



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:04 AM UTC

PDB ID : 1LD9 / pdb_00001ld9
Title : THE THREE-DIMENSIONAL STRUCTURE OF AN H-2LD PEPTIDE COMPLEX EXPLAINS THE UNIQUE INTERACTION OF LD WITH BETA2M AND PEPTIDE
Authors : Balendiran, G.K.; Solheim, J.C.; Young, A.C.M.; Hansen, T.H.; Nathenson, S.G.; Sacchettini, J.C.
Deposited on : 1997-04-24
Resolution : 2.40 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

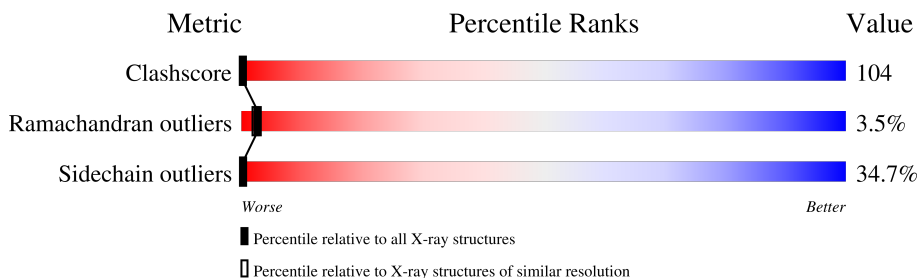
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	A	268	15% 33% 28% 24%
1	D	268	15% 32% 29% 24%
2	B	99	12% 34% 32% 21%
2	E	99	11% 34% 33% 21%
3	C	9	56% 44%
3	F	9	56% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6168 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 MHC CLASS I H-2LD HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2184	1381	381	412	10			
1	D	268	Total	C	N	O	S	0	0	0
			2184	1381	381	412	10			

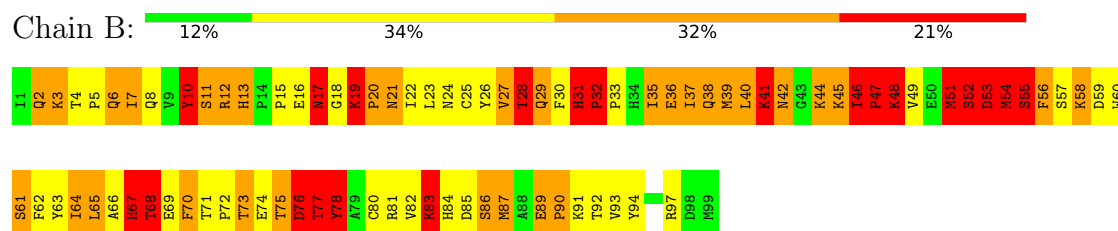
- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	E	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

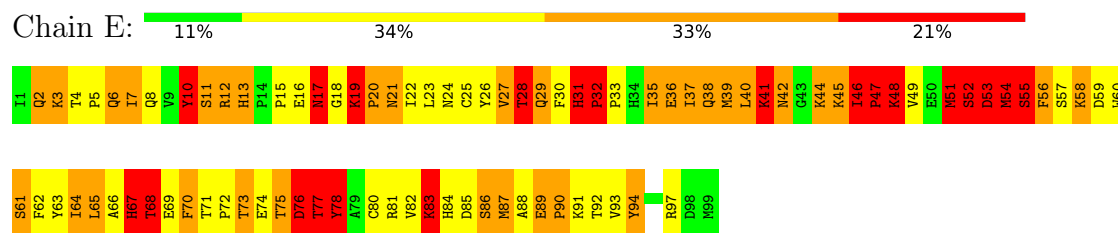
- Molecule 3 is a protein called NANO-PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			80	52	14	14			
3	F	9	Total	C	N	O	0	0	0
			80	52	14	14			

• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 3: NANO-PEPTIDE



• Molecule 3: NANO-PEPTIDE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.10Å 87.20Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	75.0 ((Not available)-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	75/2248 (3.3%)	3.77	165/3056 (5.4%)
1	D	2.22	75/2248 (3.3%)	3.77	165/3056 (5.4%)
2	B	2.43	29/846 (3.4%)	3.48	68/1148 (5.9%)
2	E	2.43	29/846 (3.4%)	3.48	68/1148 (5.9%)
3	C	1.70	1/83 (1.2%)	2.18	7/112 (6.2%)
3	F	1.70	1/83 (1.2%)	2.18	7/112 (6.2%)
All	All	2.27	210/6354 (3.3%)	3.67	480/8632 (5.6%)

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
1	A	0	60
1	D	0	60
2	B	0	12
2	E	0	12
3	C	0	2
3	F	0	2
All	All	0	148

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	LYS	C-O	-26.73	0.89	1.24
2	E	19	LYS	C-O	-26.71	0.89	1.24
1	A	254	GLU	C-O	-24.13	0.92	1.24
1	D	254	GLU	C-O	-24.08	0.93	1.24
2	E	20	PRO	N-CD	20.22	1.76	1.47
2	B	20	PRO	N-CD	20.19	1.76	1.47
2	E	47	PRO	N-CD	19.66	1.75	1.47
2	B	47	PRO	N-CD	19.64	1.75	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	LYS	C-N	-19.42	1.05	1.33
1	D	131	LYS	C-N	-19.41	1.05	1.33
1	A	175	GLY	C-N	17.02	1.59	1.33
1	D	175	GLY	C-N	17.01	1.59	1.33
1	D	226	GLN	N-CA	-16.22	1.26	1.46
1	A	226	GLN	N-CA	-16.20	1.26	1.46
1	D	30	ASN	N-CA	-15.75	1.28	1.46
1	A	30	ASN	N-CA	-15.69	1.28	1.46
2	B	19	LYS	N-CA	14.63	1.59	1.46
2	E	19	LYS	N-CA	14.61	1.59	1.46
1	A	263	HIS	C-N	13.87	1.53	1.33
1	D	263	HIS	C-N	13.83	1.53	1.33
1	A	128	GLU	C-N	13.74	1.52	1.33
1	D	128	GLU	C-N	13.71	1.52	1.33
1	D	110	LEU	C-N	12.91	1.51	1.33
1	A	110	LEU	C-N	12.87	1.51	1.33
2	B	31	HIS	CA-C	-12.41	1.37	1.52
2	E	31	HIS	CA-C	-12.38	1.37	1.52
1	D	225	THR	C-N	-12.13	1.18	1.33
1	A	225	THR	C-N	-12.13	1.18	1.33
1	A	29	ASP	CA-C	-12.12	1.36	1.52
1	D	29	ASP	CA-C	-12.12	1.36	1.52
2	B	16	GLU	C-N	12.09	1.50	1.33
2	E	16	GLU	C-N	12.06	1.50	1.33
1	D	193	PRO	C-N	11.91	1.48	1.33
1	A	193	PRO	C-N	11.85	1.48	1.33
1	A	225	THR	CA-C	-11.70	1.34	1.52
1	D	225	THR	CA-C	-11.70	1.34	1.52
2	E	17	ASN	CA-C	-11.24	1.38	1.52
2	B	17	ASN	CA-C	-11.22	1.38	1.52
1	D	56	GLY	C-N	11.06	1.42	1.33
1	A	164	CYS	C-N	-11.02	1.20	1.33
1	D	129	ASP	C-N	11.01	1.48	1.33
1	A	129	ASP	C-N	10.99	1.48	1.33
1	D	164	CYS	C-N	-10.99	1.20	1.33
1	A	56	GLY	C-N	10.97	1.42	1.33
1	D	227	ASP	CA-C	10.90	1.66	1.52
1	A	256	ASN	C-N	10.89	1.47	1.33
1	A	227	ASP	CA-C	10.88	1.66	1.52
1	D	256	ASN	C-N	10.82	1.47	1.33
1	D	4	SER	N-CA	10.69	1.59	1.46
1	A	4	SER	N-CA	10.67	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	N-CA	10.64	1.59	1.46
1	D	229	GLU	N-CA	10.60	1.59	1.46
1	D	267	PRO	CA-C	10.29	1.61	1.53
2	E	18	GLY	CA-C	10.21	1.66	1.51
1	A	267	PRO	CA-C	10.20	1.61	1.53
2	B	18	GLY	CA-C	10.20	1.66	1.51
2	B	51	MET	SD-CE	10.12	2.04	1.79
2	E	51	MET	SD-CE	10.11	2.04	1.79
1	D	2	PRO	CA-C	9.96	1.66	1.52
1	A	2	PRO	CA-C	9.93	1.66	1.52
1	A	3	HIS	N-CA	9.92	1.58	1.46
1	D	3	HIS	N-CA	9.88	1.58	1.46
1	D	3	HIS	CA-C	9.63	1.65	1.52
1	A	3	HIS	CA-C	9.61	1.65	1.52
1	D	196	LYS	N-CA	-9.57	1.33	1.46
1	A	196	LYS	N-CA	-9.54	1.33	1.46
2	E	18	GLY	N-CA	-9.54	1.31	1.45
2	B	18	GLY	N-CA	-9.50	1.31	1.45
1	D	210	PRO	N-CA	-9.36	1.36	1.46
1	A	210	PRO	N-CA	-9.35	1.36	1.46
1	D	228	MET	N-CA	9.27	1.58	1.46
1	A	228	MET	N-CA	9.23	1.58	1.46
1	D	228	MET	CA-C	9.19	1.65	1.52
1	A	195	SER	CA-C	-9.15	1.41	1.53
1	D	195	SER	CA-C	-9.15	1.41	1.53
1	D	49	ALA	C-N	9.14	1.45	1.33
1	A	228	MET	CA-C	9.13	1.65	1.52
1	A	49	ALA	C-N	9.11	1.45	1.33
2	B	31	HIS	C-N	-8.96	1.22	1.33
2	B	42	ASN	N-CA	-8.94	1.34	1.46
2	E	31	HIS	C-N	-8.92	1.22	1.33
2	E	42	ASN	N-CA	-8.92	1.34	1.46
2	B	20	PRO	CG-CD	8.90	1.81	1.50
2	E	20	PRO	CG-CD	8.89	1.80	1.50
2	B	41	LYS	CA-C	-8.89	1.40	1.52
2	E	41	LYS	CA-C	-8.87	1.40	1.52
1	D	25	VAL	CA-CB	8.86	1.64	1.54
1	A	229	GLU	C-N	-8.84	1.20	1.33
1	D	229	GLU	C-N	-8.84	1.20	1.33
1	A	25	VAL	CA-CB	8.82	1.64	1.54
1	D	218	GLN	C-N	-8.81	1.21	1.33
1	A	218	GLN	C-N	-8.80	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ASN	C-N	8.68	1.45	1.33
2	E	31	HIS	C-O	-8.68	1.13	1.24
2	B	47	PRO	CG-CD	8.68	1.80	1.50
