.85
1:A:47:VAL:HA	1:A:198:LEU:HB2	1.59	0.85
1:B:18:GLY:O	1:B:20:PRO:HD3	1.75	0.85
1:A:108:SER:O	1:A:195:PHE:HA	1.75	0.85
1:B:122:GLN:O	1:B:123:THR:HB	1.75	0.85
1:A:13:PRO:HB3	1:A:22:TYR:CA	2.05	0.85
1:A:59:LYS:O	1:A:59:LYS:CG	2.24	0.85
1:B:103:THR:O	1:B:199:ILE:HG23	1.77	0.85
1:A:182:TRP:CD1	1:A:183:GLU:N	2.44	0.85
1:B:104:ASN:CB	1:B:210:ILE:HD11	2.07	0.85
1:B:56:SER:HB2	1:B:189:VAL:H	1.41	0.85
1:B:55:ASN:CB	1:B:58:ASP:HB2	2.06	0.85
1:A:222:PRO:HG3	1:A:225:SER:HB3	1.56	0.84
1:B:200:LYS:O	1:B:201:SER:HB3	1.76	0.84
1:A:137:GLN:HB3	1:A:140:LEU:H	1.42	0.84
1:B:22:TYR:CE1	1:B:39:LYS:HD3	2.12	0.84
1:A:88:TRP:CZ3	1:A:182:TRP:CH2	2.65	0.84
1:A:88:TRP:CD2	1:A:182:TRP:CZ3	2.66	0.84
1:A:231:GLY:C	1:A:232:LEU:HD23	1.97	0.84
1:B:117:SER:HB3	1:B:187:ALA:HB3	1.59	0.84
1:B:23:PRO:HG2	1:B:40:TRP:O	1.77	0.84
1:B:4:ILE:HG22	1:B:215:SER:HB3	1.59	0.84
1:B:5:VAL:HG11	1:B:81:LEU:HD11	1.57	0.84
1:B:87:GLU:HG3	1:B:182:TRP:CG	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HB3	1:B:131:ASN:HB2	1.59	0.83
1:A:93:LEU:HD22	1:A:212:PHE:CD1	2.13	0.83
1:B:127:HIS:C	1:B:127:HIS:ND1	2.31	0.83
1:B:148:THR:O	1:B:148:THR:HG22	1.76	0.83
1:A:32:VAL:HG22	1:A:233:PHE:CB	2.07	0.83
1:B:225:SER:HA	1:B:229:LEU:HB3	1.60	0.83
1:B:87:GLU:CG	1:B:182:TRP:CD2	2.60	0.83
1:B:205:HIS:N	1:B:206:PRO:CD	2.40	0.83
1:A:225:SER:CB	1:A:231:GLY:CA	2.51	0.83
1:B:55:ASN:HB2	1:B:58:ASP:HB3	1.60	0.83
1:A:64:VAL:HA	1:A:73:THR:O	1.78	0.83
1:B:2:ASP:HA	1:B:216:ASN:ND2	1.94	0.83
1:B:9:LEU:CD2	1:B:25:ILE:HG22	2.08	0.83
1:A:29:ILE:HG12	1:A:35:LYS:NZ	1.94	0.83
1:B:172:ARG:HH21	1:B:220:SER:C	1.82	0.83
1:B:179:VAL:HG12	1:B:180:HIS:H	1.43	0.83
1:A:28:ASP:C	1:A:29:ILE:HD13	1.99	0.83
1:A:126:LEU:HD11	1:A:175:PHE:HE1	1.42	0.82
1:A:105:THR:CG2	1:A:198:LEU:HD22	2.09	0.82
1:A:229:LEU:CG	1:A:235:ASP:HA	2.09	0.82
1:B:205:HIS:N	1:B:206:PRO:HD2	1.95	0.82
1:A:84:VAL:C	1:A:85:LEU:HD23	1.99	0.82
1:A:92:GLY:O	1:A:93:LEU:HD23	1.79	0.82
1:A:5:VAL:HG21	1:A:84:VAL:HG11	1.62	0.82
1:B:172:ARG:NH2	1:B:220:SER:C	2.32	0.82
1:B:137:GLN:CG	1:B:140:LEU:HD22	2.09	0.82
1:A:32:VAL:HA	1:A:233:PHE:CE2	2.14	0.82
1:A:45:GLY:HA3	1:A:200:LYS:CE	2.09	0.81
1:B:14:ASN:H	1:B:19:ASP:CB	1.85	0.81
1:A:45:GLY:HA3	1:A:200:LYS:HE3	1.61	0.81
1:B:210:ILE:HG22	1:B:211:ALA:N	1.92	0.81
1:A:234:PRO:O	1:A:235:ASP:HB3	1.78	0.81
1:B:22:TYR:CE1	1:B:39:LYS:CD	2.63	0.81
1:A:50:ALA:HB3	1:A:195:PHE:CE1	2.15	0.81
1:B:160:SER:HB3	1:B:164:SER:O	1.80	0.81
1:A:115:LEU:HD23	1:A:183:GLU:OE1	1.80	0.81
1:A:231:GLY:O	1:A:232:LEU:HD23	1.79	0.81
1:B:55:ASN:CB	1:B:58:ASP:CB	2.58	0.81
1:B:181:ILE:HG22	1:B:189:VAL:CG1	2.10	0.81
1:B:88:TRP:CZ2	1:B:182:TRP:CH2	2.63	0.81
1:B:9:LEU:HB3	1:B:40:TRP:CH2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:H	1:B:229:LEU:CD1	1.93	0.81
1:B:226:THR:N	1:B:229:LEU:HD13	1.96	0.80
1:B:103:THR:C	1:B:199:ILE:HG23	2.01	0.80
1:B:172:ARG:HD2	1:B:174:LEU:HD21	1.63	0.80
1:A:211:ALA:CB	1:A:230:LEU:HD12	2.07	0.80
1:B:225:SER:HA	1:B:229:LEU:CD2	2.12	0.80
1:B:235:ASP:CG	1:B:236:ALA:H	1.85	0.80
1:A:181:ILE:HG22	1:A:189:VAL:HG11	1.62	0.80
1:A:117:SER:OG	1:A:186:ALA:HA	1.81	0.80
1:B:95:ALA:HB2	1:B:210:ILE:CG2	2.10	0.80
1:B:9:LEU:HD13	1:B:40:TRP:HH2	1.43	0.80
1:A:139:ASP:O	1:A:176:TYR:HB2	1.80	0.80
1:B:88:TRP:CD2	1:B:182:TRP:CH2	2.69	0.80
1:A:119:SER:C	1:A:121:HIS:H	1.80	0.80
1:B:51:HIS:C	1:B:52:ILE:HG12	2.01	0.80
1:A:172:ARG:HH21	1:A:219:SER:HB3	1.45	0.80
1:A:66:SER:CA	1:A:72:ALA:HB2	2.11	0.80
1:A:16:ASP:HB2	1:A:228:ARG:HH12	1.47	0.79
1:B:8:GLU:HB2	1:B:211:ALA:HB2	1.63	0.79
1:B:137:GLN:NE2	1:B:137:GLN:CA	2.34	0.79
1:A:32:VAL:HG13	1:A:233:PHE:HD2	1.48	0.79
1:A:235:ASP:CG	1:A:236:ALA:N	2.35	0.79
1:B:6:ALA:HB1	1:B:213:PHE:CA	2.11	0.79
1:A:84:VAL:O	1:A:85:LEU:HD23	1.81	0.79
1:B:52:ILE:HG13	1:B:212:PHE:CD2	2.17	0.79
1:A:133:PHE:CE1	1:A:154:LEU:HB2	2.17	0.79
1:B:151:ASP:OD2	1:B:153:ASN:HB2	1.82	0.79
1:A:143:GLN:HB3	1:A:172:ARG:HB3	1.63	0.79
1:B:104:ASN:HB3	1:B:210:ILE:CD1	2.12	0.79
1:B:222:PRO:HG3	1:B:232:LEU:O	1.82	0.79
1:A:40:TRP:HA	1:A:73:THR:HG21	1.65	0.79
1:A:45:GLY:HA2	1:A:200:LYS:CD	2.12	0.79
1:B:210:ILE:CG2	1:B:211:ALA:H	1.93	0.79
1:B:91:VAL:CG2	1:B:214:ILE:HG23	2.12	0.79
1:A:53:ILE:CD1	1:A:53:ILE:N	2.43	0.79
1:B:136:ASP:OD1	1:B:136:ASP:O	2.00	0.78
1:A:88:TRP:CG	1:B:138:LYS:HD2	2.18	0.78
1:B:181:ILE:HG22	1:B:189:VAL:CG2	2.12	0.78
1:B:35:LYS:HD2	1:B:35:LYS:N	1.97	0.78
1:B:21:SER:HB3	1:B:22:TYR:CE2	2.17	0.78
1:A:88:TRP:CZ3	1:A:182:TRP:HH2	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:OD2	1:A:158:ARG:HD2	1.83	0.78
1:A:229:LEU:HD21	1:A:235:ASP:CA	2.12	0.78
1:B:127:HIS:C	1:B:127:HIS:HD1	1.87	0.78
1:B:56:SER:CB	1:B:189:VAL:N	2.44	0.78
1:B:95:ALA:HB1	1:B:210:ILE:HG12	1.65	0.78
1:A:74:SER:O	1:A:75:VAL:HG23	1.84	0.78
1:B:8:GLU:HA	1:B:211:ALA:HB2	1.63	0.78
1:A:115:LEU:HD12	1:A:189:VAL:CG2	2.13	0.78
1:A:229:LEU:HD21	1:A:235:ASP:HB2	1.66	0.78
1:B:228:ARG:O	1:B:230:LEU:N	2.17	0.78
1:A:116:LYS:HB3	1:A:123:THR:HA	1.66	0.77
1:A:56:SER:OG	1:A:189:VAL:HB	1.84	0.77
1:B:158:ARG:O	1:B:159:VAL:HG12	1.83	0.77
1:A:93:LEU:HD21	1:A:109:TRP:CE2	2.17	0.77
1:A:224:GLY:CA	1:A:229:LEU:HD23	2.15	0.77
1:A:118:ASN:HB3	1:A:185:SER:HB2	1.65	0.77
1:B:137:GLN:HB3	1:B:140:LEU:CB	2.10	0.77
1:B:231:GLY:O	1:B:232:LEU:HG	1.84	0.77
1:B:87:GLU:HG2	1:B:182:TRP:CE3	2.19	0.77
1:B:103:THR:C	1:B:105:THR:H	1.88	0.77
1:A:225:SER:HA	1:A:229:LEU:HB3	1.65	0.77
1:A:118:ASN:HB3	1:A:185:SER:CB	2.15	0.77
1:B:207:ALA:CB	1:B:208:ASP:CA	2.60	0.77
1:A:143:GLN:NE2	1:A:144:GLY:N	2.32	0.77
1:A:157:THR:OG1	1:A:169:SER:CB	2.32	0.77
1:A:42:MET:CG	1:A:43:GLN:H	1.97	0.77
1:A:14:ASN:O	1:A:17:ILE:HG23	1.85	0.76
1:A:17:ILE:CG2	1:A:228:ARG:HD3	2.15	0.76
1:A:92:GLY:C	1:A:93:LEU:HD23	2.06	0.76
1:B:94:SER:O	1:B:210:ILE:HG23	1.85	0.76
1:B:29:ILE:O	1:B:30:LYS:HG3	1.86	0.76
1:A:45:GLY:CA	1:A:200:LYS:CE	2.64	0.76
1:A:198:LEU:C	1:A:198:LEU:HD23	2.04	0.76
1:B:45:GLY:O	1:B:46:LYS:HD3	1.85	0.76
1:A:20:PRO:CG	1:A:24:HIS:CG	2.69	0.76
1:B:65:VAL:HG23	1:B:73:THR:HG23	1.68	0.76
1:A:127:HIS:C	1:A:127:HIS:ND1	2.39	0.76
1:B:102:GLU:OE1	1:B:199:ILE:HG21	1.86	0.76
1:B:10:ASP:HB2	1:B:24:HIS:O	1.85	0.76
1:A:61:LEU:HD12	1:A:62:SER:N	2.01	0.75
1:B:86:PRO:HG2	1:B:89:VAL:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:CD1	1:A:189:VAL:HG22	2.15	0.75
1:A:157:THR:HG1	1:A:169:SER:CB	1.98	0.75
1:B:62:SER:OG	1:B:76:SER:HB3	1.86	0.75
1:B:157:THR:HG23	1:B:158:ARG:N	2.01	0.75
1:A:137:GLN:CG	1:A:140:LEU:HB2	2.16	0.75
1:B:94:SER:HB3	1:B:172:ARG:HG2	1.66	0.75
1:B:118:ASN:HB2	1:B:120:THR:OG1	1.87	0.74
1:A:14:ASN:HB3	1:A:228:ARG:NE	2.02	0.74
1:B:42:MET:HE1	1:B:206:PRO:O	1.86	0.74
1:B:14:ASN:HB3	1:B:228:ARG:NH2	2.02	0.74
1:B:86:PRO:O	1:B:89:VAL:HG23	1.85	0.74
1:B:101:LYS:H	1:B:101:LYS:CD	1.99	0.74
1:A:166:GLU:CG	1:A:167:GLY:N	2.44	0.74
1:A:109:TRP:CZ3	1:A:140:LEU:HD11	2.23	0.74
1:A:174:LEU:H	1:A:174:LEU:HD23	1.51	0.74
1:B:2:ASP:OD2	1:B:219:SER:HA	1.87	0.74
1:A:118:ASN:CB	1:A:185:SER:HB2	2.18	0.74
1:A:64:VAL:HA	1:A:74:SER:HA	1.69	0.74
1:B:52:ILE:HD13	1:B:63:ALA:HB2	1.68	0.74
1:B:32:VAL:CA	1:B:233:PHE:HE2	1.97	0.74
1:A:142:LEU:N	1:A:142:LEU:HD23	2.03	0.74
1:B:95:ALA:HB1	1:B:210:ILE:HA	1.68	0.74
1:A:49:THR:HA	1:A:195:PHE:O	1.87	0.74
1:A:157:THR:HG23	1:A:158:ARG:O	1.87	0.73
1:A:16:ASP:C	1:A:18:GLY:H	1.91	0.73
1:B:204:SER:C	1:B:206:PRO:HD2	2.08	0.73
1:A:170:VAL:O	1:A:170:VAL:HG23	1.86	0.73
1:B:9:LEU:CA	1:B:40:TRP:HZ3	2.00	0.73
1:A:56:SER:HB2	1:A:189:VAL:N	2.03	0.73
1:A:97:THR:OG1	1:A:167:GLY:HA2	1.87	0.73
1:A:87:GLU:O	1:A:182:TRP:CE3	2.41	0.73
1:A:44:ASP:OD1	1:A:200:LYS:HG2	1.88	0.73
1:A:115:LEU:HD22	1:A:180:HIS:CE1	2.22	0.73
1:B:91:VAL:HG21	1:B:214:ILE:HG23	1.71	0.73
1:B:21:SER:HB3	1:B:22:TYR:CD2	2.23	0.73
1:B:65:VAL:HG23	1:B:73:THR:CG2	2.19	0.73
1:A:32:VAL:HG22	1:A:233:PHE:CG	2.23	0.73
1:A:180:HIS:HB2	1:A:182:TRP:CD2	2.23	0.73
1:B:174:LEU:CD2	1:B:213:PHE:HZ	2.02	0.73
1:A:20:PRO:HG3	1:A:24:HIS:CG	2.24	0.73
1:A:4:ILE:CD1	1:A:232:LEU:CB	2.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HG2	1:A:225:SER:HB3	0.75	0.73
1:B:25:ILE:N	1:B:25:ILE:CD1	2.51	0.73
1:A:87:GLU:CD	1:A:182:TRP:CB	2.56	0.72
1:A:145:ASP:OD1	1:A:169:SER:HA	1.90	0.72
1:B:61:LEU:CD2	1:B:81:LEU:HD13	2.17	0.72
1:A:182:TRP:HD1	1:A:183:GLU:H	1.33	0.72
1:A:55:ASN:HB2	1:A:58:ASP:CB	2.20	0.72
1:B:17:ILE:O	1:B:33:ARG:HG2	1.89	0.72
1:B:145:ASP:HB3	1:B:158:ARG:HG3	1.72	0.72
1:A:32:VAL:HA	1:A:233:PHE:CD2	2.25	0.72
1:B:25:ILE:H	1:B:25:ILE:CD1	2.02	0.72
1:B:53:ILE:O	1:B:53:ILE:HD12	1.88	0.72
1:A:180:HIS:CA	1:A:182:TRP:CZ3	2.71	0.72
1:A:225:SER:HB2	1:A:231:GLY:N	2.05	0.72
1:A:20:PRO:HG3	1:A:24:HIS:CB	2.19	0.72
1:B:230:LEU:HD13	1:B:230:LEU:O	1.89	0.72
1:A:137:GLN:C	1:A:139:ASP:H	1.88	0.71
1:B:174:LEU:N	1:B:174:LEU:HD23	2.03	0.71
1:B:17:ILE:HG22	1:B:237:ASN:OD1	1.89	0.71
1:A:106:ILE:HD12	1:A:154:LEU:HB3	1.73	0.71
1:B:56:SER:CB	1:B:188:THR:CA	2.66	0.71
1:B:145:ASP:OD2	1:B:169:SER:HB2	1.90	0.71
1:A:122:GLN:HG2	1:B:131:ASN:CB	2.08	0.71
1:B:26:GLY:HA3	1:B:34:SER:OG	1.91	0.71
1:A:116:LYS:HG2	1:A:117:SER:N	2.06	0.71
1:A:170:VAL:O	1:A:170:VAL:CG2	2.39	0.71
1:A:17:ILE:HA	1:A:33:ARG:CZ	2.21	0.71
1:B:7:VAL:HG21	1:B:52:ILE:CD1	2.20	0.71
1:B:58:ASP:O	1:B:59:LYS:HG3	1.89	0.71
1:B:143:GLN:NE2	1:B:221:ILE:HB	2.05	0.71
1:A:137:GLN:CB	1:A:140:LEU:HB2	2.20	0.70
1:A:52:ILE:C	1:A:53:ILE:HD12	2.11	0.70
1:A:54:TYR:HB3	1:A:191:PHE:CZ	2.25	0.70
1:B:100:TYR:O	1:B:167:GLY:HA3	1.91	0.70
1:A:10:ASP:CB	1:A:24:HIS:CE1	2.73	0.70
1:B:9:LEU:HB3	1:B:40:TRP:HH2	1.56	0.70
1:A:17:ILE:HD11	1:A:19:ASP:OD2	1.91	0.70
1:B:141:ILE:CG2	1:B:174:LEU:HB2	2.20	0.70
1:B:213:PHE:C	1:B:213:PHE:CD2	2.63	0.70
1:B:60:ARG:HG2	1:B:62:SER:OG	1.90	0.70
1:B:79:VAL:HG22	1:B:80:ASP:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLN:O	1:B:138:LYS:CB	2.39	0.70
1:A:157:THR:HG1	1:A:169:SER:HB2	1.53	0.70
1:B:52:ILE:HG13	1:B:212:PHE:HD2	1.57	0.70
1:B:87:GLU:CG	1:B:182:TRP:CG	2.75	0.70
1:B:35:LYS:HD2	1:B:35:LYS:H	1.54	0.70
1:A:52:ILE:O	1:A:53:ILE:HG13	1.91	0.70
1:B:93:LEU:O	1:B:213:PHE:HE1	1.75	0.70
1:B:71:ASP:N	1:B:71:ASP:OD2	2.25	0.70
1:A:180:HIS:CD2	1:A:182:TRP:CE2	2.79	0.70
1:B:180:HIS:CD2	1:B:182:TRP:CZ3	2.78	0.70
1:B:51:HIS:O	1:B:63:ALA:HB1	1.92	0.70
1:B:8:GLU:HA	1:B:211:ALA:CA	2.21	0.70
1:B:102:GLU:HG3	1:B:199:ILE:CG2	2.21	0.70
1:A:117:SER:HB3	1:A:187:ALA:N	2.07	0.69
1:A:21:SER:O	1:A:22:TYR:HB3	1.92	0.69
1:A:5:VAL:CG2	1:A:84:VAL:HG11	2.20	0.69
1:B:141:ILE:CG2	1:B:141:ILE:O	2.39	0.69
1:A:50:ALA:CB	1:A:195:PHE:CZ	2.75	0.69
1:B:146:ALA:CB	1:B:156:LEU:HA	2.22	0.69
1:A:118:ASN:HA	1:A:185:SER:CB	2.22	0.69
1:A:116:LYS:CG	1:A:117:SER:H	2.03	0.69
1:A:106:ILE:CD1	1:A:154:LEU:HD13	2.12	0.69
1:B:19:ASP:CG	1:B:24:HIS:HE1	1.95	0.69
1:A:59:LYS:HE2	1:A:78:ASP:CB	2.15	0.69
1:A:88:TRP:CH2	1:B:137:GLN:O	2.45	0.69
1:B:216:ASN:N	1:B:216:ASN:OD1	2.21	0.69
1:B:105:THR:HG22	1:B:105:THR:O	1.93	0.69
1:A:115:LEU:CD1	1:A:189:VAL:CG2	2.69	0.69
1:B:22:TYR:CB	1:B:23:PRO:CD	2.50	0.69
1:B:101:LYS:H	1:B:101:LYS:HD3	1.57	0.69
1:B:2:ASP:CA	1:B:216:ASN:HD21	2.02	0.69
1:B:145:ASP:OD2	1:B:169:SER:HA	1.92	0.69
1:B:180:HIS:ND1	1:B:182:TRP:CZ3	2.60	0.69
1:B:222:PRO:HG2	1:B:225:SER:HG	1.55	0.69
1:B:102:GLU:HG3	1:B:103:THR:N	2.08	0.69
1:A:62:SER:HB2	1:A:75:VAL:O	1.93	0.69
1:B:120:THR:O	1:B:122:GLN:HG3	1.93	0.69
1:A:122:GLN:HB3	1:B:131:ASN:CB	2.22	0.68
1:B:39:LYS:HG3	1:B:40:TRP:H	1.57	0.68
1:B:60:ARG:HG2	1:B:62:SER:HG	1.59	0.68
1:A:68:PRO:C	1:A:70:ALA:H	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:O	1:A:14:ASN:N	2.26	0.68
1:B:225:SER:OG	1:B:231:GLY:HA2	1.92	0.68
1:A:50:ALA:CB	1:A:195:PHE:CE1	2.77	0.68
1:B:180:HIS:ND1	1:B:182:TRP:CE3	2.62	0.68
1:B:44:ASP:O	1:B:46:LYS:HG2	1.92	0.68
1:A:181:ILE:HG22	1:A:189:VAL:CG1	2.24	0.68
1:A:229:LEU:HG	1:A:235:ASP:HA	1.75	0.68
1:B:179:VAL:HG12	1:B:180:HIS:N	2.08	0.68
1:A:12:TYR:CD2	1:A:14:ASN:ND2	2.62	0.68
1:B:91:VAL:HG22	1:B:92:GLY:H	1.59	0.68
1:B:225:SER:HA	1:B:229:LEU:CB	2.22	0.68
1:B:93:LEU:C	1:B:213:PHE:CE1	2.67	0.68
1:A:115:LEU:O	1:A:123:THR:HA	1.92	0.68
1:B:106:ILE:HD11	1:B:156:LEU:HD11	1.76	0.68
1:A:180:HIS:HB3	1:A:182:TRP:CZ3	2.15	0.68
1:A:166:GLU:CG	1:A:167:GLY:H	2.00	0.68
1:B:9:LEU:HA	1:B:40:TRP:HZ3	1.59	0.68
1:B:121:HIS:C	1:B:122:GLN:CG	2.59	0.68
1:A:180:HIS:CD2	1:A:182:TRP:CZ2	2.81	0.68
1:A:225:SER:CA	1:A:231:GLY:H	2.07	0.68
1:A:52:ILE:N	1:A:52:ILE:CD1	2.57	0.68
1:A:65:VAL:C	1:A:72:ALA:HB1	2.15	0.67
1:B:94:SER:HB3	1:B:172:ARG:CG	2.24	0.67
1:B:145:ASP:HB2	1:B:170:VAL:O	1.92	0.67
1:A:106:ILE:HD12	1:A:154:LEU:HD22	1.75	0.67
1:A:113:SER:HA	1:A:191:PHE:HA	1.76	0.67
1:B:45:GLY:C	1:B:46:LYS:HD3	2.14	0.67
1:A:180:HIS:C	1:A:181:ILE:HG13	2.13	0.67
1:A:66:SER:CA	1:A:72:ALA:CB	2.71	0.67
1:A:182:TRP:HD1	1:A:183:GLU:N	1.87	0.67
1:B:95:ALA:HB2	1:B:210:ILE:HA	1.76	0.67
1:A:162:ASN:CG	1:A:163:GLY:N	2.47	0.67
1:A:117:SER:HB3	1:A:186:ALA:C	2.14	0.67
1:A:32:VAL:HG13	1:A:233:PHE:CD2	2.30	0.67
1:A:106:ILE:CD1	1:A:154:LEU:HB3	2.25	0.67
1:A:52:ILE:CG2	1:A:61:LEU:HD11	2.25	0.67
1:A:140:LEU:HD12	1:A:174:LEU:O	1.95	0.67
1:A:93:LEU:CD2	1:A:212:PHE:CD1	2.78	0.67
1:A:106:ILE:CD1	1:A:154:LEU:CD2	2.73	0.67
1:A:172:ARG:CD	1:A:213:PHE:CZ	2.78	0.67
1:A:20:PRO:HG3	1:A:24:HIS:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG23	1:A:7:VAL:O	1.94	0.67
1:A:88:TRP:CZ2	1:A:182:TRP:CH2	2.83	0.66
1:B:112:THR:HG23	1:B:127:HIS:CB	2.24	0.66
1:A:115:LEU:CG	1:A:180:HIS:CE1	2.78	0.66
1:A:25:ILE:HG13	1:A:38:ALA:O	1.95	0.66
1:A:29:ILE:HG22	1:A:84:VAL:CG1	2.25	0.66
1:B:225:SER:HB2	1:B:231:GLY:H	1.60	0.66
1:B:174:LEU:HD21	1:B:213:PHE:HZ	1.61	0.66
1:B:6:ALA:HB2	1:B:213:PHE:CA	2.13	0.66
1:A:109:TRP:HH2	1:A:174:LEU:HA	1.60	0.66
1:B:115:LEU:HD21	1:B:183:GLU:HB3	1.76	0.66
1:B:198:LEU:O	1:B:198:LEU:HG	1.95	0.66
1:A:17:ILE:HG21	1:A:228:ARG:HD3	1.76	0.66
1:B:87:GLU:HG2	1:B:182:TRP:CE2	2.31	0.66
1:B:89:VAL:O	1:B:179:VAL:HB	1.95	0.66
1:B:225:SER:HB2	1:B:231:GLY:N	2.11	0.66
1:A:27:ILE:O	1:A:27:ILE:HG22	1.95	0.66
1:A:3:THR:C	1:A:4:ILE:HG22	2.16	0.66
1:B:23:PRO:CG	1:B:40:TRP:O	2.44	0.66
1:B:103:THR:H	1:B:199:ILE:HG22	1.59	0.66
1:B:103:THR:OG1	1:B:199:ILE:HA	1.94	0.66
1:B:237:ASN:N	1:B:237:ASN:HD22	1.92	0.66
1:B:40:TRP:HD1	1:B:41:ASN:H	1.42	0.66
1:B:158:ARG:HB2	1:B:169:SER:HB3	1.76	0.66
1:A:52:ILE:O	1:A:53:ILE:HG23	1.96	0.65
1:A:52:ILE:HG22	1:A:53:ILE:H	1.60	0.65
1:B:143:GLN:HE22	1:B:221:ILE:HB	1.60	0.65
1:B:221:ILE:HD12	1:B:222:PRO:HD2	1.78	0.65
1:A:119:SER:C	1:A:121:HIS:N	2.48	0.65
1:A:106:ILE:CD1	1:A:156:LEU:HG	2.19	0.65
1:A:180:HIS:HB2	1:A:182:TRP:CZ2	2.30	0.65
1:A:33:ARG:HH21	1:A:237:ASN:HB3	1.60	0.65
1:A:45:GLY:CA	1:A:200:LYS:CD	2.75	0.65
1:B:8:GLU:O	1:B:25:ILE:HA	1.96	0.65
1:B:201:SER:OG	1:B:206:PRO:HB3	1.97	0.65
1:A:134:SER:O	1:A:148:THR:HG22	1.97	0.65
1:B:180:HIS:CE1	1:B:182:TRP:CD2	2.84	0.65
1:B:145:ASP:OD2	1:B:158:ARG:HD2	1.97	0.65