2	E	47	PRO	CG-CD	8.67	1.80	1.50
1	D	176	ASN	C-N	8.65	1.45	1.33
2	B	31	HIS	C-O	-8.64	1.13	1.24
3	C	5	ASN	C-N	-8.59	1.22	1.33
3	F	5	ASN	C-N	-8.57	1.22	1.33
1	A	195	SER	C-N	-8.49	1.21	1.33
1	D	195	SER	C-N	-8.45	1.21	1.33
1	D	177	ALA	C-N	8.36	1.45	1.33
1	A	177	ALA	C-N	8.32	1.45	1.33
1	A	208	PHE	N-CA	8.27	1.56	1.46
1	D	208	PHE	N-CA	8.24	1.56	1.46
2	B	46	ILE	C-N	8.03	1.45	1.33
1	D	209	TYR	CA-C	-8.02	1.42	1.52
1	A	209	TYR	CA-C	-8.01	1.42	1.52
2	E	46	ILE	C-N	8.01	1.45	1.33
2	E	28	THR	C-N	-7.76	1.22	1.33
2	B	28	THR	C-N	-7.76	1.22	1.33
1	A	27	TYR	C-N	7.71	1.44	1.33
1	D	27	TYR	C-N	7.70	1.44	1.33
2	E	87	MET	SD-CE	-7.47	1.60	1.79
2	B	87	MET	SD-CE	-7.45	1.60	1.79
1	D	207	GLY	CA-C	7.21	1.62	1.51
1	A	207	GLY	CA-C	7.19	1.62	1.51
1	D	105	SER	C-N	7.19	1.44	1.33
1	A	105	SER	C-N	7.16	1.44	1.33
1	A	255	GLN	N-CA	7.03	1.55	1.46
1	D	255	GLN	N-CA	6.97	1.55	1.46
1	D	182	THR	C-N	-6.86	1.24	1.33
1	D	178	THR	C-N	-6.85	1.24	1.33
1	A	182	THR	C-N	-6.85	1.24	1.33
1	A	178	THR	C-N	-6.82	1.24	1.33
1	A	185	PRO	C-N	-6.63	1.21	1.33
1	D	185	PRO	C-N	-6.63	1.21	1.33
1	A	138	MET	SD-CE	6.46	1.95	1.79
1	D	138	MET	SD-CE	6.45	1.95	1.79
1	A	208	PHE	CA-C	-6.42	1.44	1.52
1	D	208	PHE	CA-C	-6.39	1.44	1.52
1	A	5	MET	N-CA	6.35	1.54	1.46
1	D	5	MET	N-CA	6.33	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	17	ASN	C-N	6.24	1.42	1.33
1	D	180	LEU	C-N	-6.23	1.25	1.33
1	D	160	LEU	C-N	-6.20	1.24	1.33
1	A	180	LEU	C-N	-6.20	1.25	1.33
2	B	17	ASN	C-N	6.20	1.42	1.33
1	A	160	LEU	C-N	-6.16	1.24	1.33
1	A	197	GLY	C-N	-6.14	1.25	1.33
1	D	197	GLY	C-N	-6.09	1.25	1.33
2	B	53	ASP	N-CA	6.08	1.52	1.46
2	E	53	ASP	N-CA	6.06	1.52	1.46
1	D	63	ILE	CA-CB	6.00	1.61	1.54
1	A	227	ASP	N-CA	5.94	1.53	1.45
1	A	63	ILE	CA-CB	5.94	1.61	1.54
1	D	123	TYR	C-N	-5.94	1.25	1.33
1	A	123	TYR	C-N	-5.92	1.25	1.33
1	D	140	ALA	CA-CB	-5.91	1.43	1.53
2	E	20	PRO	CB-CG	5.91	1.79	1.49
2	B	20	PRO	CB-CG	5.91	1.79	1.49
1	D	227	ASP	N-CA	5.89	1.53	1.45
1	A	140	ALA	CA-CB	-5.88	1.43	1.53
1	A	127	ASN	C-N	5.84	1.42	1.33
2	E	39	MET	SD-CE	5.81	1.94	1.79
1	D	127	ASN	C-N	5.80	1.42	1.33
1	D	230	LEU	C-N	-5.80	1.26	1.33
2	B	39	MET	SD-CE	5.80	1.94	1.79
1	A	259	CYS	CA-C	5.79	1.59	1.52
1	A	230	LEU	C-N	-5.78	1.26	1.33
1	D	259	CYS	CA-C	5.77	1.59	1.52
1	D	4	SER	CA-C	5.76	1.60	1.52
1	A	4	SER	CA-C	5.75	1.60	1.52
1	A	61	GLU	CA-C	-5.73	1.45	1.52
1	D	61	GLU	CA-C	-5.69	1.45	1.52
1	D	163	GLU	C-N	-5.69	1.26	1.33
1	A	163	GLU	C-N	-5.68	1.26	1.33
1	D	62	ARG	CB-CG	5.67	1.69	1.52
1	A	62	ARG	CB-CG	5.65	1.69	1.52
1	D	209	TYR	N-CA	-5.62	1.38	1.46
1	A	209	TYR	N-CA	-5.60	1.38	1.46
1	A	258	THR	CA-CB	5.54	1.61	1.53
1	D	29	ASP	N-CA	5.52	1.53	1.46
1	D	237	GLY	C-N	5.52	1.41	1.33
1	A	237	GLY	C-N	5.51	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	ASP	N-CA	5.50	1.53	1.46
1	D	258	THR	CA-CB	5.50	1.61	1.53
2	B	68	THR	CA-C	5.45	1.58	1.53
2	E	68	THR	CA-C	5.44	1.58	1.53
1	D	204	TRP	NE1-CE2	-5.43	1.31	1.37
1	D	166	GLU	CG-CD	5.39	1.65	1.52
1	A	204	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	166	GLU	CG-CD	5.38	1.65	1.52
1	D	253	LYS	C-N	-5.38	1.26	1.33
1	D	28	VAL	CA-C	5.35	1.59	1.52
1	D	179	LEU	C-N	-5.34	1.26	1.33
1	A	179	LEU	C-N	-5.33	1.26	1.33
1	A	253	LYS	C-N	-5.32	1.26	1.33
2	B	47	PRO	CB-CG	5.31	1.76	1.49
1	A	28	VAL	CA-C	5.30	1.59	1.52
2	E	47	PRO	CB-CG	5.30	1.76	1.49
2	E	17	ASN	CA-CB	5.29	1.59	1.53
2	B	55	SER	C-N	-5.28	1.26	1.33
2	B	17	ASN	CA-CB	5.27	1.59	1.53
2	E	53	ASP	CB-CG	5.26	1.65	1.52
2	B	53	ASP	CB-CG	5.26	1.65	1.52
1	D	197	GLY	N-CA	5.23	1.52	1.45
1	D	256	ASN	CA-C	-5.22	1.45	1.52
1	A	197	GLY	N-CA	5.22	1.52	1.45
1	A	256	ASN	CA-C	-5.22	1.45	1.52
2	E	55	SER	C-N	-5.22	1.26	1.33
2	E	13	HIS	CA-C	-5.21	1.47	1.52
2	B	13	HIS	CA-C	-5.18	1.47	1.52
1	A	3	HIS	C-N	5.17	1.40	1.33
1	D	3	HIS	C-N	5.15	1.40	1.33
1	D	213	ILE	CA-CB	5.05	1.60	1.55
1	A	213	ILE	CA-CB	5.01	1.60	1.55
1	D	139	ALA	CA-C	-5.01	1.46	1.52
1	A	75	ARG	CA-C	-5.00	1.46	1.52

All (480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ALA	O-C-N	-79.33	23.52	122.68
1	A	236	ALA	O-C-N	-79.30	23.55	122.68
1	D	206	LEU	O-C-N	-59.78	45.30	123.01
1	A	206	LEU	O-C-N	-59.76	45.33	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	ILE	O-C-N	-54.98	69.99	121.12
2	E	46	ILE	O-C-N	-54.98	69.99	121.12
1	D	264	GLU	O-C-N	-52.05	50.57	122.41
1	A	264	GLU	O-C-N	-52.04	50.59	122.41
1	A	256	ASN	O-C-N	-46.74	60.42	122.59
1	D	256	ASN	O-C-N	-46.72	60.45	122.59
1	A	28	VAL	O-C-N	-37.80	75.32	122.57
1	D	28	VAL	O-C-N	-37.80	75.32	122.57
1	A	131	LYS	O-C-N	-36.89	79.06	122.22
1	D	131	LYS	O-C-N	-36.88	79.07	122.22
2	B	46	ILE	CA-C-N	-31.36	86.62	119.24
2	B	46	ILE	C-N-CA	-31.36	86.62	119.24
2	E	46	ILE	CA-C-N	-31.34	86.64	119.24
2	E	46	ILE	C-N-CA	-31.34	86.64	119.24
1	A	236	ALA	CA-C-N	-31.33	60.00	121.41
1	A	236	ALA	C-N-CA	-31.33	60.00	121.41
1	D	236	ALA	CA-C-N	-31.32	60.02	121.41
1	D	236	ALA	C-N-CA	-31.32	60.02	121.41
1	A	129	ASP	O-C-N	-26.88	92.18	122.55
1	D	129	ASP	O-C-N	-26.83	92.23	122.55
2	B	52	SER	O-C-N	-24.54	93.03	122.97
2	E	52	SER	O-C-N	-24.52	93.05	122.97
1	A	211	ALA	O-C-N	21.77	147.02	122.20
1	D	211	ALA	O-C-N	21.76	147.00	122.20
1	A	206	LEU	CA-C-N	21.45	163.46	121.41
1	A	206	LEU	C-N-CA	21.45	163.46	121.41
1	D	206	LEU	CA-C-N	21.43	163.42	121.41
1	D	206	LEU	C-N-CA	21.43	163.42	121.41
1	A	205	ALA	O-C-N	-21.04	98.17	122.15
1	D	205	ALA	O-C-N	-21.03	98.18	122.15