1:A:65:VAL:O	1:A:72:ALA:HA	1.97	0.65
1:B:173:ALA:O	1:B:174:LEU:HD23	1.96	0.65
1:A:172:ARG:CZ	1:A:213:PHE:CE2	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:SER:O	1:B:75:VAL:HG22	1.97	0.65
1:B:8:GLU:CB	1:B:211:ALA:HB2	2.26	0.65
1:B:160:SER:HB3	1:B:164:SER:HB2	1.79	0.65
1:A:89:VAL:HG21	1:A:214:ILE:HG22	1.77	0.65
1:B:141:ILE:HG21	1:B:174:LEU:CB	2.27	0.65
1:B:225:SER:CA	1:B:229:LEU:HD22	2.25	0.65
1:A:53:ILE:O	1:A:53:ILE:HD13	1.97	0.64
1:B:137:GLN:CB	1:B:140:LEU:CB	2.73	0.64
1:B:88:TRP:CD2	1:B:182:TRP:HH2	2.10	0.64
1:B:48:GLY:O	1:B:197:PHE:CE1	2.50	0.64
1:B:154:LEU:HD22	1:B:155:GLU:N	2.12	0.64
1:A:106:ILE:HD12	1:A:154:LEU:C	2.18	0.64
1:A:137:GLN:O	1:A:139:ASP:N	2.30	0.64
1:B:224:GLY:O	1:B:229:LEU:HD22	1.98	0.64
1:B:226:THR:N	1:B:229:LEU:HB2	2.11	0.64
1:B:237:ASN:N	1:B:237:ASN:ND2	2.46	0.64
1:B:110:SER:HB3	1:B:194:THR:CG2	2.28	0.64
1:A:180:HIS:HD2	1:A:182:TRP:CZ2	2.16	0.64
1:A:88:TRP:CE2	1:B:138:LYS:HD2	2.33	0.64
1:A:17:ILE:C	1:A:19:ASP:H	1.99	0.64
1:A:6:ALA:HA	1:A:212:PHE:O	1.96	0.64
1:B:18:GLY:O	1:B:20:PRO:CD	2.44	0.64
1:A:135:LYS:HG3	1:A:149:GLY:HA3	1.79	0.64
1:A:29:ILE:N	1:A:35:LYS:HE3	2.12	0.64
1:B:193:ALA:O	1:B:194:THR:HB	1.98	0.64
1:A:127:HIS:ND1	1:A:128:PHE:N	2.45	0.64
1:A:95:ALA:HB2	1:A:210:ILE:HG23	1.80	0.64
1:A:133:PHE:CE2	1:A:154:LEU:HD12	2.32	0.64
1:B:7:VAL:O	1:B:212:PHE:N	2.30	0.64
1:B:22:TYR:HE1	1:B:39:LYS:HB2	1.61	0.64
1:B:110:SER:HB3	1:B:194:THR:HG22	1.79	0.64
1:A:60:ARG:HA	1:A:77:TYR:O	1.98	0.63
1:B:8:GLU:HA	1:B:211:ALA:HA	1.80	0.63
1:B:91:VAL:HG23	1:B:214:ILE:CG2	2.27	0.63
1:A:88:TRP:CE3	1:A:182:TRP:CZ3	2.86	0.63
1:A:93:LEU:HD21	1:A:109:TRP:CZ2	2.34	0.63
1:A:141:ILE:HG22	1:A:174:LEU:CD2	2.28	0.63
1:A:106:ILE:HD12	1:A:154:LEU:CB	2.29	0.63
1:B:122:GLN:NE2	1:B:122:GLN:N	2.45	0.63
1:A:159:VAL:HA	1:A:165:PRO:HA	1.80	0.63
1:A:89:VAL:HG23	1:A:215:SER:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASN:O	1:B:17:ILE:HG13	1.98	0.63
1:B:93:LEU:O	1:B:213:PHE:CE1	2.52	0.63
1:B:88:TRP:CZ3	1:B:180:HIS:HB2	2.34	0.63
1:B:91:VAL:CG2	1:B:214:ILE:CG2	2.77	0.63
1:A:26:GLY:C	1:A:27:ILE:HD12	2.19	0.63
1:A:122:GLN:O	1:A:123:THR:HG22	1.99	0.63
1:A:8:GLU:O	1:A:25:ILE:HG22	1.98	0.63
1:A:42:MET:CG	1:A:43:GLN:N	2.56	0.63
1:A:10:ASP:HB2	1:A:24:HIS:CE1	2.34	0.63
1:B:8:GLU:CA	1:B:211:ALA:HB2	2.29	0.63
1:A:93:LEU:HD21	1:A:109:TRP:NE1	2.13	0.62
1:B:63:ALA:C	1:B:64:VAL:HG12	2.20	0.62
1:B:55:ASN:O	1:B:59:LYS:HA	1.98	0.62
1:B:141:ILE:O	1:B:173:ALA:CA	2.36	0.62
1:A:128:PHE:CE2	1:A:175:PHE:CE1	2.86	0.62
1:A:23:PRO:HB2	1:A:40:TRP:O	2.00	0.62
1:A:87:GLU:CG	1:A:182:TRP:CB	2.77	0.62
1:A:20:PRO:HG2	1:A:24:HIS:CG	2.33	0.62
1:B:93:LEU:C	1:B:213:PHE:HE1	2.00	0.62
1:B:181:ILE:HG22	1:B:189:VAL:HG21	1.81	0.62
1:B:25:ILE:HD13	1:B:25:ILE:C	2.17	0.62
1:B:63:ALA:O	1:B:64:VAL:HG12	1.99	0.62
1:A:87:GLU:CG	1:A:182:TRP:HB3	2.29	0.62
1:A:56:SER:CB	1:A:189:VAL:N	2.63	0.62
1:A:141:ILE:CG2	1:A:141:ILE:O	2.48	0.62
1:A:172:ARG:NH1	1:A:213:PHE:CE1	2.68	0.62
1:A:17:ILE:O	1:A:33:ARG:HD3	2.00	0.62
1:B:29:ILE:C	1:B:30:LYS:HG3	2.19	0.62
1:A:18:GLY:O	1:A:19:ASP:O	2.17	0.62
1:B:74:SER:O	1:B:75:VAL:CG1	2.47	0.62
1:B:95:ALA:CB	1:B:210:ILE:HG12	2.28	0.62
1:A:137:GLN:HB3	1:A:139:ASP:OD2	1.99	0.62
1:A:89:VAL:O	1:A:179:VAL:HG23	1.99	0.62
1:B:51:HIS:O	1:B:63:ALA:CB	2.48	0.62
1:B:90:ARG:HG3	1:B:91:VAL:N	2.14	0.62
1:A:89:VAL:CG2	1:A:214:ILE:HG22	2.30	0.61
1:A:32:VAL:CG1	1:A:233:PHE:HD2	2.12	0.61
1:A:51:HIS:O	1:A:52:ILE:HD13	1.99	0.61
1:B:91:VAL:HG22	1:B:213:PHE:O	2.00	0.61
1:B:4:ILE:HG22	1:B:215:SER:CB	2.28	0.61
1:B:39:LYS:CG	1:B:40:TRP:N	2.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASN:N	1:B:82:ASN:OD1	2.33	0.61
1:B:45:GLY:C	1:B:46:LYS:HE2	2.21	0.61
1:B:6:ALA:HB1	1:B:212:PHE:C	2.19	0.61
1:B:157:THR:CG2	1:B:158:ARG:N	2.62	0.61
1:A:12:TYR:C	1:A:12:TYR:CD2	2.74	0.61
1:A:143:GLN:O	1:A:171:GLY:HA2	2.00	0.61
1:A:54:TYR:CB	1:A:191:PHE:CZ	2.83	0.61
1:A:13:PRO:CB	1:A:21:SER:C	2.68	0.61
1:B:187:ALA:O	1:B:188:THR:HG22	2.00	0.61
1:B:225:SER:CA	1:B:229:LEU:HB3	2.29	0.61
1:A:111:PHE:HB3	1:A:128:PHE:CZ	2.36	0.61
1:A:22:TYR:CB	1:A:23:PRO:CD	2.54	0.61
1:A:35:LYS:N	1:A:35:LYS:HD3	2.16	0.61
1:B:38:ALA:HB2	1:B:75:VAL:HG13	1.76	0.61
1:B:38:ALA:HB3	1:B:75:VAL:HG11	1.80	0.61
1:B:92:GLY:CA	1:B:174:LEU:HA	2.26	0.61
1:B:9:LEU:HD22	1:B:25:ILE:CG2	2.25	0.61
1:B:101:LYS:HB3	1:B:165:PRO:HB2	1.82	0.61
1:A:122:GLN:NE2	1:B:132:GLN:NE2	2.45	0.61
1:B:54:TYR:OH	1:B:81:LEU:HB3	2.01	0.61
1:B:120:THR:O	1:B:121:HIS:CD2	2.54	0.61
1:A:11:THR:HG23	1:A:209:GLY:CA	2.28	0.61
1:A:115:LEU:C	1:A:116:LYS:CD	2.66	0.60
1:B:188:THR:HG23	1:B:188:THR:O	2.01	0.60
1:B:9:LEU:CD1	1:B:40:TRP:CH2	2.83	0.60
1:A:180:HIS:CB	1:A:182:TRP:CE3	2.60	0.60
1:A:42:MET:O	1:A:43:GLN:HG2	2.00	0.60
1:B:122:GLN:HE21	1:B:122:GLN:H	1.47	0.60
1:B:205:HIS:O	1:B:206:PRO:C	2.38	0.60
1:A:62:SER:CB	1:A:76:SER:HA	2.28	0.60
1:B:143:GLN:N	1:B:172:ARG:O	2.34	0.60
1:B:184:SER:C	1:B:186:ALA:H	2.05	0.60
1:B:9:LEU:CD1	1:B:40:TRP:HH2	2.13	0.60
1:A:48:GLY:O	1:A:196:ALA:HA	1.99	0.60
1:B:120:THR:O	1:B:121:HIS:O	2.20	0.60
1:A:24:HIS:O	1:A:25:ILE:HG12	2.02	0.60
1:A:29:ILE:CG2	1:A:84:VAL:HG11	2.32	0.60
1:B:44:ASP:O	1:B:46:LYS:CE	2.50	0.60
1:A:101:LYS:O	1:A:102:GLU:HG2	2.01	0.60
1:A:13:PRO:CB	1:A:22:TYR:HA	2.30	0.60
1:B:79:VAL:CG2	1:B:80:ASP:N	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLY:O	1:A:212:PHE:CD1	2.55	0.60
1:B:53:ILE:CD1	1:B:62:SER:HB2	2.24	0.60
1:A:29:ILE:HD13	1:A:29:ILE:N	2.15	0.59
1:B:19:ASP:CG	1:B:24:HIS:CE1	2.75	0.59
1:B:94:SER:O	1:B:95:ALA:HB2	2.00	0.59
1:A:69:ASN:N	1:A:69:ASN:ND2	2.49	0.59
1:A:225:SER:O	1:A:231:GLY:N	2.35	0.59
1:A:61:LEU:HD12	1:A:62:SER:H	1.66	0.59
1:B:181:ILE:HG22	1:B:189:VAL:HG11	1.83	0.59
1:B:9:LEU:HB3	1:B:40:TRP:CZ3	2.37	0.59
1:A:173:ALA:C	1:A:174:LEU:CD2	2.71	0.59
1:A:27:ILE:O	1:A:29:ILE:CD1	2.51	0.59
1:A:29:ILE:O	1:A:30:LYS:HG3	2.02	0.59
1:A:29:ILE:CG1	1:A:35:LYS:CE	2.52	0.59
1:B:53:ILE:CD1	1:B:62:SER:O	2.51	0.59
1:A:169:SER:C	1:A:170:VAL:HG13	2.23	0.59
1:A:222:PRO:HG2	1:A:225:SER:OG	2.01	0.59
1:B:42:MET:CE	1:B:206:PRO:O	2.50	0.59
1:A:65:VAL:O	1:A:72:ALA:CA	2.51	0.59
1:B:180:HIS:CE1	1:B:182:TRP:CE3	2.90	0.59
1:B:95:ALA:HB2	1:B:210:ILE:CB	2.32	0.59
1:A:195:PHE:O	1:A:195:PHE:CD1	2.56	0.59
1:A:116:LYS:HB3	1:A:123:THR:CA	2.31	0.59
1:A:160:SER:HB3	1:A:164:SER:H	1.67	0.59
1:A:116:LYS:O	1:A:117:SER:CB	2.47	0.59
1:A:117:SER:HA	1:A:187:ALA:HB3	1.83	0.59
1:A:158:ARG:NH1	1:A:158:ARG:CG	2.41	0.59
1:A:93:LEU:HD22	1:A:212:PHE:HD1	1.64	0.59
1:A:10:ASP:HB3	1:A:24:HIS:CE1	2.38	0.59
1:B:180:HIS:ND1	1:B:180:HIS:C	2.56	0.59
1:B:100:TYR:C	1:B:101:LYS:HD2	2.23	0.59
1:A:235:ASP:OD1	1:A:236:ALA:N	2.36	0.59
1:A:29:ILE:H	1:A:35:LYS:CE	2.15	0.59
1:B:22:TYR:HE1	1:B:39:LYS:HD3	1.64	0.59
1:A:80:ASP:O	1:A:81:LEU:CB	2.49	0.59
1:A:117:SER:CB	1:A:187:ALA:N	2.65	0.59
1:A:143:GLN:CB	1:A:172:ARG:HB3	2.32	0.59
1:A:145:ASP:OD1	1:A:169:SER:HB3	2.03	0.59
1:A:27:ILE:O	1:A:29:ILE:HD13	2.03	0.59
1:B:172:ARG:HD3	1:B:213:PHE:CZ	2.38	0.59
1:A:33:ARG:HH21	1:A:237:ASN:CB	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:SER:HB2	1:B:37:THR:HG22	1.85	0.58
1:A:11:THR:N	1:A:208:ASP:O	2.32	0.58
1:B:13:PRO:HG3	1:B:22:TYR:HA	1.85	0.58
1:B:39:LYS:HG3	1:B:40:TRP:N	2.17	0.58
1:A:56:SER:HB3	1:A:187:ALA:O	2.03	0.58
1:A:29:ILE:HG22	1:A:84:VAL:HG13	1.86	0.58
1:B:40:TRP:CD1	1:B:41:ASN:N	2.72	0.58
1:B:74:SER:C	1:B:75:VAL:HG22	2.24	0.58
1:B:118:ASN:OD1	1:B:121:HIS:N	2.36	0.58
1:A:17:ILE:HG12	1:A:19:ASP:HB2	1.84	0.58
1:B:215:SER:HB2	1:B:216:ASN:OD1	2.03	0.58
1:A:107:LEU:HB2	1:A:196:ALA:O	2.03	0.58
1:A:115:LEU:CD2	1:A:180:HIS:CE1	2.85	0.58
1:A:12:TYR:C	1:A:12:TYR:HD2	2.05	0.58
1:A:172:ARG:NH1	1:A:213:PHE:CE2	2.71	0.58
1:B:92:GLY:CA	1:B:109:TRP:HH2	2.01	0.58
1:B:120:THR:HB	1:B:122:GLN:OE1	2.03	0.58
1:A:120:THR:C	1:A:121:HIS:CG	2.76	0.58
1:A:180:HIS:CB	1:A:182:TRP:CZ2	2.83	0.58
1:A:118:ASN:CB	1:A:185:SER:CB	2.80	0.58
1:A:52:ILE:O	1:A:53:ILE:CG1	2.51	0.58
1:B:162:ASN:O	1:B:162:ASN:CG	2.42	0.58
1:A:116:LYS:CG	1:A:117:SER:N	2.64	0.58
1:A:120:THR:O	1:A:120:THR:HG22	2.02	0.58
1:A:88:TRP:CE3	1:A:182:TRP:CH2	2.91	0.58
1:A:137:GLN:HB3	1:A:140:LEU:N	2.17	0.58
1:A:172:ARG:NH1	1:A:213:PHE:CZ	2.71	0.58
1:B:141:ILE:CG2	1:B:174:LEU:CB	2.81	0.58
1:B:87:GLU:CG	1:B:182:TRP:CE2	2.87	0.58
1:A:137:GLN:O	1:B:88:TRP:CH2	2.57	0.58
1:B:12:TYR:HB2	1:B:207:ALA:HB2	1.86	0.58
1:B:180:HIS:NE2	1:B:182:TRP:CZ2	2.72	0.57
1:A:133:PHE:CZ	1:A:154:LEU:HB2	2.38	0.57
1:B:128:PHE:CD2	1:B:175:PHE:CZ	2.92	0.57
1:B:180:HIS:NE2	1:B:182:TRP:CH2	2.72	0.57
1:B:8:GLU:CA	1:B:211:ALA:CB	2.79	0.57
1:B:201:SER:HB2	1:B:206:PRO:HB3	1.86	0.57
1:A:130:PHE:CE2	1:A:140:LEU:HD22	2.38	0.57
1:A:27:ILE:CG2	1:A:29:ILE:CD1	2.78	0.57
1:B:226:THR:H	1:B:229:LEU:HB2	1.69	0.57
1:B:234:PRO:O	1:B:235:ASP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:CB	1:B:40:TRP:CH2	2.87	0.57
1:A:88:TRP:CE2	1:A:182:TRP:CH2	2.92	0.57
1:A:106:ILE:HD11	1:A:156:LEU:HD21	1.83	0.57
1:A:106:ILE:HD13	1:A:154:LEU:CG	2.33	0.57
1:A:35:LYS:HB3	1:A:77:TYR:CZ	2.40	0.57
1:B:49:THR:CG2	1:B:51:HIS:CE1	2.87	0.57
1:B:44:ASP:O	1:B:46:LYS:CG	2.52	0.57
1:A:56:SER:HB2	1:A:189:VAL:H	1.69	0.57
1:A:145:ASP:OD1	1:A:169:SER:CA	2.52	0.57
1:A:17:ILE:HA	1:A:33:ARG:NH2	2.18	0.57
1:A:6:ALA:CB	1:A:212:PHE:O	2.52	0.57
1:B:141:ILE:HG23	1:B:141:ILE:O	2.03	0.57
1:B:7:VAL:HG11	1:B:52:ILE:CD1	2.34	0.57
1:B:63:ALA:C	1:B:64:VAL:CG1	2.72	0.57
1:A:109:TRP:HZ3	1:A:140:LEU:HD11	1.68	0.57
1:A:199:ILE:HD11	1:A:210:ILE:HD11	1.86	0.57
1:B:212:PHE:CD1	1:B:213:PHE:N	2.73	0.57
1:A:113:SER:HB3	1:A:191:PHE:HB3	1.86	0.57
1:A:6:ALA:CA	1:A:212:PHE:O	2.52	0.57
1:B:32:VAL:CA	1:B:233:PHE:CE2	2.81	0.57
1:B:110:SER:CB	1:B:194:THR:HG23	2.34	0.57
1:A:88:TRP:CG	1:B:138:LYS:CD	2.86	0.57
1:A:24:HIS:C	1:A:25:ILE:CG1	2.73	0.57
1:A:126:LEU:HD11	1:A:175:PHE:CE1	2.33	0.56
1:A:128:PHE:CE2	1:A:175:PHE:CD1	2.93	0.56
1:A:106:ILE:CB	1:A:154:LEU:HB3	2.31	0.56
1:A:141:ILE:O	1:A:174:LEU:HD23	2.05	0.56
1:A:32:VAL:CG2	1:A:233:PHE:CD2	2.86	0.56
1:A:32:VAL:CA	1:A:233:PHE:CD2	2.87	0.56
1:B:7:VAL:O	1:B:211:ALA:HB1	2.04	0.56
1:B:203:ASP:HB2	1:B:206:PRO:HD3	1.87	0.56
1:B:134:SER:O	1:B:148:THR:HG23	2.04	0.56
1:B:172:ARG:CD	1:B:174:LEU:HD21	2.35	0.56
1:A:177:ALA:HB2	1:B:177:ALA:HB2	1.87	0.56
1:A:95:ALA:HB1	1:A:104:ASN:ND2	2.20	0.56
1:A:132:GLN:HB3	1:B:183:GLU:OE2	2.04	0.56
1:A:91:VAL:HG22	1:A:214:ILE:HG23	1.87	0.56
1:B:172:ARG:HH21	1:B:221:ILE:N	2.03	0.56
1:B:52:ILE:CG1	1:B:212:PHE:HD2	2.18	0.56
1:B:217:ILE:HG23	1:B:217:ILE:O	2.06	0.56
1:B:117:SER:HB3	1:B:187:ALA:CB	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TRP:CG	1:B:183:GLU:N	2.73	0.56
1:B:3:THR:O	1:B:4:ILE:CG2	2.54	0.56
1:A:88:TRP:CE2	1:A:182:TRP:CZ3	2.94	0.56
1:A:28:ASP:O	1:A:29:ILE:HD13	2.05	0.56
1:A:5:VAL:HG12	1:A:5:VAL:O	2.05	0.56
1:B:31:SER:C	1:B:233:PHE:CE2	2.79	0.56
1:B:52:ILE:CD1	1:B:212:PHE:HD2	2.18	0.56
1:A:106:ILE:CD1	1:A:156:LEU:HD21	2.36	0.56
1:A:93:LEU:CD2	1:A:212:PHE:HD1	2.18	0.56
1:B:9:LEU:HA	1:B:40:TRP:CZ3	2.39	0.56
1:B:160:SER:HB3	1:B:164:SER:C	2.25	0.56
1:A:128:PHE:N	1:A:128:PHE:CD2	2.74	0.56
1:A:16:ASP:HB2	1:A:228:ARG:HH11	1.69	0.56
1:B:183:GLU:O	1:B:186:ALA:CB	2.54	0.56
1:B:30:LYS:O	1:B:31:SER:HB2	2.04	0.56
1:B:34:SER:HB2	1:B:37:THR:CG2	2.36	0.56
1:B:133:PHE:HB3	1:B:153:ASN:O	2.05	0.56
1:B:201:SER:CB	1:B:206:PRO:CB	2.82	0.56
1:A:91:VAL:HG13	1:A:212:PHE:CZ	2.41	0.56
1:B:222:PRO:HG3	1:B:232:LEU:N	2.21	0.56
1:A:133:PHE:CZ	1:A:154:LEU:HD12	2.41	0.55
1:A:224:GLY:C	1:A:226:THR:H	2.09	0.55
1:A:24:HIS:C	1:A:25:ILE:HG13	2.27	0.55
1:B:151:ASP:N	1:B:151:ASP:OD2	2.40	0.55
1:B:61:LEU:CD2	1:B:81:LEU:CD1	2.84	0.55
1:B:45:GLY:CA	1:B:46:LYS:HE2	2.37	0.55
1:A:111:PHE:HE2	1:A:179:VAL:HG11	1.71	0.55
1:B:212:PHE:CD1	1:B:212:PHE:C	2.70	0.55
1:A:139:ASP:OD2	1:A:140:LEU:N	2.39	0.55
1:A:3:THR:HG23	1:A:216:ASN:OD1	2.06	0.55
1:A:145:ASP:OD1	1:A:169:SER:CB	2.55	0.55
1:A:133:PHE:CD1	1:A:154:LEU:HB2	2.42	0.55
1:B:121:HIS:O	1:B:122:GLN:CG	2.52	0.55
1:B:65:VAL:CG2	1:B:73:THR:CG2	2.85	0.55
1:A:150:THR:OG1	1:A:153:ASN:HB2	2.07	0.55
1:A:222:PRO:HD2	1:A:231:GLY:O	2.06	0.55
1:A:29:ILE:C	1:A:30:LYS:HG3	2.26	0.55
1:B:217:ILE:CG2	1:B:217:ILE:O	2.55	0.55
1:B:9:LEU:CB	1:B:40:TRP:CZ3	2.90	0.55
1:B:233:PHE:CD1	1:B:233:PHE:N	2.74	0.55
1:B:34:SER:CB	1:B:37:THR:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:CB	1:B:75:VAL:HG13	2.34	0.54
1:B:9:LEU:HD22	1:B:40:TRP:CZ3	2.42	0.54
1:B:230:LEU:CD1	1:B:230:LEU:O	2.55	0.54
1:B:154:LEU:HD22	1:B:154:LEU:C	2.27	0.54
1:B:74:SER:OG	1:B:75:VAL:N	2.36	0.54
1:A:115:LEU:HB2	1:A:180:HIS:CE1	2.43	0.54
1:A:24:HIS:O	1:A:25:ILE:CG1	2.56	0.54
1:B:7:VAL:HG22	1:B:212:PHE:CB	2.29	0.54
1:A:58:ASP:O	1:A:59:LYS:CG	2.53	0.54
1:A:145:ASP:CB	1:A:169:SER:HB3	2.36	0.54
1:A:92:GLY:HA2	1:A:174:LEU:HA	1.90	0.54
1:A:27:ILE:N	1:A:27:ILE:CD1	2.71	0.54
1:B:181:ILE:CG2	1:B:189:VAL:CG2	2.84	0.54
1:B:189:VAL:CG1	1:B:189:VAL:O	2.54	0.54
1:B:65:VAL:CG2	1:B:73:THR:HG23	2.35	0.54
1:B:183:GLU:O	1:B:186:ALA:HB2	2.08	0.54
1:B:54:TYR:OH	1:B:81:LEU:CB	2.56	0.54
1:A:6:ALA:HB1	1:A:212:PHE:O	2.07	0.54
1:B:103:THR:O	1:B:105:THR:N	2.40	0.54
1:A:184:SER:O	1:A:186:ALA:N	2.41	0.54
1:A:166:GLU:OE1	1:A:168:SER:HB2	2.07	0.54
1:A:29:ILE:CG1	1:A:35:LYS:NZ	2.70	0.54
1:A:32:VAL:HG22	1:A:233:PHE:HB3	1.89	0.54
1:A:6:ALA:HB2	1:A:213:PHE:HB3	1.89	0.54
1:A:29:ILE:HG22	1:A:84:VAL:HG11	1.88	0.54
1:B:88:TRP:CH2	1:B:180:HIS:HD2	2.26	0.54
1:B:182:TRP:CD1	1:B:183:GLU:N	2.75	0.54
1:B:111:PHE:HE2	1:B:113:SER:HG	1.55	0.54
1:A:88:TRP:CZ2	1:A:182:TRP:CZ2	2.96	0.54
1:B:141:ILE:HG22	1:B:174:LEU:CA	2.37	0.54
1:B:88:TRP:NE1	1:B:182:TRP:CH2	2.72	0.54
1:B:95:ALA:CB	1:B:210:ILE:CG1	2.86	0.54
1:A:150:THR:HG1	1:A:153:ASN:HB2	1.73	0.54
1:A:56:SER:HB2	1:A:188:THR:C	2.27	0.53
1:A:27:ILE:N	1:A:27:ILE:HD12	2.23	0.53
1:A:91:VAL:O	1:A:174:LEU:HB2	2.08	0.53
1:B:19:ASP:OD1	1:B:24:HIS:CE1	2.60	0.53
1:A:87:GLU:CB	1:A:182:TRP:HB3	2.39	0.53
1:A:141:ILE:O	1:A:141:ILE:HG22	2.08	0.53
1:A:54:TYR:CB	1:A:191:PHE:CE2	2.84	0.53
1:A:199:ILE:CD1	1:A:210:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HA	1:B:127:HIS:HB2	1.90	0.53
1:B:214:ILE:O	1:B:215:SER:HB3	2.08	0.53
1:A:44:ASP:OD1	1:A:200:LYS:CG	2.57	0.53
1:B:160:SER:CB	1:B:164:SER:O	2.54	0.53
1:B:68:PRO:O	1:B:70:ALA:N	2.42	0.53
1:A:120:THR:CG2	1:A:122:GLN:NE2	2.71	0.53
1:A:10:ASP:OD1	1:A:19:ASP:OD2	2.26	0.53
1:A:213:PHE:CD1	1:A:232:LEU:HD13	2.42	0.53
1:A:105:THR:CG2	1:A:198:LEU:CD2	2.84	0.53
1:B:222:PRO:HG2	1:B:225:SER:CB	2.36	0.53
1:B:31:SER:O	1:B:233:PHE:CE2	2.62	0.53
1:A:14:ASN:HB3	1:A:228:ARG:NH1	2.21	0.53
1:B:92:GLY:HA3	1:B:173:ALA:O	2.08	0.53
1:A:7:VAL:CG2	1:A:7:VAL:O	2.57	0.53
1:A:88:TRP:CZ2	1:B:137:GLN:O	2.62	0.53
1:A:27:ILE:CG2	1:A:29:ILE:HD11	2.23	0.53
1:A:32:VAL:CB	1:A:233:PHE:HD2	2.22	0.53
1:B:52:ILE:HD13	1:B:63:ALA:CB	2.36	0.53
1:B:158:ARG:HB2	1:B:169:SER:CB	2.37	0.53