1	D	254	GLU	CA-C-N	20.75	150.17	120.28
1	D	254	GLU	C-N-CA	20.75	150.17	120.28
1	A	254	GLU	CA-C-N	20.75	150.15	120.28
1	A	254	GLU	C-N-CA	20.75	150.15	120.28
1	A	196	LYS	CA-C-N	19.53	159.68	121.41
1	A	196	LYS	C-N-CA	19.53	159.68	121.41
1	D	196	LYS	CA-C-N	19.52	159.68	121.41
1	D	196	LYS	C-N-CA	19.52	159.68	121.41
1	D	1	GLY	CA-C-N	19.52	144.24	119.84
1	D	1	GLY	C-N-CA	19.52	144.24	119.84
1	A	1	GLY	CA-C-N	19.50	144.22	119.84
1	A	1	GLY	C-N-CA	19.50	144.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASN	O-C-N	-19.47	100.65	122.85
1	D	127	ASN	O-C-N	-19.47	100.66	122.85
1	D	197	GLY	O-C-N	-18.14	99.12	122.70
1	A	197	GLY	O-C-N	-18.13	99.12	122.70
2	B	53	ASP	O-C-N	-18.03	98.12	121.74
2	E	53	ASP	O-C-N	-18.02	98.13	121.74
2	B	47	PRO	N-CD-CG	-17.60	76.80	103.20
2	E	47	PRO	N-CD-CG	-17.59	76.81	103.20
2	B	20	PRO	N-CD-CG	-17.21	77.38	103.20
2	E	20	PRO	N-CD-CG	-17.21	77.38	103.20
1	D	1	GLY	O-C-N	-16.96	95.86	123.00
1	A	1	GLY	O-C-N	-16.96	95.87	123.00
1	A	252	GLY	O-C-N	-16.60	101.12	122.70
1	D	252	GLY	O-C-N	-16.59	101.14	122.70
1	D	128	GLU	O-C-N	16.48	145.03	122.46
1	A	128	GLU	O-C-N	16.46	145.01	122.46
1	A	237	GLY	O-C-N	-16.27	101.54	122.70
1	D	237	GLY	O-C-N	-16.26	101.56	122.70
2	E	18	GLY	CA-C-N	16.21	145.57	122.06
2	E	18	GLY	C-N-CA	16.21	145.57	122.06
2	B	18	GLY	CA-C-N	16.20	145.56	122.06
2	B	18	GLY	C-N-CA	16.20	145.56	122.06
1	A	28	VAL	CB-CA-C	-15.10	86.53	111.29
1	A	266	LEU	O-C-N	-15.09	103.97	121.32
1	D	28	VAL	CB-CA-C	-15.09	86.55	111.29
1	D	266	LEU	O-C-N	-15.05	104.01	121.32
1	D	179	LEU	O-C-N	-14.94	102.90	122.33
2	B	19	LYS	O-C-N	-14.94	106.77	121.56
1	A	179	LEU	O-C-N	-14.93	102.92	122.33
2	E	19	LYS	O-C-N	-14.91	106.80	121.56
2	B	20	PRO	CA-N-CD	14.57	132.39	112.00
2	E	20	PRO	CA-N-CD	14.57	132.39	112.00
2	B	48	LYS	CA-C-N	-14.37	103.56	123.10
2	B	48	LYS	C-N-CA	-14.37	103.56	123.10
2	E	48	LYS	CA-C-N	-14.36	103.57	123.10
2	E	48	LYS	C-N-CA	-14.36	103.57	123.10
1	A	209	TYR	CA-C-N	13.97	138.12	120.51
1	A	209	TYR	C-N-CA	13.97	138.12	120.51
1	D	209	TYR	CA-C-N	13.97	138.12	120.51
1	D	209	TYR	C-N-CA	13.97	138.12	120.51
1	A	127	ASN	CA-C-N	13.94	146.20	121.66
1	A	127	ASN	C-N-CA	13.94	146.20	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ASN	CA-C-N	13.92	146.16	121.66
1	D	127	ASN	C-N-CA	13.92	146.16	121.66
1	D	174	ASN	O-C-N	13.29	139.33	122.19
1	A	174	ASN	O-C-N	13.28	139.32	122.19
1	D	17	LEU	O-C-N	-13.20	105.03	122.59
1	A	17	LEU	O-C-N	-13.16	105.09	122.59
1	A	131	LYS	CA-C-N	12.84	142.97	122.81
1	A	131	LYS	C-N-CA	12.84	142.97	122.81
1	D	131	LYS	CA-C-N	12.82	142.94	122.81
1	D	131	LYS	C-N-CA	12.82	142.94	122.81
1	D	17	LEU	CA-C-O	-12.58	102.52	120.51
1	A	17	LEU	CA-C-O	-12.57	102.54	120.51
2	E	19	LYS	CA-C-O	-12.55	109.14	120.56
1	D	176	ASN	O-C-N	-12.54	105.16	122.46
1	A	176	ASN	O-C-N	-12.52	105.18	122.46
2	B	19	LYS	CA-C-O	-12.50	109.18	120.56
2	E	90	PRO	N-CA-C	12.48	129.17	111.33
2	B	90	PRO	N-CA-C	12.46	129.15	111.33
1	A	192	HIS	O-C-N	12.45	131.26	121.55
1	A	227	ASP	O-C-N	-12.43	108.12	123.17
1	D	227	ASP	O-C-N	-12.42	108.14	123.17
1	D	192	HIS	O-C-N	12.39	131.22	121.55
1	A	58	GLU	N-CA-C	-11.99	95.78	112.45
1	D	58	GLU	N-CA-C	-11.99	95.79	112.45
1	D	16	GLY	O-C-N	-11.92	107.20	122.70
1	A	16	GLY	O-C-N	-11.90	107.23	122.70
2	B	10	TYR	N-CA-C	11.88	127.54	108.76
2	E	10	TYR	N-CA-C	11.87	127.51	108.76
1	D	209	TYR	O-C-N	-11.54	108.06	121.32
1	A	209	TYR	O-C-N	-11.53	108.06	121.32
2	E	42	ASN	O-C-N	11.49	137.87	122.59
2	B	76	ASP	N-CA-C	11.49	127.22	110.10
2	B	42	ASN	O-C-N	11.48	137.86	122.59
2	E	76	ASP	N-CA-C	11.48	127.20	110.10
2	B	32	PRO	O-C-N	-11.42	107.98	121.46
2	E	32	PRO	O-C-N	-11.41	108.00	121.46
1	A	263	HIS	CA-C-N	-11.25	102.52	122.32
1	A	263	HIS	C-N-CA	-11.25	102.52	122.32
1	D	263	HIS	CA-C-N	-11.24	102.53	122.32
1	D	263	HIS	C-N-CA	-11.24	102.53	122.32
2	E	47	PRO	CA-C-N	11.23	140.32	122.34
2	E	47	PRO	C-N-CA	11.23	140.32	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	PRO	CA-C-N	11.21	140.28	122.34
2	B	47	PRO	C-N-CA	11.21	140.28	122.34
1	A	164	CYS	O-C-N	11.19	134.12	122.03
1	D	164	CYS	O-C-N	11.18	134.10	122.03
1	D	205	ALA	CA-C-N	11.11	139.58	123.14
1	D	205	ALA	C-N-CA	11.11	139.58	123.14
1	A	205	ALA	CA-C-N	11.09	139.56	123.14
1	A	205	ALA	C-N-CA	11.09	139.56	123.14
1	A	175	GLY	CA-C-N	-11.07	101.77	121.14
1	A	175	GLY	C-N-CA	-11.07	101.77	121.14
1	D	175	GLY	CA-C-N	-11.05	101.80	121.14
1	D	175	GLY	C-N-CA	-11.05	101.80	121.14
1	D	251	LEU	O-C-N	-10.98	109.76	122.93
1	A	251	LEU	O-C-N	-10.96	109.78	122.93
1	D	46	GLU	CA-C-N	10.65	131.08	119.90
1	D	46	GLU	C-N-CA	10.65	131.08	119.90
1	A	210	PRO	CA-C-N	10.64	135.91	120.38
1	A	210	PRO	C-N-CA	10.64	135.91	120.38
1	A	46	GLU	CA-C-N	10.64	131.07	119.90
1	A	46	GLU	C-N-CA	10.64	131.07	119.90
1	D	210	PRO	CA-C-N	10.63	135.91	120.38
1	D	210	PRO	C-N-CA	10.63	135.91	120.38
1	A	175	GLY	O-C-N	-10.56	108.97	122.70
1	D	175	GLY	O-C-N	-10.55	108.99	122.70
1	D	211	ALA	CA-C-N	-10.48	106.37	121.99
1	D	211	ALA	C-N-CA	-10.48	106.37	121.99
1	A	211	ALA	CA-C-N	-10.47	106.38	121.99
1	A	211	ALA	C-N-CA	-10.47	106.38	121.99
1	A	176	ASN	N-CA-C	10.46	125.87	112.89
1	D	176	ASN	N-CA-C	10.46	125.86	112.89
1	D	181	ARG	CA-C-N	-10.20	101.09	122.41
1	D	181	ARG	C-N-CA	-10.20	101.09	122.41
1	A	181	ARG	CA-C-N	-10.20	101.10	122.41
1	A	181	ARG	C-N-CA	-10.20	101.10	122.41
1	A	219	LEU	O-C-N	9.88	135.73	122.59