1:A:80:ASP:O	1:A:81:LEU:HB2	2.06	0.53
1:A:101:LYS:O	1:A:102:GLU:CB	2.57	0.53
1:A:106:ILE:HD12	1:A:154:LEU:O	2.09	0.53
1:A:172:ARG:HG3	1:A:213:PHE:HZ	1.73	0.53
1:A:225:SER:H	1:A:229:LEU:HB3	1.73	0.53
1:B:17:ILE:O	1:B:33:ARG:CG	2.57	0.53
1:B:174:LEU:HD22	1:B:213:PHE:HZ	1.73	0.53
1:B:101:LYS:O	1:B:102:GLU:HB3	2.09	0.53
1:A:87:GLU:HG2	1:A:182:TRP:CB	2.38	0.52
1:B:117:SER:CB	1:B:187:ALA:N	2.72	0.52
1:B:22:TYR:CD1	1:B:39:LYS:HD2	2.44	0.52
1:A:88:TRP:CD1	1:B:138:LYS:HD2	2.43	0.52
1:A:105:THR:HG22	1:A:198:LEU:CD2	2.39	0.52
1:A:172:ARG:NH1	1:A:213:PHE:CG	2.77	0.52
1:A:45:GLY:CA	1:A:200:LYS:HE3	2.32	0.52
1:A:20:PRO:CG	1:A:24:HIS:HB3	2.39	0.52
1:A:72:ALA:O	1:A:73:THR:CG2	2.57	0.52
1:A:17:ILE:CD1	1:A:19:ASP:OD2	2.58	0.52
1:B:221:ILE:O	1:B:221:ILE:CG2	2.57	0.52
1:B:8:GLU:O	1:B:8:GLU:HG2	2.03	0.52
1:A:172:ARG:NH1	1:A:213:PHE:CD1	2.78	0.52
1:B:222:PRO:HG3	1:B:232:LEU:CA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:OD2	1:B:169:SER:CB	2.57	0.52
1:B:142:LEU:HD11	1:B:148:THR:HB	1.91	0.52
1:B:56:SER:OG	1:B:188:THR:HA	2.09	0.52
1:B:230:LEU:HB3	1:B:232:LEU:HD12	1.91	0.52
1:A:107:LEU:HD23	1:A:153:ASN:OD1	2.08	0.52
1:A:49:THR:N	1:A:197:PHE:CE1	2.78	0.52
1:B:44:ASP:OD2	1:B:200:LYS:HA	2.10	0.52
1:A:180:HIS:HA	1:A:182:TRP:CZ3	2.43	0.52
1:A:115:LEU:HD11	1:A:189:VAL:HG21	1.92	0.52
1:B:95:ALA:CB	1:B:210:ILE:CA	2.84	0.52
1:A:162:ASN:OD1	1:A:163:GLY:N	2.43	0.52
1:A:120:THR:O	1:A:121:HIS:CG	2.63	0.52
1:A:106:ILE:CD1	1:A:154:LEU:CG	2.87	0.52
1:A:12:TYR:HB2	1:A:207:ALA:HA	1.92	0.52
1:B:121:HIS:O	1:B:121:HIS:CD2	2.63	0.52
1:A:215:SER:O	1:A:216:ASN:O	2.28	0.52
1:A:222:PRO:CG	1:A:225:SER:CB	2.38	0.52
1:B:14:ASN:C	1:B:16:ASP:H	2.13	0.52
1:A:137:GLN:O	1:A:138:LYS:HB2	2.09	0.51
1:A:142:LEU:CD2	1:A:142:LEU:N	2.72	0.51
1:A:12:TYR:HB3	1:A:14:ASN:HD21	1.75	0.51
1:A:172:ARG:NH2	1:A:219:SER:HB3	2.19	0.51
1:B:88:TRP:CH2	1:B:182:TRP:HH2	2.27	0.51
1:B:187:ALA:O	1:B:188:THR:HB	2.09	0.51
1:B:91:VAL:CG2	1:B:213:PHE:O	2.57	0.51
1:B:133:PHE:CD1	1:B:154:LEU:HB2	2.46	0.51
1:B:137:GLN:HB2	1:B:140:LEU:CD2	2.41	0.51
1:A:228:ARG:O	1:A:230:LEU:HD23	2.11	0.51
1:B:11:THR:N	1:B:208:ASP:O	2.36	0.51
1:B:91:VAL:HG23	1:B:214:ILE:HG23	1.90	0.51
1:B:3:THR:C	1:B:4:ILE:HG23	2.31	0.51
1:B:99:LEU:O	1:B:100:TYR:CG	2.63	0.51
1:A:120:THR:O	1:A:121:HIS:CD2	2.63	0.51
1:A:137:GLN:HB3	1:A:140:LEU:HB2	1.92	0.51
1:B:104:ASN:CA	1:B:210:ILE:HD11	2.40	0.51
1:B:145:ASP:OD2	1:B:158:ARG:HG3	2.11	0.51
1:A:172:ARG:HD2	1:A:213:PHE:CE1	2.44	0.51
1:A:9:LEU:CD2	1:A:25:ILE:CG2	2.75	0.51
1:B:193:ALA:O	1:B:194:THR:CB	2.58	0.51
1:B:174:LEU:HD22	1:B:213:PHE:CZ	2.46	0.51
1:B:87:GLU:OE2	1:B:182:TRP:CE2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:O	1:B:66:SER:HB3	2.10	0.51
1:A:180:HIS:HB2	1:A:182:TRP:CE2	2.46	0.51
1:A:20:PRO:O	1:A:22:TYR:N	2.43	0.51
1:A:4:ILE:HA	1:A:215:SER:HB3	1.92	0.51
1:B:143:GLN:CB	1:B:172:ARG:HB3	2.41	0.51
1:B:25:ILE:HD12	1:B:25:ILE:N	2.09	0.51
1:B:51:HIS:C	1:B:52:ILE:CG1	2.77	0.51
1:A:233:PHE:O	1:A:234:PRO:C	2.49	0.51
1:B:184:SER:C	1:B:186:ALA:N	2.64	0.51
1:B:29:ILE:O	1:B:30:LYS:CG	2.57	0.51
1:B:160:SER:CB	1:B:164:SER:HB2	2.39	0.51
1:A:180:HIS:C	1:A:181:ILE:CG1	2.77	0.51
1:A:143:GLN:HE22	1:A:144:GLY:CA	2.24	0.51
1:A:158:ARG:HD3	1:A:166:GLU:OE2	2.11	0.51
1:A:225:SER:CB	1:A:231:GLY:N	2.73	0.50
1:A:224:GLY:O	1:A:226:THR:N	2.44	0.50
1:B:172:ARG:HH21	1:B:220:SER:CA	2.24	0.50
1:B:128:PHE:CE2	1:B:175:PHE:CZ	2.98	0.50
1:B:231:GLY:C	1:B:232:LEU:HG	2.31	0.50
1:A:122:GLN:CG	1:B:131:ASN:CB	2.81	0.50
1:A:115:LEU:HD12	1:A:189:VAL:HG13	1.92	0.50
1:A:52:ILE:HG23	1:A:61:LEU:HD11	1.93	0.50
1:B:86:PRO:O	1:B:89:VAL:CG2	2.56	0.50
1:B:42:MET:HE1	1:B:206:PRO:HG2	1.93	0.50
1:A:127:HIS:CE1	1:A:129:MET:HG2	2.45	0.50
1:A:29:ILE:H	1:A:35:LYS:HE3	1.76	0.50
1:B:22:TYR:CE1	1:B:39:LYS:HD2	2.45	0.50
1:B:129:MET:HE2	1:B:131:ASN:OD1	2.11	0.50
1:A:101:LYS:O	1:A:102:GLU:HB3	2.10	0.50
1:A:8:GLU:HG3	1:A:10:ASP:H	1.75	0.50
1:B:49:THR:O	1:B:49:THR:HG22	2.11	0.50
1:A:100:TYR:N	1:A:100:TYR:CD2	2.79	0.50
1:B:11:THR:OG1	1:B:207:ALA:HA	2.11	0.50
1:B:117:SER:HB2	1:B:186:ALA:HA	1.93	0.50
1:B:9:LEU:CA	1:B:40:TRP:CZ3	2.89	0.50
1:A:106:ILE:CD1	1:A:154:LEU:CB	2.89	0.50
1:B:88:TRP:CE3	1:B:179:VAL:O	2.65	0.50
1:B:65:VAL:O	1:B:66:SER:CB	2.58	0.50
1:A:96:SER:O	1:A:96:SER:OG	2.28	0.50
1:B:54:TYR:HB2	1:B:191:PHE:CE2	2.47	0.50
1:B:110:SER:CB	1:B:194:THR:CG2	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:CD1	1:A:156:LEU:CD2	2.81	0.50
1:A:172:ARG:NH1	1:A:213:PHE:CD2	2.79	0.50
1:B:187:ALA:O	1:B:188:THR:CB	2.59	0.50
1:B:54:TYR:OH	1:B:80:ASP:O	2.30	0.50
1:A:48:GLY:CA	1:A:197:PHE:CZ	2.87	0.50
1:B:160:SER:OG	1:B:161:SER:N	2.44	0.50
1:A:122:GLN:O	1:A:123:THR:O	2.30	0.49
1:A:171:GLY:O	1:A:172:ARG:HB2	2.12	0.49
1:A:91:VAL:CG1	1:A:212:PHE:CZ	2.95	0.49
1:B:182:TRP:O	1:B:183:GLU:O	2.30	0.49
1:B:14:ASN:N	1:B:19:ASP:O	2.45	0.49
1:B:27:ILE:HD13	1:B:77:TYR:HB2	1.93	0.49
1:A:105:THR:HG22	1:A:198:LEU:HD22	1.92	0.49
1:A:122:GLN:NE2	1:B:132:GLN:OE1	2.45	0.49
1:A:29:ILE:HG12	1:A:35:LYS:HZ2	1.76	0.49
1:A:51:HIS:C	1:A:52:ILE:CD1	2.67	0.49
1:B:226:THR:O	1:B:228:ARG:C	2.51	0.49
1:A:184:SER:C	1:A:186:ALA:H	2.15	0.49
1:A:181:ILE:CG2	1:A:189:VAL:HG11	2.40	0.49
1:B:137:GLN:O	1:B:138:LYS:HB2	2.10	0.49
1:A:213:PHE:CD1	1:A:232:LEU:CD1	2.96	0.49
1:A:51:HIS:O	1:A:63:ALA:HB1	2.12	0.49
1:A:40:TRP:CA	1:A:73:THR:HG21	2.39	0.49
1:B:92:GLY:CA	1:B:109:TRP:CH2	2.82	0.49
1:B:32:VAL:CG2	1:B:233:PHE:HD2	2.15	0.49
1:B:22:TYR:CD1	1:B:39:LYS:CD	2.94	0.49
1:B:7:VAL:HG11	1:B:52:ILE:HD12	1.93	0.49
1:A:225:SER:C	1:A:229:LEU:HB3	2.31	0.49
1:B:126:LEU:HD23	1:B:179:VAL:HG13	1.94	0.49
1:B:143:GLN:HB2	1:B:172:ARG:HB3	1.92	0.49
1:A:42:MET:HG2	1:A:43:GLN:N	2.06	0.49
1:B:102:GLU:CG	1:B:103:THR:N	2.74	0.49
1:A:117:SER:OG	1:A:187:ALA:N	2.45	0.49
1:A:221:ILE:HG13	1:A:222:PRO:HD2	1.95	0.49
1:A:29:ILE:CB	1:A:35:LYS:HE3	2.42	0.49
1:B:180:HIS:CE1	1:B:182:TRP:CZ3	3.00	0.49
1:B:116:LYS:HB2	1:B:188:THR:CG2	2.42	0.49
1:A:55:ASN:HD22	1:A:58:ASP:CG	2.16	0.49
1:A:29:ILE:H	1:A:35:LYS:HE2	1.76	0.49
1:B:111:PHE:O	1:B:112:THR:OG1	2.29	0.49
1:B:56:SER:OG	1:B:188:THR:CA	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:O	1:A:5:VAL:HG23	2.12	0.49
1:A:93:LEU:CD2	1:A:212:PHE:CE1	2.96	0.49
1:B:191:PHE:C	1:B:191:PHE:CD1	2.85	0.49
1:B:93:LEU:HD23	1:B:212:PHE:HA	1.95	0.49
1:B:29:ILE:C	1:B:30:LYS:CG	2.78	0.49
1:A:32:VAL:CB	1:A:233:PHE:CD2	2.95	0.49
1:B:12:TYR:C	1:B:12:TYR:CD2	2.86	0.49
1:B:95:ALA:HB2	1:B:210:ILE:CA	2.41	0.49
1:A:128:PHE:CD2	1:A:175:PHE:CE1	3.01	0.49
1:A:137:GLN:C	1:A:139:ASP:N	2.64	0.48
1:A:4:ILE:HD11	1:A:232:LEU:CB	2.43	0.48
1:A:89:VAL:HG22	1:A:215:SER:H	1.77	0.48
1:B:53:ILE:O	1:B:53:ILE:CD1	2.60	0.48
1:B:81:LEU:C	1:B:82:ASN:OD1	2.50	0.48
1:B:162:ASN:O	1:B:162:ASN:ND2	2.46	0.48
1:A:53:ILE:O	1:A:53:ILE:CD1	2.61	0.48
1:A:59:LYS:O	1:A:78:ASP:HA	2.13	0.48
1:B:133:PHE:H	1:B:152:GLY:HA2	1.77	0.48
1:B:122:GLN:HE21	1:B:123:THR:H	1.59	0.48
1:A:13:PRO:HB3	1:A:21:SER:O	2.13	0.48
1:A:101:LYS:CG	1:A:102:GLU:N	2.74	0.48
1:A:159:VAL:HG23	1:A:165:PRO:HD3	1.95	0.48
1:B:117:SER:OG	1:B:187:ALA:N	2.46	0.48
1:A:233:PHE:O	1:A:235:ASP:N	2.47	0.48
1:A:91:VAL:O	1:A:174:LEU:CB	2.62	0.48
1:A:112:THR:OG1	1:A:127:HIS:CD2	2.66	0.48
1:A:141:ILE:O	1:A:174:LEU:CD2	2.62	0.48
1:B:150:THR:O	1:B:151:ASP:CB	2.58	0.48
1:A:115:LEU:O	1:A:116:LYS:HB3	2.13	0.48
1:A:88:TRP:CZ3	1:B:138:LYS:HB3	2.48	0.48
1:A:128:PHE:CA	1:B:125:ALA:O	2.61	0.48
1:A:17:ILE:CG1	1:A:19:ASP:CG	2.82	0.48
1:A:65:VAL:N	1:A:73:THR:O	2.47	0.48
1:A:139:ASP:OD1	1:B:88:TRP:CH2	2.66	0.48
1:B:145:ASP:OD2	1:B:169:SER:CA	2.59	0.48
1:A:80:ASP:CG	1:A:82:ASN:ND2	2.67	0.48
1:B:114:LYS:HG2	1:B:116:LYS:HE3	1.96	0.48
1:B:56:SER:HB2	1:B:188:THR:C	2.33	0.48
1:B:158:ARG:HB3	1:B:158:ARG:HH11	1.79	0.48
1:A:182:TRP:HD1	1:A:183:GLU:CA	2.27	0.48
1:A:88:TRP:CD2	1:A:182:TRP:CH2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:CB	1:B:131:ASN:CB	2.90	0.48
1:A:225:SER:C	1:A:231:GLY:H	2.17	0.48
1:A:3:THR:C	1:A:4:ILE:CG2	2.82	0.48
1:A:51:HIS:O	1:A:52:ILE:CD1	2.60	0.48
1:A:51:HIS:O	1:A:63:ALA:CB	2.62	0.48
1:A:65:VAL:O	1:A:72:ALA:HB1	2.14	0.48
1:B:88:TRP:CD2	1:B:182:TRP:CZ3	3.01	0.48
1:B:159:VAL:CA	1:B:165:PRO:HA	2.27	0.48
1:A:11:THR:CG2	1:A:209:GLY:HA2	2.34	0.47
1:B:44:ASP:O	1:B:46:LYS:HE3	2.14	0.47
1:A:95:ALA:CB	1:A:104:ASN:ND2	2.77	0.47
1:A:128:PHE:CZ	1:A:175:PHE:CD1	3.02	0.47
1:A:20:PRO:CG	1:A:24:HIS:CD2	2.97	0.47
1:B:104:ASN:OD1	1:B:210:ILE:CG1	2.62	0.47
1:B:179:VAL:O	1:B:180:HIS:HB2	2.14	0.47
1:B:180:HIS:HE1	1:B:183:GLU:H	1.62	0.47
1:B:9:LEU:CD2	1:B:25:ILE:CG2	2.88	0.47
1:B:99:LEU:O	1:B:100:TYR:CD1	2.67	0.47
1:B:45:GLY:C	1:B:46:LYS:CD	2.82	0.47
1:A:160:SER:HB2	1:A:164:SER:CB	2.44	0.47
1:A:143:GLN:NE2	1:A:144:GLY:CA	2.77	0.47
1:B:222:PRO:CG	1:B:232:LEU:N	2.77	0.47
1:B:222:PRO:CG	1:B:232:LEU:O	2.59	0.47
1:B:90:ARG:HD2	1:B:175:PHE:O	2.14	0.47
1:B:121:HIS:O	1:B:121:HIS:HD2	1.95	0.47
1:A:181:ILE:CG2	1:A:189:VAL:CG1	2.92	0.47
1:B:7:VAL:O	1:B:211:ALA:CA	2.63	0.47
1:B:110:SER:HB2	1:B:194:THR:HG23	1.95	0.47
1:A:118:ASN:O	1:A:119:SER:HB3	2.14	0.47
1:A:229:LEU:O	1:A:231:GLY:N	2.47	0.47
1:B:136:ASP:OD1	1:B:136:ASP:C	2.52	0.47
1:B:137:GLN:CB	1:B:140:LEU:CD2	2.93	0.47
1:A:4:ILE:HG12	1:A:5:VAL:N	2.28	0.47
1:B:148:THR:O	1:B:148:THR:CG2	2.46	0.47
1:A:122:GLN:HB2	1:A:122:GLN:HE21	1.58	0.47
1:A:56:SER:CB	1:A:188:THR:CA	2.75	0.47
1:B:139:ASP:OD2	1:B:139:ASP:N	2.47	0.47
1:A:116:LYS:CB	1:A:123:THR:HA	2.40	0.47
1:A:101:LYS:HA	1:A:166:GLU:O	2.15	0.47
1:A:132:GLN:O	1:A:134:SER:N	2.47	0.47
1:A:137:GLN:O	1:A:139:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ALA:C	1:A:174:LEU:HD22	2.34	0.47
1:A:214:ILE:O	1:A:215:SER:CB	2.60	0.47
1:A:29:ILE:CG2	1:A:84:VAL:CG1	2.91	0.47
1:A:137:GLN:O	1:B:88:TRP:CZ3	2.68	0.47
1:B:92:GLY:HA2	1:B:109:TRP:CZ2	2.46	0.47
1:B:95:ALA:CB	1:B:210:ILE:CB	2.92	0.47
1:A:130:PHE:HE2	1:A:140:LEU:HD22	1.78	0.47
1:A:17:ILE:HD11	1:A:19:ASP:CG	2.35	0.47
1:A:29:ILE:O	1:A:30:LYS:CB	2.63	0.47
1:B:145:ASP:CB	1:B:158:ARG:HG3	2.42	0.47
1:A:94:SER:HA	1:A:156:LEU:HD13	1.95	0.47
1:B:226:THR:O	1:B:229:LEU:HD12	2.15	0.47
1:B:228:ARG:H	1:B:228:ARG:HG2	1.54	0.47
1:B:197:PHE:N	1:B:197:PHE:CD1	2.83	0.47
1:B:110:SER:HB2	1:B:194:THR:O	2.15	0.47
1:A:116:LYS:O	1:A:117:SER:HB2	2.14	0.47
1:A:52:ILE:CG2	1:A:61:LEU:CD1	2.92	0.47
1:A:44:ASP:O	1:A:46:LYS:N	2.48	0.47
1:A:201:SER:HA	1:A:202:PRO:HD2	1.54	0.47
1:A:184:SER:C	1:A:186:ALA:N	2.68	0.47
1:A:210:ILE:HG22	1:A:211:ALA:H	1.80	0.47
1:B:106:ILE:HG13	1:B:154:LEU:HD13	1.96	0.47
1:B:133:PHE:CB	1:B:153:ASN:O	2.63	0.47
1:B:101:LYS:HA	1:B:166:GLU:O	2.15	0.47
1:A:39:LYS:O	1:A:73:THR:HG21	2.14	0.46
1:B:12:TYR:C	1:B:12:TYR:HD2	2.18	0.46
1:B:181:ILE:CG2	1:B:189:VAL:HG22	2.46	0.46
1:A:150:THR:C	1:A:151:ASP:OD1	2.53	0.46
1:A:88:TRP:CH2	1:A:182:TRP:CZ2	3.03	0.46
1:B:90:ARG:CB	1:B:217:ILE:HG13	2.46	0.46
1:B:103:THR:H	1:B:199:ILE:CG2	2.26	0.46
1:A:225:SER:N	1:A:229:LEU:HD23	2.29	0.46
1:A:35:LYS:N	1:A:35:LYS:CD	2.79	0.46
1:B:219:SER:OG	1:B:219:SER:O	2.33	0.46
1:B:51:HIS:O	1:B:52:ILE:HD13	2.16	0.46
1:A:139:ASP:OD1	1:B:88:TRP:CZ3	2.69	0.46
1:A:4:ILE:CD1	1:A:232:LEU:HB2	2.44	0.46
1:B:12:TYR:HD2	1:B:13:PRO:N	2.13	0.46
1:B:94:SER:HB3	1:B:213:PHE:HE1	1.81	0.46
1:A:80:ASP:OD2	1:A:82:ASN:ND2	2.49	0.46
1:B:62:SER:HA	1:B:76:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASN:HB2	1:A:58:ASP:CG	2.35	0.46
1:B:159:VAL:HB	1:B:165:PRO:HB3	1.98	0.46
1:B:137:GLN:HB2	1:B:140:LEU:HD23	1.98	0.46
1:A:137:GLN:CB	1:A:140:LEU:CB	2.91	0.46
1:A:169:SER:C	1:A:170:VAL:CG1	2.84	0.46
1:A:32:VAL:CG2	1:A:233:PHE:HD2	2.28	0.46
1:B:116:LYS:O	1:B:117:SER:CB	2.63	0.46
1:A:116:LYS:HB3	1:A:123:THR:OG1	2.15	0.46
1:A:221:ILE:HA	1:A:222:PRO:HD2	1.64	0.46
1:A:4:ILE:HB	1:A:215:SER:HB3	1.97	0.46
1:B:181:ILE:HG22	1:B:189:VAL:HG13	1.92	0.46
1:B:112:THR:O	1:B:191:PHE:HA	2.16	0.46
1:A:160:SER:N	1:A:164:SER:O	2.49	0.46
1:A:117:SER:CB	1:A:186:ALA:HA	2.45	0.46
1:A:143:GLN:O	1:A:171:GLY:CA	2.62	0.46
1:B:180:HIS:CE1	1:B:182:TRP:CE2	3.03	0.46
1:B:29:ILE:O	1:B:30:LYS:CB	2.63	0.46
1:B:3:THR:O	1:B:4:ILE:HG22	2.15	0.46
1:A:44:ASP:C	1:A:46:LYS:N	2.69	0.46
1:B:160:SER:HB3	1:B:164:SER:CB	2.45	0.46
1:A:56:SER:OG	1:A:189:VAL:N	2.49	0.46
1:A:89:VAL:CG2	1:A:215:SER:O	2.64	0.46
1:A:225:SER:H	1:A:229:LEU:HD23	1.81	0.46
1:A:33:ARG:HH21	1:A:237:ASN:CG	2.18	0.46
1:B:235:ASP:OD2	1:B:236:ALA:CB	2.64	0.46
1:B:74:SER:O	1:B:75:VAL:CG2	2.64	0.46
1:A:50:ALA:N	1:A:195:PHE:O	2.48	0.46
1:B:158:ARG:C	1:B:159:VAL:HG12	2.36	0.46
1:A:119:SER:O	1:A:121:HIS:N	2.49	0.46
1:A:127:HIS:C	1:A:128:PHE:CD2	2.89	0.46
1:A:158:ARG:O	1:A:159:VAL:CB	2.64	0.46
1:A:66:SER:HA	1:A:72:ALA:CA	2.46	0.46
1:B:115:LEU:CD1	1:B:180:HIS:CE1	2.99	0.46
1:B:116:LYS:HB2	1:B:188:THR:HG23	1.98	0.46
1:B:95:ALA:CB	1:B:210:ILE:HG23	2.27	0.46
1:B:106:ILE:N	1:B:154:LEU:O	2.38	0.46
1:A:117:SER:CB	1:A:186:ALA:CA	2.94	0.45
1:A:117:SER:HG	1:A:186:ALA:HA	1.79	0.45
1:A:154:LEU:HD22	1:A:156:LEU:HD23	1.98	0.45
1:A:158:ARG:HB2	1:A:166:GLU:OE2	2.16	0.45
1:A:18:GLY:N	1:A:33:ARG:NH1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:HA	1:A:73:THR:CG2	2.42	0.45
1:B:157:THR:HG23	1:B:158:ARG:O	2.16	0.45
1:A:98:GLY:C	1:A:100:TYR:N	2.69	0.45
1:A:154:LEU:HD22	1:A:156:LEU:CD2	2.46	0.45
1:B:141:ILE:HG22	1:B:141:ILE:O	2.16	0.45
1:A:45:GLY:HA3	1:A:200:LYS:HE2	1.97	0.45
1:B:50:ALA:N	1:B:197:PHE:HE1	2.13	0.45
1:A:125:ALA:O	1:B:128:PHE:HA	2.16	0.45
1:A:229:LEU:CD2	1:A:235:ASP:CA	2.80	0.45
1:B:137:GLN:CB	1:B:140:LEU:HD22	2.45	0.45
1:A:117:SER:CB	1:A:186:ALA:C	2.84	0.45
1:A:101:LYS:O	1:A:102:GLU:CG	2.64	0.45
1:A:17:ILE:CG2	1:A:228:ARG:CD	2.89	0.45
1:A:225:SER:CB	1:A:231:GLY:H	2.29	0.45
1:A:52:ILE:HG22	1:A:61:LEU:CD1	2.46	0.45
1:A:101:LYS:HE3	1:A:101:LYS:HB3	1.45	0.45
1:A:94:SER:OG	1:A:232:LEU:HD21	2.17	0.45
1:B:157:THR:CG2	1:B:158:ARG:O	2.65	0.45
1:A:12:TYR:O	1:A:14:ASN:CG	2.55	0.45
1:A:52:ILE:O	1:A:53:ILE:CG2	2.65	0.45
1:A:35:LYS:HG3	1:A:77:TYR:OH	2.17	0.45
1:A:128:PHE:HA	1:B:125:ALA:O	2.17	0.45
1:B:187:ALA:O	1:B:188:THR:CG2	2.63	0.45
1:B:166:GLU:CG	1:B:167:GLY:N	2.63	0.45
1:A:218:ASP:N	1:A:218:ASP:OD2	2.49	0.45
1:A:115:LEU:HD11	1:A:189:VAL:CG2	2.45	0.45
1:A:87:GLU:CG	1:A:182:TRP:HB2	2.42	0.45
1:A:141:ILE:C	1:A:142:LEU:HD23	2.36	0.45
1:B:12:TYR:CD2	1:B:13:PRO:O	2.69	0.45
1:A:43:GLN:OE1	1:A:46:LYS:HG2	2.17	0.45
1:B:130:PHE:CZ	1:B:139:ASP:OD1	2.70	0.45
1:A:14:ASN:C	1:A:16:ASP:N	2.69	0.45
1:B:13:PRO:C	1:B:14:ASN:ND2	2.70	0.45
1:B:225:SER:CA	1:B:229:LEU:CB	2.92	0.45
1:B:133:PHE:CG	1:B:154:LEU:HB2	2.52	0.45
1:A:136:ASP:O	1:A:136:ASP:OD1	2.35	0.45
1:A:180:HIS:HD2	1:A:182:TRP:CE2	2.28	0.45
1:A:185:SER:O	1:A:186:ALA:O	2.34	0.45
1:B:53:ILE:HD12	1:B:62:SER:O	2.17	0.45
1:B:67:TYR:HB3	1:B:68:PRO:HD2	1.99	0.45
1:A:204:SER:O	1:A:206:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:O	1:A:14:ASN:ND2	2.51	0.44