1	D	219	LEU	O-C-N	9.87	135.72	122.59
1	A	202	ARG	N-CA-C	9.85	125.68	109.24
2	E	28	THR	CA-C-N	9.85	140.34	121.54
2	E	28	THR	C-N-CA	9.85	140.34	121.54
1	D	202	ARG	N-CA-C	9.84	125.68	109.24
2	B	28	THR	CA-C-N	9.84	140.33	121.54
2	B	28	THR	C-N-CA	9.84	140.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	O-C-N	-9.82	114.03	123.26
1	D	182	THR	O-C-N	-9.80	114.05	123.26
1	D	174	ASN	CA-C-N	-9.74	102.33	121.41
1	D	174	ASN	C-N-CA	-9.74	102.33	121.41
1	A	174	ASN	CA-C-N	-9.73	102.33	121.41
1	A	174	ASN	C-N-CA	-9.73	102.33	121.41
1	A	178	THR	O-C-N	-9.71	110.42	122.17
1	D	178	THR	O-C-N	-9.70	110.44	122.17
3	F	6	ILE	O-C-N	-9.68	110.47	122.57
3	C	6	ILE	O-C-N	-9.66	110.49	122.57
2	E	52	SER	CA-C-N	-9.61	106.00	121.86
2	E	52	SER	C-N-CA	-9.61	106.00	121.86
2	B	52	SER	CA-C-N	-9.61	106.01	121.86
2	B	52	SER	C-N-CA	-9.61	106.01	121.86
1	A	18	GLY	O-C-N	9.51	135.06	122.70
1	D	18	GLY	O-C-N	9.50	135.05	122.70
1	D	180	LEU	O-C-N	-9.48	109.73	122.43
1	A	180	LEU	O-C-N	-9.46	109.76	122.43
1	A	5	MET	O-C-N	-9.34	108.77	122.96
1	D	5	MET	O-C-N	-9.33	108.78	122.96
1	D	63	ILE	N-CA-C	9.33	119.30	110.53
1	A	63	ILE	N-CA-C	9.33	119.30	110.53
1	D	27	TYR	O-C-N	9.19	135.25	123.12
1	A	27	TYR	O-C-N	9.18	135.24	123.12
2	B	32	PRO	CA-C-N	9.16	131.29	119.84
2	B	32	PRO	C-N-CA	9.16	131.29	119.84
2	E	32	PRO	CA-C-N	9.13	131.26	119.84
2	E	32	PRO	C-N-CA	9.13	131.26	119.84
1	D	1	GLY	C-N-CD	-9.12	87.59	125.00
1	A	1	GLY	C-N-CD	-9.12	87.63	125.00
1	D	193	PRO	CA-C-N	-9.10	105.75	121.85
1	D	193	PRO	C-N-CA	-9.10	105.75	121.85
1	A	193	PRO	CA-C-N	-9.08	105.77	121.85
1	A	193	PRO	C-N-CA	-9.08	105.77	121.85
1	D	212	ASP	N-CA-C	9.08	122.74	108.67
1	A	212	ASP	N-CA-C	9.07	122.73	108.67
2	E	74	GLU	N-CA-C	-9.05	99.86	112.45
2	B	74	GLU	N-CA-C	-9.04	99.88	112.45
2	E	16	GLU	N-CA-C	-9.02	92.20	107.80
2	B	16	GLU	N-CA-C	-9.01	92.22	107.80
1	D	164	CYS	N-CA-C	8.95	120.96	111.03
1	A	164	CYS	N-CA-C	8.94	120.95	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASP	N-CA-C	-8.90	91.84	110.80
2	E	46	ILE	N-CA-C	8.90	117.87	107.73
2	B	46	ILE	N-CA-C	8.89	117.87	107.73
1	D	238	ASP	N-CA-C	-8.89	91.86	110.80
2	B	18	GLY	O-C-N	8.89	134.26	122.70
2	E	18	GLY	O-C-N	8.86	134.22	122.70
1	D	225	THR	O-C-N	8.54	133.51	122.06
1	A	103	VAL	N-CA-C	8.52	127.07	109.34
1	D	103	VAL	N-CA-C	8.52	127.06	109.34
1	A	225	THR	O-C-N	8.52	133.47	122.06
2	B	16	GLU	CA-C-N	-8.32	109.59	121.99
2	B	16	GLU	C-N-CA	-8.32	109.59	121.99
2	E	16	GLU	CA-C-N	-8.32	109.60	121.99
2	E	16	GLU	C-N-CA	-8.32	109.60	121.99
1	A	29	ASP	CA-C-N	8.21	134.09	120.70
1	A	29	ASP	C-N-CA	8.21	134.09	120.70
1	D	29	ASP	CA-C-N	8.20	134.07	120.70
1	D	29	ASP	C-N-CA	8.20	134.07	120.70
1	A	228	MET	O-C-N	-8.17	111.72	122.59
1	D	228	MET	O-C-N	-8.17	111.73	122.59
2	E	44	LYS	N-CA-C	8.05	121.54	109.95
2	E	53	ASP	N-CA-C	8.05	122.35	109.79
2	B	53	ASP	N-CA-C	8.03	122.32	109.79
2	B	44	LYS	N-CA-C	8.03	121.51	109.95
2	E	42	ASN	CB-CA-C	8.00	126.34	110.42
2	B	42	ASN	CB-CA-C	7.99	126.32	110.42
2	E	89	GLU	CB-CA-C	7.94	121.07	109.48
2	B	89	GLU	CB-CA-C	7.93	121.06	109.48
1	D	196	LYS	O-C-N	-7.93	110.63	122.28
1	A	196	LYS	O-C-N	-7.92	110.63	122.28
1	A	210	PRO	O-C-N	-7.78	112.62	123.05
1	D	210	PRO	O-C-N	-7.78	112.63	123.05
1	A	27	TYR	CA-C-N	-7.74	108.04	121.97
1	A	27	TYR	C-N-CA	-7.74	108.04	121.97
1	D	27	TYR	CA-C-N	-7.73	108.06	121.97
1	D	27	TYR	C-N-CA	-7.73	108.06	121.97
2	E	55	SER	N-CA-C	-7.64	97.78	109.85
2	B	55	SER	N-CA-C	-7.62	97.81	109.85
1	D	111	ARG	N-CA-C	7.58	121.58	108.76
1	A	111	ARG	N-CA-C	7.57	121.56	108.76
1	A	150	ALA	N-CA-C	7.57	122.18	112.34
1	D	150	ALA	N-CA-C	7.57	122.18	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	PRO	CA-N-CD	7.52	122.53	112.00
1	A	150	ALA	CA-C-N	-7.51	106.70	121.41
1	A	150	ALA	C-N-CA	-7.51	106.70	121.41
1	D	150	ALA	CA-C-N	-7.51	106.70	121.41
1	D	150	ALA	C-N-CA	-7.51	106.70	121.41
1	D	152	ALA	N-CA-C	-7.49	103.75	113.12
2	E	47	PRO	CA-N-CD	7.49	122.48	112.00
1	A	152	ALA	N-CA-C	-7.47	103.78	113.12
1	A	5	MET	CA-C-N	-7.44	108.68	121.85
1	A	5	MET	C-N-CA	-7.44	108.68	121.85
1	D	5	MET	CA-C-N	-7.43	108.70	121.85
1	D	5	MET	C-N-CA	-7.43	108.70	121.85
3	F	6	ILE	N-CA-C	7.37	124.66	109.34
1	D	166	GLU	N-CA-C	-7.36	102.28	111.11
1	A	166	GLU	N-CA-C	-7.34	102.30	111.11
3	C	6	ILE	N-CA-C	7.34	124.60	109.34
1	A	246	SER	N-CA-C	7.33	119.30	108.60
1	D	246	SER	N-CA-C	7.33	119.30	108.60
2	E	13	HIS	CA-C-N	-7.29	112.87	120.38
2	E	13	HIS	C-N-CA	-7.29	112.87	120.38
2	B	13	HIS	CA-C-N	-7.27	112.89	120.38
2	B	13	HIS	C-N-CA	-7.27	112.89	120.38
1	D	261	VAL	CB-CA-C	7.26	120.71	110.84
1	A	261	VAL	CB-CA-C	7.23	120.67	110.84
1	D	150	ALA	O-C-N	-7.20	112.97	122.33
3	C	5	ASN	O-C-N	-7.20	113.46	122.17
3	F	5	ASN	O-C-N	-7.18	113.48	122.17
1	A	209	TYR	C-N-CD	-7.17	95.58	125.00
1	D	209	TYR	C-N-CD	-7.17	95.59	125.00
1	D	11	ALA	N-CA-C	-7.17	96.65	108.76
2	E	56	PHE	N-CA-C	-7.17	98.41	109.52
1	A	150	ALA	O-C-N	-7.16	113.02	122.33
1	A	11	ALA	N-CA-C	-7.16	96.66	108.76
2	B	41	LYS	CB-CA-C	7.14	124.62	110.42
2	B	56	PHE	N-CA-C	-7.13	98.46	109.52
1	D	247	VAL	N-CA-C	7.13	118.99	108.65
1	A	247	VAL	N-CA-C	7.13	118.99	108.65
2	E	41	LYS	CB-CA-C	7.12	124.58	110.42
2	B	19	LYS	CA-C-N	6.98	128.45	120.98
2	B	19	LYS	C-N-CA	6.98	128.45	120.98
2	E	19	LYS	CA-C-N	6.98	128.45	120.98
2	E	19	LYS	C-N-CA	6.98	128.45	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	THR	N-CA-C	6.96	118.67	108.86
2	E	73	THR	N-CA-C	6.96	118.67	108.86
2	E	52	SER	N-CA-C	6.87	119.92	110.24
2	B	52	SER	N-CA-C	6.86	119.91	110.24
1	A	193	PRO	O-C-N	6.82	131.84	122.64
1	D	193	PRO	O-C-N	6.81	131.83	122.64
1	D	173	LYS	CA-C-N	-6.75	112.43	122.83
1	D	173	LYS	C-N-CA	-6.75	112.43	122.83
2	E	54	MET	N-CA-C	6.74	120.65	109.46
1	A	173	LYS	CA-C-N	-6.74	112.45	122.83
1	A	173	LYS	C-N-CA	-6.74	112.45	122.83
2	B	54	MET	N-CA-C	6.74	120.65	109.46
1	D	249	VAL	CA-C-N	-6.70	111.47	119.84
1	D	249	VAL	C-N-CA	-6.70	111.47	119.84
1	A	249	VAL	CA-C-N	-6.69	111.47	119.84
1	A	249	VAL	C-N-CA	-6.69	111.47	119.84
1	A	181	ARG	O-C-N	6.69	131.49	122.59
1	D	181	ARG	O-C-N	6.69	131.49	122.59
2	B	17	ASN	O-C-N	6.65	131.47	122.82
3	C	7	HIS	N-CA-CB	6.64	121.72	110.49
2	E	17	ASN	O-C-N	6.63	131.44	122.82
1	A	174	ASN	N-CA-C	-6.63	105.08	112.57
3	F	7	HIS	N-CA-CB	6.63	121.70	110.49
1	A	78	LEU	N-CA-C	-6.62	103.33	111.40
1	D	174	ASN	N-CA-C	-6.62	105.09	112.57
1	D	68	LYS	N-CA-C	-6.59	104.02	111.07
1	D	78	LEU	N-CA-C	-6.58	103.37	111.40
1	A	68	LYS	N-CA-C	-6.55	104.06	111.07
1	A	161	GLU	CA-C-N	-6.51	108.65	121.41
1	A	161	GLU	C-N-CA	-6.51	108.65	121.41
1	D	161	GLU	CA-C-N	-6.50	108.67	121.41
1	D	161	GLU	C-N-CA	-6.50	108.67	121.41
1	A	216	THR	N-CA-C	6.48	119.73	109.50
1	D	216	THR	N-CA-C	6.47	119.72	109.50
1	D	197	GLY	CA-C-N	6.46	133.88	121.54
1	D	197	GLY	C-N-CA	6.46	133.88	121.54
1	D	255	GLN	CA-C-N	-6.45	109.21	121.54
1	D	255	GLN	C-N-CA	-6.45	109.21	121.54
1	A	197	GLY	CA-C-N	6.45	133.86	121.54
1	A	197	GLY	C-N-CA	6.45	133.86	121.54
1	A	255	GLN	CA-C-N	-6.45	109.22	121.54
1	A	255	GLN	C-N-CA	-6.45	109.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	N-CA-C	6.40	120.19	112.38
1	D	130	LEU	N-CA-C	6.40	120.19	112.38
1	D	14	ARG	N-CA-C	-6.36	102.05	109.93
1	D	35	ARG	N-CA-C	-6.35	99.49	108.96
1	A	14	ARG	N-CA-C	-6.35	102.06	109.93
1	A	187	ALA	N-CA-C	6.34	119.75	110.17
1	A	36	PHE	N-CA-C	-6.34	98.74	108.76
1	D	187	ALA	N-CA-C	6.34	119.74	110.17
1	A	127	ASN	N-CA-C	6.33	119.10	110.55
1	A	35	ARG	N-CA-C	-6.33	99.53	108.96
1	D	36	PHE	N-CA-C	-6.33	98.75	108.76
1	D	127	ASN	N-CA-C	6.33	119.10	110.55
2	B	19	LYS	C-N-CD	-6.32	99.08	125.00
2	E	19	LYS	C-N-CD	-6.32	99.08	125.00
2	E	70	PHE	N-CA-C	6.30	118.75	108.55
2	B	70	PHE	N-CA-C	6.29	118.75	108.55
1	D	25	VAL	N-CA-C	6.23	116.84	107.80
1	A	25	VAL	N-CA-C	6.19	116.77	107.80
2	B	67	HIS	N-CA-C	6.14	123.87	110.80
2	E	67	HIS	N-CA-C	6.13	123.86	110.80
1	A	29	ASP	O-C-N	6.02	130.60	122.59
1	D	29	ASP	O-C-N	6.01	130.58	122.59
1	A	62	ARG	N-CA-C	-6.00	101.48	111.37
1	D	62	ARG	N-CA-C	-6.00	101.48	111.37
2	B	68	THR	N-CA-C	5.99	119.73	108.65
1	A	223	GLU	CB-CA-C	-5.98	100.94	110.81
1	D	223	GLU	CB-CA-C	-5.98	100.95	110.81
2	E	68	THR	N-CA-C	5.97	119.70	108.65
1	A	231	VAL	CA-C-N	5.92	129.17	120.82
1	A	231	VAL	C-N-CA	5.92	129.17	120.82
2	E	13	HIS	N-CA-C	-5.92	98.82	108.82
1	A	57	PRO	N-CA-C	-5.90	107.90	114.92
2	B	13	HIS	N-CA-C	-5.90	98.85	108.82
1	D	231	VAL	CA-C-N	5.89	129.13	120.82
1	D	231	VAL	C-N-CA	5.89	129.13	120.82
1	D	57	PRO	N-CA-C	-5.89	107.91	114.92
1	A	222	GLU	CB-CA-C	5.86	121.03	109.66
3	C	5	ASN	N-CA-CB	-5.85	101.47	110.13
3	F	5	ASN	N-CA-CB	-5.85	101.48	110.13
1	D	222	GLU	CB-CA-C	5.83	120.98	109.66
1	A	125	ALA	N-CA-C	5.82	118.96	109.06
1	D	125	ALA	N-CA-C	5.79	118.90	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	CA-CB-CG	5.78	125.66	114.10
1	D	62	ARG	CA-CB-CG	5.77	125.65	114.10
2	E	75	THR	N-CA-C	5.76	123.08	110.80
1	A	32	GLU	O-C-N	-5.76	114.93	122.59
2	B	75	THR	N-CA-C	5.76	123.07	110.80
1	D	247	VAL	CB-CA-C	-5.73	101.52	110.52
1	D	32	GLU	O-C-N	-5.73	114.97	122.59
1	A	56	GLY	CA-C-N	5.73	127.64	121.00
1	A	56	GLY	C-N-CA	5.73	127.64	121.00
2	E	83	LYS	N-CA-C	-5.73	100.34	109.96
1	A	247	VAL	CB-CA-C	-5.72	101.54	110.52
2	B	83	LYS	N-CA-C	-5.71	100.36	109.96
1	D	56	GLY	CA-C-N	5.70	127.61	121.00
1	D	56	GLY	C-N-CA	5.70	127.61	121.00
1	A	264	GLU	CA-C-N	5.66	132.51	121.41
1	A	264	GLU	C-N-CA	5.66	132.51	121.41
1	D	264	GLU	CA-C-N	5.66	132.50	121.41
1	D	264	GLU	C-N-CA	5.66	132.50	121.41
2	B	35	ILE	N-CA-C	5.60	116.74	108.45
1	D	211	ALA	N-CA-C	5.57	118.88	111.75
1	A	211	ALA	N-CA-C	5.57	118.88	111.75
2	E	35	ILE	N-CA-C	5.57	116.69	108.45
1	D	39	ASP	N-CA-C	5.56	118.27	111.82
1	A	62	ARG	CG-CD-NE	5.55	124.20	112.00
1	D	62	ARG	CG-CD-NE	5.55	124.20	112.00
2	E	77	THR	CB-CA-C	-5.54	100.60	109.75
1	A	156	TYR	CA-C-N	5.53	129.12	120.82
1	A	156	TYR	C-N-CA	5.53	129.12	120.82
1	D	156	TYR	CA-C-N	5.53	129.11	120.82
1	D	156	TYR	C-N-CA	5.53	129.11	120.82
2	B	77	THR	CB-CA-C	-5.53	100.63	109.75
1	A	39	ASP	N-CA-C	5.52	118.22	111.82
2	B	59	ASP	N-CA-C	-5.52	105.86	112.59
1	A	213	ILE	CB-CA-C	-5.50	104.15	111.80
2	E	59	ASP	N-CA-C	-5.50	105.88	112.59
1	A	177	ALA	O-C-N	5.50	127.94	122.12
1	D	213	ILE	CB-CA-C	-5.50	104.16	111.80
1	D	177	ALA	O-C-N	5.49	127.94	122.12
1	D	194	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	A	133	TRP	N-CA-C	5.41	118.53	110.14
1	D	133	TRP	N-CA-C	5.41	118.53	110.14
1	A	30	ASN	CB-CA-C	5.41	118.70	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ASN	CB-CA-C	5.40	118.69	110.37
1	D	235	PRO	O-C-N	5.40	129.93	122.64
1	A	235	PRO	O-C-N	5.40	129.93	122.64
1	A	244	TRP	CA-CB-CG	5.39	123.85	113.60
3	C	9	PHE	N-CA-C	5.39	126.11	111.00
1	D	214	THR	N-CA-C	-5.39	99.90	109.06
1	D	244	TRP	CA-CB-CG	5.39	123.84	113.60
3	F	9	PHE	N-CA-C	5.39	126.09	111.00