1:A:22:TYR:CE1	1:A:39:LYS:CA	2.85	0.44
1:A:13:PRO:C	1:A:15:THR:H	2.21	0.44
1:A:158:ARG:H	1:A:169:SER:CB	2.29	0.44
1:B:226:THR:O	1:B:228:ARG:N	2.50	0.44
1:B:54:TYR:CZ	1:B:81:LEU:HB3	2.51	0.44
1:B:54:TYR:HD2	1:B:61:LEU:HD13	1.81	0.44
1:B:120:THR:C	1:B:122:GLN:HG3	2.37	0.44
1:A:29:ILE:CD1	1:A:35:LYS:HE3	2.45	0.44
1:B:3:THR:C	1:B:4:ILE:CG2	2.85	0.44
1:B:156:LEU:HB3	1:B:171:GLY:O	2.17	0.44
1:A:122:GLN:NE2	1:B:132:GLN:CD	2.70	0.44
1:A:225:SER:C	1:A:229:LEU:CB	2.86	0.44
1:B:191:PHE:O	1:B:191:PHE:CG	2.70	0.44
1:B:226:THR:H	1:B:229:LEU:CB	2.28	0.44
1:B:118:ASN:O	1:B:119:SER:HB2	2.17	0.44
1:A:118:ASN:C	1:A:120:THR:H	2.20	0.44
1:A:56:SER:CB	1:A:189:VAL:H	2.29	0.44
1:A:88:TRP:CH2	1:A:182:TRP:HH2	2.22	0.44
1:B:112:THR:CG2	1:B:127:HIS:HB2	2.33	0.44
1:B:228:ARG:O	1:B:230:LEU:CA	2.65	0.44
1:A:195:PHE:O	1:A:195:PHE:HD1	2.01	0.44
1:B:200:LYS:O	1:B:201:SER:CB	2.53	0.44
1:A:126:LEU:HD23	1:A:179:VAL:HG13	2.00	0.44
1:B:231:GLY:O	1:B:232:LEU:CG	2.62	0.44
1:A:115:LEU:HD12	1:A:189:VAL:CG1	2.46	0.44
1:A:14:ASN:C	1:A:16:ASP:H	2.20	0.44
1:A:224:GLY:CA	1:A:229:LEU:CD2	2.92	0.44
1:A:222:PRO:CD	1:A:231:GLY:O	2.66	0.44
1:A:91:VAL:CG1	1:A:212:PHE:HZ	2.30	0.44
1:B:14:ASN:O	1:B:19:ASP:HB2	2.17	0.44
1:B:25:ILE:HD13	1:B:25:ILE:N	2.33	0.44
1:A:141:ILE:HG22	1:A:174:LEU:HD21	1.96	0.44
1:B:230:LEU:HD22	1:B:230:LEU:HA	1.86	0.44
1:B:41:ASN:HD22	1:B:41:ASN:HA	1.26	0.44
1:A:42:MET:HB3	1:A:42:MET:HE2	1.68	0.44
1:B:154:LEU:CD1	1:B:156:LEU:HD21	2.48	0.44
1:B:158:ARG:C	1:B:159:VAL:CG1	2.86	0.44
1:A:13:PRO:CB	1:A:22:TYR:N	2.72	0.44
1:B:145:ASP:OD2	1:B:158:ARG:CD	2.66	0.44
1:B:122:GLN:CA	1:B:122:GLN:HE21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:NE2	1:B:132:GLN:HE22	1.89	0.43
1:B:14:ASN:HB3	1:B:228:ARG:HH21	1.79	0.43
1:B:229:LEU:O	1:B:233:PHE:CD2	2.71	0.43
1:A:93:LEU:N	1:A:173:ALA:O	2.43	0.43
1:A:90:ARG:NH1	1:A:176:TYR:O	2.52	0.43
1:B:6:ALA:HB1	1:B:213:PHE:N	2.33	0.43
1:B:108:SER:O	1:B:195:PHE:CB	2.66	0.43
1:A:102:GLU:OE1	1:A:104:ASN:OD1	2.36	0.43
1:A:143:GLN:C	1:A:143:GLN:CD	2.75	0.43
1:A:224:GLY:O	1:A:225:SER:OG	2.33	0.43
1:A:27:ILE:O	1:A:29:ILE:HD11	2.18	0.43
1:A:93:LEU:HD22	1:A:212:PHE:CE1	2.52	0.43
1:B:141:ILE:CG2	1:B:174:LEU:N	2.63	0.43
1:B:94:SER:HB3	1:B:213:PHE:CE1	2.54	0.43
1:A:195:PHE:C	1:A:195:PHE:CD1	2.91	0.43
1:A:49:THR:CA	1:A:195:PHE:O	2.62	0.43
1:B:103:THR:O	1:B:105:THR:HB	2.18	0.43
1:A:54:TYR:HB2	1:A:191:PHE:CZ	2.53	0.43
1:A:89:VAL:CG2	1:A:215:SER:H	2.31	0.43
1:A:92:GLY:CA	1:A:174:LEU:CB	2.87	0.43
1:B:98:GLY:O	1:B:99:LEU:CD2	2.51	0.43
1:A:17:ILE:HG12	1:A:19:ASP:CB	2.48	0.43
1:A:74:SER:OG	1:A:75:VAL:N	2.49	0.43
1:B:233:PHE:HA	1:B:234:PRO:HD2	1.84	0.43
1:B:7:VAL:HA	1:B:26:GLY:O	2.18	0.43
1:B:77:TYR:CD1	1:B:77:TYR:C	2.92	0.43
1:B:101:LYS:CG	1:B:165:PRO:O	2.67	0.43
1:A:122:GLN:CB	1:B:131:ASN:HB3	2.48	0.43
1:A:111:PHE:HB3	1:A:128:PHE:CE1	2.54	0.43
1:A:13:PRO:O	1:A:15:THR:HG23	2.19	0.43
1:A:215:SER:C	1:A:216:ASN:O	2.56	0.43
1:A:222:PRO:C	1:A:224:GLY:H	2.21	0.43
1:B:146:ALA:HB1	1:B:156:LEU:HA	2.00	0.43
1:A:116:LYS:CD	1:A:116:LYS:N	2.50	0.43
1:B:51:HIS:O	1:B:52:ILE:HG12	2.18	0.43
1:A:131:ASN:HD22	1:A:131:ASN:HA	1.68	0.43
1:A:134:SER:OG	1:A:135:LYS:N	2.49	0.43
1:A:237:ASN:HD22	1:A:237:ASN:HA	1.49	0.43
1:A:29:ILE:C	1:A:30:LYS:CG	2.87	0.43
1:A:49:THR:HA	1:A:196:ALA:HA	2.00	0.43
1:B:127:HIS:ND1	1:B:128:PHE:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HD11	1:B:75:VAL:HG21	2.01	0.43
1:B:52:ILE:HG13	1:B:212:PHE:CE2	2.52	0.43
1:A:151:ASP:OD2	1:A:153:ASN:CG	2.57	0.43
1:B:48:GLY:C	1:B:197:PHE:CZ	2.92	0.43
1:A:106:ILE:HD13	1:A:154:LEU:CD2	2.46	0.43
1:B:95:ALA:HB1	1:B:210:ILE:CG1	2.41	0.43
1:A:205:HIS:HA	1:A:206:PRO:HD2	1.70	0.43
1:A:99:LEU:HD13	1:A:99:LEU:HA	1.69	0.43
1:A:189:VAL:HG12	1:A:189:VAL:O	2.19	0.42
1:A:106:ILE:HD12	1:A:154:LEU:CD2	2.43	0.42
1:A:111:PHE:O	1:A:127:HIS:HA	2.18	0.42
1:A:66:SER:CB	1:A:72:ALA:HB2	2.48	0.42
1:B:36:LYS:HD3	1:B:37:THR:O	2.17	0.42
1:B:65:VAL:CG2	1:B:73:THR:HG21	2.49	0.42
1:A:160:SER:OG	1:A:161:SER:N	2.52	0.42
1:A:88:TRP:CH2	1:B:138:LYS:HB3	2.54	0.42
1:A:142:LEU:HD11	1:A:148:THR:HB	2.01	0.42
1:A:112:THR:O	1:A:191:PHE:HA	2.18	0.42
1:A:65:VAL:O	1:A:72:ALA:CB	2.67	0.42
1:B:226:THR:H	1:B:229:LEU:CG	2.30	0.42
1:B:58:ASP:O	1:B:59:LYS:CE	2.66	0.42
1:B:48:GLY:O	1:B:197:PHE:CD1	2.72	0.42
1:A:112:THR:CB	1:A:127:HIS:HB2	2.48	0.42
1:A:135:LYS:HB2	1:A:135:LYS:HZ2	1.85	0.42
1:B:115:LEU:HG	1:B:189:VAL:HG23	2.01	0.42
1:B:19:ASP:O	1:B:20:PRO:O	2.36	0.42
1:B:79:VAL:CG2	1:B:80:ASP:H	2.30	0.42
1:B:117:SER:HB3	1:B:187:ALA:N	2.34	0.42
1:B:89:VAL:O	1:B:179:VAL:CB	2.66	0.42
1:B:94:SER:O	1:B:95:ALA:CB	2.66	0.42
1:A:106:ILE:N	1:A:154:LEU:O	2.42	0.42
1:A:23:PRO:O	1:A:40:TRP:N	2.53	0.42
1:B:104:ASN:HA	1:B:210:ILE:HD11	2.00	0.42
1:A:45:GLY:CA	1:A:200:LYS:HG3	2.48	0.42
1:B:159:VAL:HG23	1:B:160:SER:O	2.19	0.42
1:A:93:LEU:O	1:A:156:LEU:HD13	2.19	0.42
1:B:7:VAL:O	1:B:211:ALA:CB	2.68	0.42
1:B:146:ALA:HB2	1:B:156:LEU:HA	1.97	0.42
1:B:130:PHE:CE1	1:B:137:GLN:OE1	2.72	0.42
1:A:17:ILE:C	1:A:19:ASP:N	2.69	0.42
1:A:27:ILE:O	1:A:27:ILE:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:CA	1:A:33:ARG:CZ	2.93	0.42
1:B:36:LYS:HB2	1:B:77:TYR:HD2	1.84	0.42
1:B:139:ASP:O	1:B:176:TYR:CB	2.57	0.42
1:A:158:ARG:O	1:A:159:VAL:HB	2.20	0.42
1:A:222:PRO:HG3	1:A:232:LEU:N	2.35	0.42
1:B:12:TYR:O	1:B:14:ASN:ND2	2.53	0.42
1:A:59:LYS:CE	1:A:78:ASP:HB3	2.19	0.42
1:B:158:ARG:O	1:B:159:VAL:CG1	2.62	0.42
1:A:120:THR:O	1:A:120:THR:CG2	2.65	0.42
1:B:88:TRP:CH2	1:B:180:HIS:CD2	3.06	0.42
1:B:88:TRP:HE3	1:B:179:VAL:O	2.02	0.42
1:B:55:ASN:O	1:B:59:LYS:CA	2.67	0.42
1:B:9:LEU:CG	1:B:40:TRP:CH2	3.03	0.41
1:B:76:SER:O	1:B:77:TYR:HB2	2.19	0.41
1:B:87:GLU:OE2	1:B:182:TRP:CZ2	2.73	0.41
1:A:48:GLY:N	1:A:197:PHE:O	2.34	0.41
1:B:102:GLU:HG3	1:B:103:THR:H	1.85	0.41
1:B:135:LYS:HG2	1:B:135:LYS:H	1.56	0.41
1:A:130:PHE:HA	1:A:130:PHE:HD1	1.60	0.41
1:A:158:ARG:O	1:A:159:VAL:HG12	2.20	0.41
1:A:24:HIS:CG	1:A:25:ILE:N	2.87	0.41
1:A:29:ILE:O	1:A:30:LYS:CG	2.68	0.41
1:B:210:ILE:CG2	1:B:211:ALA:N	2.62	0.41
1:A:80:ASP:C	1:A:82:ASN:H	2.24	0.41
1:A:182:TRP:CG	1:A:183:GLU:N	2.77	0.41
1:A:17:ILE:HG12	1:A:19:ASP:CG	2.40	0.41
1:B:7:VAL:N	1:B:212:PHE:O	2.53	0.41
1:B:101:LYS:O	1:B:102:GLU:CB	2.67	0.41
1:A:116:LYS:HB3	1:A:123:THR:CB	2.50	0.41
1:A:137:GLN:CB	1:A:140:LEU:H	2.24	0.41
1:A:173:ALA:C	1:A:174:LEU:HD23	2.29	0.41
1:B:14:ASN:N	1:B:19:ASP:CB	2.61	0.41
1:B:5:VAL:O	1:B:214:ILE:HG12	2.20	0.41
1:B:154:LEU:HD13	1:B:156:LEU:HD21	2.03	0.41
1:B:160:SER:HB3	1:B:164:SER:CA	2.50	0.41
1:B:43:GLN:OE1	1:B:46:LYS:HG3	2.20	0.41
1:A:141:ILE:HG22	1:A:174:LEU:HG	2.03	0.41
1:A:222:PRO:C	1:A:224:GLY:N	2.74	0.41
1:A:4:ILE:HD13	1:A:233:PHE:CE1	2.55	0.41
1:B:226:THR:O	1:B:227:GLY:C	2.58	0.41
1:B:205:HIS:H	1:B:206:PRO:CD	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:HB3	1:A:77:TYR:CE2	2.55	0.41
1:A:72:ALA:O	1:A:73:THR:HG23	2.20	0.41
1:B:88:TRP:CE3	1:B:180:HIS:HB2	2.55	0.41
1:B:3:THR:O	1:B:215:SER:HB2	2.21	0.41
1:B:91:VAL:O	1:B:174:LEU:HB3	2.20	0.41
1:A:115:LEU:CD2	1:A:183:GLU:HB2	2.51	0.41
1:B:90:ARG:HB3	1:B:217:ILE:HG13	2.03	0.41
1:B:35:LYS:HG3	1:B:35:LYS:HZ3	1.78	0.41
1:A:79:VAL:CG1	1:A:81:LEU:HD12	2.51	0.41
1:A:126:LEU:CD2	1:A:179:VAL:HG13	2.51	0.41
1:A:91:VAL:HG21	1:A:179:VAL:HG21	1.94	0.41
1:A:32:VAL:HG22	1:A:233:PHE:HB2	1.98	0.41
1:A:52:ILE:O	1:A:53:ILE:CB	2.69	0.41