1	A	214	THR	N-CA-C	-5.39	99.90	109.06
1	A	194	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	D	234	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	234	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	B	58	LYS	N-CA-C	5.30	122.10	110.80
1	D	181	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	E	58	LYS	N-CA-C	5.30	122.08	110.80
1	A	181	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	251	LEU	CA-C-N	-5.28	111.06	121.41
1	A	251	LEU	C-N-CA	-5.28	111.06	121.41
1	D	251	LEU	CA-C-N	-5.27	111.08	121.41
1	D	251	LEU	C-N-CA	-5.27	111.08	121.41
2	B	48	LYS	O-C-N	5.27	129.28	122.43
2	E	48	LYS	O-C-N	5.24	129.24	122.43
1	A	49	ALA	N-CA-C	-5.21	100.01	109.44
1	D	45	TYR	N-CA-C	-5.20	101.24	109.76
1	A	220	ASN	N-CA-C	-5.19	108.70	114.62
3	C	5	ASN	N-CA-C	5.19	117.73	111.40
1	D	49	ALA	N-CA-C	-5.19	100.04	109.44
1	A	45	TYR	N-CA-C	-5.18	101.26	109.76
3	F	5	ASN	N-CA-C	5.17	117.71	111.40
1	D	72	GLN	N-CA-C	5.17	119.07	112.87
1	D	220	ASN	N-CA-C	-5.17	108.73	114.62
1	A	198	GLU	N-CA-C	-5.16	99.82	110.80
1	D	198	GLU	N-CA-C	-5.15	99.83	110.80
2	E	51	MET	CA-C-N	5.15	128.16	120.90
2	E	51	MET	C-N-CA	5.15	128.16	120.90
2	B	51	MET	CA-C-N	5.15	128.16	120.90
2	B	51	MET	C-N-CA	5.15	128.16	120.90
2	E	51	MET	N-CA-C	5.14	116.99	107.73
1	A	72	GLN	N-CA-C	5.14	119.03	112.87
2	B	51	MET	N-CA-C	5.13	116.97	107.73
1	A	257	TYR	N-CA-C	-5.13	100.81	109.07
1	A	252	GLY	N-CA-C	-5.12	101.04	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	GLY	N-CA-C	-5.12	101.04	113.18
1	D	257	TYR	N-CA-C	-5.12	100.82	109.07
2	E	54	MET	CB-CG-SD	-5.11	97.38	112.70
2	B	54	MET	CB-CG-SD	-5.10	97.41	112.70
1	A	193	PRO	N-CA-C	-5.09	101.99	112.47
1	D	193	PRO	N-CA-C	-5.08	101.99	112.47
1	A	161	GLU	O-C-N	-5.04	115.07	122.43
2	E	71	THR	CA-C-N	5.04	125.03	119.89
2	E	71	THR	C-N-CA	5.04	125.03	119.89
1	D	161	GLU	O-C-N	-5.03	115.09	122.43
2	B	94	TYR	N-CA-C	5.02	118.25	110.17
2	E	94	TYR	N-CA-C	5.01	118.24	110.17
2	B	71	THR	CA-C-N	5.01	125.00	119.89
2	B	71	THR	C-N-CA	5.01	125.00	119.89

There are no chirality outliers.

All (148) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	Mainchain,Peptide
1	A	127	ASN	Mainchain,Peptide
1	A	128	GLU	Mainchain
1	A	129	ASP	Mainchain,Peptide
1	A	130	LEU	Mainchain
1	A	131	LYS	Mainchain
1	A	150	ALA	Mainchain
1	A	16	GLY	Mainchain,Peptide
1	A	163	GLU	Mainchain
1	A	17	LEU	Mainchain,Peptide
1	A	173	LYS	Mainchain
1	A	175	GLY	Mainchain,Peptide
1	A	176	ASN	Mainchain
1	A	177	ALA	Mainchain
1	A	179	LEU	Mainchain
1	A	180	LEU	Mainchain,Peptide
1	A	181	ARG	Mainchain
1	A	182	THR	Mainchain
1	A	195	SER	Peptide
1	A	196	LYS	Mainchain,Peptide
1	A	197	GLY	Mainchain
1	A	2	PRO	Peptide
1	A	205	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	206	LEU	Mainchain
1	A	209	TYR	Mainchain,Peptide
1	A	210	PRO	Peptide
1	A	218	GLN	Mainchain
1	A	219	LEU	Peptide
1	A	224	LEU	Peptide
1	A	227	ASP	Peptide
1	A	229	GLU	Mainchain
1	A	233	THR	Mainchain
1	A	236	ALA	Mainchain,Peptide
1	A	237	GLY	Mainchain,Peptide
1	A	251	LEU	Mainchain
1	A	252	GLY	Mainchain
1	A	254	GLU	Peptide
1	A	255	GLN	Mainchain
1	A	256	ASN	Mainchain,Peptide
1	A	263	HIS	Mainchain
1	A	264	GLU	Mainchain
1	A	266	LEU	Mainchain
1	A	28	VAL	Mainchain
1	A	29	ASP	Mainchain
1	A	3	HIS	Peptide
1	A	30	ASN	Mainchain
1	A	32	GLU	Mainchain
1	A	85	TYR	Sidechain
2	B	10	TYR	Sidechain
2	B	19	LYS	Mainchain
2	B	31	HIS	Mainchain,Peptide
2	B	46	ILE	Mainchain
2	B	47	PRO	Mainchain,Peptide
2	B	48	LYS	Mainchain
2	B	52	SER	Mainchain,Peptide
2	B	53	ASP	Mainchain
2	B	78	TYR	Sidechain
3	C	5	ASN	Mainchain
3	C	6	ILE	Mainchain
1	D	1	GLY	Mainchain,Peptide
1	D	127	ASN	Mainchain,Peptide
1	D	128	GLU	Mainchain
1	D	129	ASP	Mainchain,Peptide
1	D	130	LEU	Mainchain
1	D	131	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	D	150	ALA	Mainchain
1	D	16	GLY	Mainchain,Peptide
1	D	163	GLU	Mainchain
1	D	17	LEU	Mainchain,Peptide
1	D	173	LYS	Mainchain
1	D	175	GLY	Mainchain,Peptide
1	D	176	ASN	Mainchain
1	D	177	ALA	Mainchain
1	D	179	LEU	Mainchain
1	D	180	LEU	Mainchain,Peptide
1	D	181	ARG	Mainchain
1	D	182	THR	Mainchain
1	D	195	SER	Peptide
1	D	196	LYS	Mainchain,Peptide
1	D	197	GLY	Mainchain
1	D	2	PRO	Peptide
1	D	205	ALA	Peptide
1	D	206	LEU	Mainchain
1	D	209	TYR	Mainchain,Peptide
1	D	210	PRO	Peptide
1	D	218	GLN	Mainchain
1	D	219	LEU	Peptide
1	D	224	LEU	Peptide
1	D	227	ASP	Peptide
1	D	229	GLU	Mainchain
1	D	233	THR	Mainchain
1	D	236	ALA	Mainchain,Peptide
1	D	237	GLY	Mainchain,Peptide
1	D	251	LEU	Mainchain
1	D	252	GLY	Mainchain
1	D	254	GLU	Peptide
1	D	255	GLN	Mainchain
1	D	256	ASN	Mainchain,Peptide
1	D	263	HIS	Mainchain
1	D	264	GLU	Mainchain
1	D	266	LEU	Mainchain
1	D	28	VAL	Mainchain
1	D	29	ASP	Mainchain
1	D	3	HIS	Peptide
1	D	30	ASN	Mainchain
1	D	32	GLU	Mainchain
1	D	85	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	E	10	TYR	Sidechain
2	E	19	LYS	Mainchain
2	E	31	HIS	Mainchain,Peptide
2	E	46	ILE	Mainchain
2	E	47	PRO	Mainchain,Peptide
2	E	48	LYS	Mainchain
2	E	52	SER	Mainchain,Peptide
2	E	53	ASP	Mainchain
2	E	78	TYR	Sidechain
3	F	5	ASN	Mainchain
3	F	6	ILE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2184	0	2043	507	14
1	D	2184	0	2045	498	17
2	B	820	0	795	144	0
2	E	820	0	795	151	2
3	C	80	0	72	22	2
3	F	80	0	72	23	2
All	All	6168	0	5822	1249	29

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 104.

All (1249) 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:2:PRO:HA	1:A:3:HIS:CD2	1.24	1.70
1:D:2:PRO:HA	1:D:3:HIS:CD2	1.25	1.65
2:B:20:PRO:CG	2:B:20:PRO:CB	1.79	1.61
2:E:47:PRO:CB	2:E:47:PRO:CG	1.76	1.59
2:E:20:PRO:CG	2:E:20:PRO:CB	1.79	1.58
2:B:47:PRO:CD	2:B:47:PRO:CG	1.80	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:CG	2:B:47:PRO:CB	1.76	1.57
2:B:20:PRO:CG	2:B:20:PRO:CD	1.81	1.57
2:E:47:PRO:CG	2:E:47:PRO:CD	1.80	1.56
2:E:20:PRO:CG	2:E:20:PRO:CD	1.81	1.56
1:D:2:PRO:CA	1:D:3:HIS:CD2	1.92	1.53
1:A:2:PRO:CA	1:A:3:HIS:CD2	1.92	1.50
2:E:47:PRO:CD	2:E:47:PRO:N	1.75	1.48
2:B:47:PRO:CD	2:B:47:PRO:N	1.75	1.46
2:E:20:PRO:CD	2:E:20:PRO:N	1.76	1.46
2:B:20:PRO:CD	2:B:20:PRO:N	1.76	1.44
2:B:51:MET:SD	2:B:51:MET:CE	2.04	1.44
2:E:51:MET:SD	2:E:51:MET:CE	2.04	1.44
1:A:3:HIS:N	1:A:103:VAL:HG11	1.29	1.43
1:D:253:LYS:CD	1:D:255:GLN:NE2	1.80	1.43
1:D:183:ASP:N	1:D:209:TYR:HB2	1.34	1.42
1:D:3:HIS:N	1:D:103:VAL:HG11	1.29	1.40
1:A:253:LYS:CD	1:A:255:GLN:NE2	1.80	1.40
1:A:181:ARG:HH12	2:E:20:PRO:CD	1.31	1.39
1:A:3:HIS:CB	1:A:103:VAL:HG21	1.53	1.39
1:A:183:ASP:N	1:A:209:TYR:HB2	1.34	1.38
1:D:3:HIS:CB	1:D:103:VAL:HG21	1.53	1.37
1:A:253:LYS:CD	1:A:255:GLN:HE21	1.34	1.37
2:B:20:PRO:HG3	1:D:181:ARG:NH1	1.39	1.33
1:D:253:LYS:CD	1:D:255:GLN:HE21	1.34	1.33
1:D:253:LYS:CE	1:D:255:GLN:HE22	1.41	1.33
1:A:253:LYS:CE	1:A:255:GLN:NE2	1.91	1.33
1:A:253:LYS:CE	1:A:255:GLN:HE22	1.41	1.32
1:D:101:CYS:SG	1:D:164:CYS:HB2	1.70	1.30
1:D:208:PHE:HD1	1:D:209:TYR:O	1.10	1.30
1:D:253:LYS:CE	1:D:255:GLN:NE2	1.91	1.30
1:A:101:CYS:SG	1:A:164:CYS:HB2	1.70	1.29
1:A:3:HIS:O	1:A:103:VAL:HB	1.13	1.26
1:A:208:PHE:HD1	1:A:209:TYR:O	1.10	1.26
1:D:3:HIS:O	1:D:103:VAL:HB	1.13	1.24
1:A:253:LYS:CG	1:A:255:GLN:NE2	2.00	1.24
1:D:253:LYS:CG	1:D:255:GLN:NE2	2.00	1.24
1:D:3:HIS:HB2	1:D:103:VAL:CG2	1.66	1.23
1:A:3:HIS:HB2	1:A:103:VAL:CG2	1.66	1.23
1:A:208:PHE:CD1	1:A:209:TYR:O	1.93	1.22
1:D:208:PHE:CD1	1:D:209:TYR:O	1.93	1.20
1:A:3:HIS:O	1:A:103:VAL:CB	1.89	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CB	1:A:210:PRO:HD3	1.70	1.20
1:A:253:LYS:CG	1:A:255:GLN:HE21	1.52	1.20
1:A:253:LYS:HE3	1:A:255:GLN:NE2	1.52	1.19
1:D:3:HIS:O	1:D:103:VAL:CB	1.89	1.19
1:D:209:TYR:CB	1:D:210:PRO:HD3	1.70	1.18
1:D:253:LYS:CG	1:D:255:GLN:HE21	1.52	1.18
1:A:183:ASP:HB2	1:A:209:TYR:N	1.57	1.17
1:D:253:LYS:HE3	1:D:255:GLN:NE2	1.52	1.17
1:D:195:SER:OG	1:D:198:GLU:HB2	1.45	1.16
1:D:237:GLY:O	1:D:238:ASP:O	1.63	1.16
1:D:183:ASP:HB2	1:D:209:TYR:N	1.57	1.15
1:A:3:HIS:H	1:A:103:VAL:CG1	1.60	1.15
1:A:237:GLY:O	1:A:238:ASP:O	1.63	1.15
1:A:195:SER:OG	1:A:198:GLU:HB2	1.45	1.14
1:D:3:HIS:H	1:D:103:VAL:CG1	1.60	1.14
1:A:181:ARG:NH1	2:E:20:PRO:CD	2.11	1.14
2:B:3:LYS:HB2	2:B:30:PHE:HA	1.28	1.14
2:B:41:LYS:O	2:B:77:THR:O	1.66	1.14
2:E:3:LYS:HB2	2:E:30:PHE:HA	1.28	1.14
2:E:41:LYS:O	2:E:77:THR:O	1.66	1.13
1:D:28:VAL:O	1:D:28:VAL:CG2	1.92	1.13
2:E:32:PRO:HD2	2:E:84:HIS:CE1	1.85	1.12
2:B:32:PRO:HD2	2:B:84:HIS:CE1	1.85	1.11
1:A:195:SER:HB3	1:A:198:GLU:O	1.50	1.11
2:B:28:THR:HG22	2:B:29:GLN:HE21	1.15	1.11
1:A:209:TYR:HB3	1:A:210:PRO:CD	1.79	1.10
1:D:180:LEU:O	1:D:181:ARG:O	1.69	1.10
1:D:209:TYR:HB3	1:D:210:PRO:CD	1.79	1.10
1:A:5:MET:CG	1:A:101:CYS:H	1.63	1.10
1:D:5:MET:CG	1:D:101:CYS:H	1.63	1.10
1:A:253:LYS:HD2	1:A:255:GLN:HE21	1.17	1.10
1:D:195:SER:HB3	1:D:198:GLU:O	1.50	1.10
2:E:28:THR:HG22	2:E:29:GLN:HE21	1.15	1.09
1:A:180:LEU:O	1:A:181:ARG:O	1.69	1.09
1:A:219:LEU:O	1:A:256:ASN:O	1.70	1.09
1:D:219:LEU:O	1:D:256:ASN:O	1.70	1.09
1:D:253:LYS:HD2	1:D:255:GLN:HE21	1.17	1.08
2:B:32:PRO:CD	2:B:84:HIS:CE1	2.37	1.07
1:D:183:ASP:N	1:D:209:TYR:CB	2.17	1.07
1:A:5:MET:HG3	1:A:100:GLY:HA2	1.35	1.07
1:D:5:MET:HG3	1:D:100:GLY:HA2	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:PRO:CD	2:E:84:HIS:CE1	2.37	1.07
1:A:28:VAL:O	1:A:28:VAL:CG2	1.92	1.07
1:A:5:MET:HG2	1:A:101:CYS:SG	1.95	1.06
1:A:183:ASP:N	1:A:209:TYR:CB	2.17	1.06
1:A:181:ARG:HH12	2:E:20:PRO:HD2	0.93	1.05
1:D:183:ASP:H	1:D:209:TYR:CB	1.69	1.05
1:D:5:MET:HG2	1:D:101:CYS:SG	1.95	1.05
1:A:183:ASP:H	1:A:209:TYR:CB	1.69	1.05
1:D:3:HIS:CD2	1:D:104:GLY:O	2.10	1.05
1:D:183:ASP:CB	1:D:209:TYR:H	1.70	1.04
2:B:47:PRO:CG	2:B:47:PRO:N	2.20	1.04
2:B:32:PRO:HD3	2:B:84:HIS:HE1	1.22	1.04
1:A:183:ASP:CB	1:A:209:TYR:H	1.70	1.04
2:E:28:THR:HG22	2:E:29:GLN:NE2	1.73	1.03
1:A:3:HIS:CD2	1:A:104:GLY:O	2.10	1.03
1:D:219:LEU:HD23	1:D:224:LEU:CD2	1.88	1.03
1:A:219:LEU:HD23	1:A:224:LEU:CD2	1.89	1.03