1:A:109:TRP:CH2	1:A:174:LEU:HA	2.47	0.41
1:A:4:ILE:HD11	1:A:232:LEU:HB2	2.03	0.41
1:A:4:ILE:CG1	1:A:5:VAL:N	2.84	0.41
1:B:172:ARG:NH2	1:B:220:SER:CA	2.83	0.41
1:B:51:HIS:O	1:B:52:ILE:CD1	2.69	0.41
1:B:46:LYS:HA	1:B:46:LYS:HD3	1.64	0.41
1:A:115:LEU:CB	1:A:180:HIS:CE1	3.03	0.41
1:A:225:SER:O	1:A:230:LEU:N	2.53	0.41
1:B:117:SER:OG	1:B:188:THR:HG22	2.20	0.41
1:B:221:ILE:HA	1:B:221:ILE:HD12	1.62	0.41
1:B:45:GLY:C	1:B:46:LYS:CE	2.89	0.41
1:A:160:SER:HB3	1:A:164:SER:N	2.33	0.41
1:A:140:LEU:HD12	1:A:174:LEU:C	2.41	0.40
1:B:53:ILE:C	1:B:53:ILE:HD12	2.39	0.40
1:A:143:GLN:CD	1:A:144:GLY:N	2.75	0.40
1:A:233:PHE:C	1:A:235:ASP:N	2.73	0.40
1:A:53:ILE:CD1	1:A:62:SER:O	2.69	0.40
1:B:111:PHE:HE2	1:B:113:SER:OG	2.05	0.40
1:B:17:ILE:O	1:B:33:ARG:CD	2.69	0.40
1:B:224:GLY:C	1:B:229:LEU:HD22	2.42	0.40
1:B:74:SER:O	1:B:75:VAL:CB	2.69	0.40
1:B:99:LEU:HA	1:B:99:LEU:HD13	1.84	0.40
1:B:65:VAL:HG23	1:B:73:THR:HG21	1.98	0.40
1:A:117:SER:HA	1:A:187:ALA:CB	2.50	0.40
1:A:159:VAL:HG23	1:A:165:PRO:CD	2.50	0.40
1:B:53:ILE:H	1:B:53:ILE:HD12	1.86	0.40
1:B:54:TYR:CB	1:B:191:PHE:CE2	3.04	0.40
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:HA	1:A:68:PRO:HD2	1.79	0.40
1:A:82:ASN:OD1	1:A:82:ASN:N	2.52	0.40
1:A:116:LYS:O	1:A:117:SER:C	2.58	0.40
1:A:120:THR:HG21	1:A:122:GLN:NE2	2.37	0.40
1:B:6:ALA:CB	1:B:212:PHE:O	2.45	0.40
1:A:116:LYS:HD3	1:A:188:THR:O	2.21	0.40
1:A:10:ASP:CB	1:A:24:HIS:HE1	2.32	0.40
1:A:12:TYR:CB	1:A:14:ASN:HD21	2.34	0.40
1:A:172:ARG:HG3	1:A:213:PHE:CZ	2.55	0.40
1:A:33:ARG:NH2	1:A:237:ASN:OD1	2.54	0.40
1:B:13:PRO:O	1:B:14:ASN:ND2	2.55	0.40
1:B:225:SER:CB	1:B:231:GLY:HA2	2.52	0.40
1:B:53:ILE:C	1:B:53:ILE:CD1	2.89	0.40
1:A:42:MET:SD	1:A:43:GLN:N	2.95	0.40
1:B:122:GLN:O	1:B:123:THR:CB	2.55	0.40

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:O	1:B:69:ASN:CG[4_455]	1.16	1.04
1:B:16:ASP:CB	1:B:69:ASN:CA[4_455]	1.20	1.00
1:B:16:ASP:O	1:B:69:ASN:ND2[4_455]	1.30	0.90
1:B:16:ASP:O	1:B:69:ASN:CB[4_455]	1.36	0.84
1:B:16:ASP:C	1:B:69:ASN:CB[4_455]	1.42	0.78
1:A:204:SER:OG	1:B:82:ASN:O[3_565]	1.45	0.75
1:B:70:ALA:CA	1:B:228:ARG:NH1[4_454]	1.48	0.72
1:B:16:ASP:CG	1:B:69:ASN:N[4_455]	1.71	0.49
1:B:16:ASP:OD2	1:B:69:ASN:N[4_455]	1.71	0.49
1:A:12:TYR:OH	1:B:184:SER:CA[3_565]	1.73	0.47
1:B:70:ALA:N	1:B:228:ARG:NH1[4_454]	1.77	0.43
1:B:16:ASP:CB	1:B:69:ASN:N[4_455]	1.83	0.37
1:A:12:TYR:OH	1:B:184:SER:CB[3_565]	1.93	0.27
1:B:16:ASP:CA	1:B:69:ASN:CA[4_455]	1.94	0.26
1:B:16:ASP:CB	1:B:69:ASN:C[4_455]	1.94	0.26
1:B:69:ASN:O	1:B:228:ARG:NH1[4_454]	1.95	0.25
1:B:16:ASP:OD2	1:B:68:PRO:C[4_455]	1.97	0.23
1:A:12:TYR:OH	1:B:184:SER:C[3_565]	2.03	0.17
1:B:16:ASP:C	1:B:69:ASN:CA[4_455]	2.06	0.14
1:B:69:ASN:C	1:B:228:ARG:NH1[4_454]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:N	1:B:69:ASN:CB[4_455]	2.10	0.10
1:A:68:PRO:CA	1:B:119:SER:OG[2_555]	2.14	0.06
1:B:69:ASN:O	1:B:228:ARG:CZ[4_454]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	235/237 (99%)	141 (60%)	52 (22%)	42 (18%)	0 0
1	B	235/237 (99%)	131 (56%)	48 (20%)	56 (24%)	0 0
All	All	470/474 (99%)	272 (58%)	100 (21%)	98 (21%)	0 0

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	17	ILE
1	A	25	ILE
1	A	42	MET
1	A	53	ILE
1	A	102	GLU
1	A	116	LYS
1	A	118	ASN
1	A	133	PHE
1	A	159	VAL
1	A	170	VAL
1	A	181	ILE
1	A	184	SER
1	A	185	SER
1	A	186	ALA
1	A	216	ASN
1	A	235	ASP

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Mol	Chain	Res	Type
1	B	19	ASP
1	B	21	SER
1	B	22	TYR
1	B	31	SER
1	B	57	VAL
1	B	58	ASP
1	B	75	VAL
1	B	82	ASN
1	B	87	GLU
1	B	102	GLU
1	B	119	SER
1	B	121	HIS
1	B	136	ASP
1	B	151	ASP
1	B	161	SER
1	B	183	GLU
1	B	187	ALA
1	B	188	THR
1	B	194	THR
1	B	216	ASN
1	B	229	LEU
1	B	230	LEU
1	A	15	THR
1	A	18	GLY
1	A	32	VAL
1	A	69	ASN
1	A	123	THR
1	A	151	ASP
1	A	163	GLY
1	A	168	SER
1	A	183	GLU
1	A	215	SER
1	A	225	SER
1	B	30	LYS
1	B	39	LYS
1	B	45	GLY
1	B	95	ALA
1	B	118	ASN
1	B	122	GLN
1	B	138	LYS
1	B	140	LEU
1	B	149	GLY

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Mol	Chain	Res	Type
1	B	185	SER
1	B	203	ASP
1	B	215	SER
1	B	227	GLY
1	B	228	ARG
1	B	232	LEU
1	B	235	ASP
1	A	22	TYR
1	A	34	SER
1	A	120	THR
1	A	172	ARG
1	B	69	ASN
1	B	98	GLY
1	B	182	TRP
1	B	211	ALA
1	B	223	SER
1	A	19	ASP
1	A	45	GLY
1	A	59	LYS
1	A	75	VAL
1	A	194	THR
1	A	230	LEU
1	B	20	PRO
1	B	77	TYR
1	B	99	LEU
1	B	104	ASN
1	B	117	SER
1	B	180	HIS
1	B	201	SER
1	A	60	ARG
1	B	15	THR
1	B	198	LEU
1	A	10	ASP
1	B	123	THR
1	A	189	VAL
1	B	205	HIS
1	B	179	VAL
1	A	179	VAL
1	B	210	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/202 (100%)	117 (58%)	85 (42%)	0 0
1	B	202/202 (100%)	118 (58%)	84 (42%)	0 0
All	All	404/404 (100%)	235 (58%)	169 (42%)	0 0

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	ILE
1	A	8	GLU
1	A	12	TYR
1	A	17	ILE
1	A	25	ILE
1	A	27	ILE
1	A	29	ILE
1	A	33	ARG
1	A	35	LYS
1	A	37	THR
1	A	42	MET
1	A	44	ASP
1	A	46	LYS
1	A	51	HIS
1	A	52	ILE
1	A	53	ILE
1	A	58	ASP
1	A	60	ARG
1	A	64	VAL
1	A	69	ASN
1	A	71	ASP
1	A	76	SER
1	A	79	VAL
1	A	81	LEU
1	A	82	ASN
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	100	TYR
1	A	101	LYS
1	A	106	ILE
1	A	110	SER
1	A	114	LYS
1	A	116	LYS
1	A	117	SER
1	A	121	HIS
1	A	122	GLN
1	A	123	THR
1	A	127	HIS
1	A	128	PHE
1	A	129	MET
1	A	135	LYS
1	A	138	LYS
1	A	140	LEU
1	A	141	ILE
1	A	142	LEU
1	A	143	GLN
1	A	151	ASP
1	A	154	LEU
1	A	157	THR
1	A	158	ARG
1	A	164	SER
1	A	166	GLU
1	A	168	SER
1	A	169	SER
1	A	172	ARG
1	A	174	LEU
1	A	179	VAL
1	A	180	HIS
1	A	181	ILE
1	A	184	SER
1	A	185	SER
1	A	188	THR
1	A	190	SER
1	A	192	GLU
1	A	194	THR
1	A	198	LEU
1	A	199	ILE
1	A	200	LYS

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Mol	Chain	Res	Type
1	A	201	SER
1	A	204	SER
1	A	208	ASP
1	A	210	ILE
1	A	214	ILE
1	A	215	SER
1	A	217	ILE
1	A	218	ASP
1	A	219	SER
1	A	220	SER
1	A	221	ILE
1	A	223	SER
1	A	226	THR
1	A	228	ARG
1	A	230	LEU
1	A	237	ASN
1	B	3	THR
1	B	4	ILE
1	B	8	GLU
1	B	10	ASP
1	B	12	TYR
1	B	16	ASP
1	B	17	ILE
1	B	19	ASP
1	B	21	SER
1	B	22	TYR
1	B	25	ILE
1	B	29	ILE
1	B	35	LYS
1	B	41	ASN
1	B	42	MET
1	B	46	LYS
1	B	49	THR
1	B	52	ILE
1	B	53	ILE
1	B	58	ASP
1	B	59	LYS
1	B	60	ARG
1	B	61	LEU
1	B	66	SER
1	B	69	ASN
1	B	71	ASP

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Mol	Chain	Res	Type
1	B	73	THR
1	B	76	SER
1	B	79	VAL
1	B	81	LEU
1	B	82	ASN
1	B	90	ARG
1	B	99	LEU
1	B	101	LYS
1	B	102	GLU
1	B	105	THR
1	B	106	ILE
1	B	110	SER
1	B	113	SER
1	B	114	LYS
1	B	117	SER
1	B	118	ASN
1	B	119	SER
1	B	120	THR
1	B	122	GLN
1	B	123	THR
1	B	126	LEU
1	B	127	HIS
1	B	129	MET
1	B	132	GLN
1	B	134	SER
1	B	135	LYS
1	B	137	GLN
1	B	139	ASP
1	B	141	ILE
1	B	143	GLN
1	B	145	ASP
1	B	147	THR
1	B	148	THR
1	B	151	ASP
1	B	154	LEU
1	B	156	LEU
1	B	157	THR
1	B	158	ARG
1	B	160	SER
1	B	169	SER
1	B	172	ARG
1	B	180	HIS

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Mol	Chain	Res	Type
1	B	181	ILE
1	B	184	SER
1	B	185	SER
1	B	189	VAL
1	B	190	SER
1	B	199	ILE
1	B	200	LYS
1	B	208	ASP
1	B	214	ILE
1	B	216	ASN
1	B	217	ILE
1	B	220	SER
1	B	221	ILE
1	B	226	THR
1	B	228	ARG
1	B	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	41	ASN
1	A	55	ASN
1	A	69	ASN
1	A	104	ASN
1	A	122	GLN
1	A	127	HIS
1	A	131	ASN
1	A	143	GLN
1	A	180	HIS
1	B	14	ASN
1	B	24	HIS
1	B	41	ASN
1	B	121	HIS
1	B	122	GLN
1	B	137	GLN
1	B	143	GLN
1	B	162	ASN
1	B	180	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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