1:A:181:ARG:NH1	2:E:20:PRO:HD3	1.72	1.02
2:B:20:PRO:CG	2:B:20:PRO:N	2.23	1.02
2:E:47:PRO:CG	2:E:47:PRO:N	2.20	1.02
1:A:2:PRO:HA	1:A:3:HIS:NE2	1.53	1.02
2:B:28:THR:HG22	2:B:29:GLN:NE2	1.73	1.02
1:D:5:MET:CB	1:D:101:CYS:H	1.72	1.02
1:D:237:GLY:O	1:D:238:ASP:C	1.94	1.02
1:A:5:MET:CB	1:A:101:CYS:H	1.72	1.01
2:E:20:PRO:CG	2:E:20:PRO:N	2.23	1.01
1:D:263:HIS:H	1:D:266:LEU:HD22	1.25	1.01
1:A:3:HIS:N	1:A:103:VAL:CG1	2.20	1.01
1:A:250:PRO:HB2	1:A:253:LYS:CB	1.91	1.00
1:A:263:HIS:H	1:A:266:LEU:HD22	1.25	1.00
1:D:220:ASN:OD1	1:D:256:ASN:CA	1.99	1.00
1:A:219:LEU:HD23	1:A:224:LEU:HD21	1.41	1.00
1:D:250:PRO:HB2	1:D:253:LYS:HB2	1.42	1.00
1:D:29:ASP:CG	1:D:179:LEU:HD13	1.87	1.00
1:D:250:PRO:HB2	1:D:253:LYS:CB	1.92	1.00
1:D:253:LYS:HG3	1:D:255:GLN:CG	1.92	1.00
1:A:220:ASN:OD1	1:A:256:ASN:CA	1.99	0.99
1:A:29:ASP:CG	1:A:179:LEU:HD13	1.87	0.99
1:A:253:LYS:HG3	1:A:255:GLN:CG	1.92	0.99
1:D:2:PRO:HA	1:D:3:HIS:NE2	1.53	0.99
2:E:32:PRO:HD3	2:E:84:HIS:HE1	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PRO:HB2	1:A:253:LYS:HB2	1.42	0.99
1:D:28:VAL:O	1:D:28:VAL:HG23	1.20	0.99
1:D:29:ASP:H	1:D:31:LYS:H	1.00	0.99
1:A:28:VAL:O	1:A:28:VAL:HG23	1.20	0.99
1:A:219:LEU:CD2	1:A:224:LEU:CD2	2.41	0.98
1:D:5:MET:O	1:D:6:ARG:NE	1.96	0.98
1:A:237:GLY:O	1:A:238:ASP:C	1.94	0.98
1:D:219:LEU:CD2	1:D:224:LEU:CD2	2.41	0.98
1:A:2:PRO:HA	1:A:3:HIS:HD2	1.24	0.97
1:D:2:PRO:HA	1:D:3:HIS:HD2	1.24	0.97
1:A:33:PHE:CD1	1:A:51:TRP:CH2	2.52	0.97
1:A:181:ARG:HB3	2:E:19:LYS:HE2	1.45	0.97
2:B:19:LYS:C	2:B:20:PRO:CD	2.38	0.97
1:D:33:PHE:CD1	1:D:51:TRP:CH2	2.52	0.97
2:E:19:LYS:C	2:E:20:PRO:CD	2.38	0.97
1:D:219:LEU:HD23	1:D:224:LEU:HD21	1.41	0.96
1:A:5:MET:O	1:A:6:ARG:NE	1.96	0.96
1:A:181:ARG:CB	2:E:19:LYS:HE2	1.48	0.96
1:D:3:HIS:CA	1:D:103:VAL:HG11	1.94	0.96
1:D:4:SER:OG	1:D:28:VAL:C	2.09	0.96
1:A:3:HIS:CA	1:A:103:VAL:HG11	1.94	0.96
1:D:3:HIS:N	1:D:103:VAL:CG1	2.20	0.96
1:D:207:GLY:HA2	1:D:241:PHE:O	1.66	0.96
1:A:172:LEU:O	1:A:176:ASN:ND2	2.00	0.95
1:A:195:SER:CB	1:A:198:GLU:HB2	1.96	0.95
1:A:4:SER:OG	1:A:28:VAL:C	2.09	0.95
1:D:58:GLU:HB2	1:D:62:ARG:CZ	1.97	0.95
1:D:195:SER:CB	1:D:198:GLU:HB2	1.96	0.95
1:D:220:ASN:OD1	1:D:256:ASN:C	2.10	0.95
1:A:207:GLY:HA2	1:A:241:PHE:O	1.66	0.94
1:D:172:LEU:O	1:D:176:ASN:ND2	2.00	0.94
1:A:29:ASP:H	1:A:31:LYS:H	1.00	0.94
1:A:220:ASN:OD1	1:A:256:ASN:C	2.10	0.94
1:D:206:LEU:HG	1:D:242:GLN:HG2	1.50	0.94
1:A:58:GLU:HB2	1:A:62:ARG:CZ	1.97	0.93
1:A:28:VAL:CG2	1:A:31:LYS:HB3	1.98	0.93
1:A:181:ARG:HH12	2:E:20:PRO:HD3	1.25	0.93
1:D:51:TRP:CZ3	1:D:52:MET:SD	2.62	0.93
1:A:181:ARG:CB	2:E:19:LYS:CE	2.36	0.93
1:A:234:ARG:NH2	2:B:10:TYR:HB3	1.83	0.93
1:A:209:TYR:HB3	1:A:210:PRO:HD3	0.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PRO:CA	1:D:3:HIS:NE2	2.02	0.92
1:D:209:TYR:HB3	1:D:210:PRO:HD3	0.94	0.92
1:A:103:VAL:HG13	1:A:104:GLY:H	1.34	0.92
1:D:28:VAL:CG2	1:D:31:LYS:HB3	1.98	0.92
1:D:234:ARG:NH2	2:E:10:TYR:HB3	1.83	0.92
1:A:2:PRO:CA	1:A:3:HIS:NE2	2.02	0.92
1:A:51:TRP:CZ3	1:A:52:MET:SD	2.62	0.92
1:A:181:ARG:NH1	2:E:20:PRO:HD2	1.77	0.92
1:A:206:LEU:HG	1:A:242:GLN:HG2	1.50	0.92
1:D:183:ASP:CA	1:D:209:TYR:HB2	2.00	0.92
1:A:253:LYS:HG3	1:A:255:GLN:HE21	1.35	0.91
1:D:3:HIS:O	1:D:103:VAL:CG1	2.18	0.91
1:D:79:ARG:HA	1:D:82:LEU:HD12	1.51	0.91
2:E:6:GLN:HE21	2:E:6:GLN:HA	1.35	0.91
1:A:79:ARG:HA	1:A:82:LEU:HD12	1.51	0.91
1:A:253:LYS:HG3	1:A:255:GLN:NE2	1.86	0.91
1:D:5:MET:HG3	1:D:100:GLY:CA	2.00	0.91
1:D:230:LEU:HA	1:D:245:ALA:HA	1.52	0.91
1:A:183:ASP:CA	1:A:209:TYR:HB2	2.00	0.91
1:A:234:ARG:NH2	2:B:10:TYR:CB	2.34	0.91
1:D:263:HIS:O	1:D:265:GLY:N	2.04	0.91
1:A:263:HIS:O	1:A:265:GLY:N	2.04	0.90
1:A:5:MET:HG3	1:A:100:GLY:CA	2.00	0.90
1:D:234:ARG:NH2	2:E:10:TYR:CB	2.34	0.90
1:D:253:LYS:HG3	1:D:255:GLN:HE21	1.35	0.90
1:D:21:ARG:HH12	2:E:54:MET:HE1	1.36	0.90
1:D:237:GLY:C	1:D:238:ASP:O	2.10	0.90
2:E:47:PRO:CG	2:E:47:PRO:CA	2.49	0.90
1:A:3:HIS:O	1:A:103:VAL:CG1	2.18	0.90
1:A:253:LYS:HD2	1:A:255:GLN:NE2	1.78	0.90
1:D:103:VAL:HG13	1:D:104:GLY:H	1.34	0.90
2:B:6:GLN:HA	2:B:6:GLN:HE21	1.35	0.90
1:D:253:LYS:HE3	1:D:255:GLN:HE22	0.73	0.90
2:B:47:PRO:CG	2:B:47:PRO:CA	2.49	0.90
2:E:32:PRO:CD	2:E:84:HIS:HE1	1.80	0.90
1:D:195:SER:OG	1:D:196:LYS:N	2.00	0.89
1:A:3:HIS:CE1	1:A:105:SER:HA	2.07	0.89
1:A:253:LYS:HE3	1:A:255:GLN:HE22	0.73	0.89
1:A:208:PHE:CZ	1:A:213:ILE:HG22	2.08	0.89
1:A:33:PHE:HD1	1:A:51:TRP:CH2	1.89	0.88
1:D:33:PHE:HD1	1:D:51:TRP:CH2	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HA	1:A:245:ALA:HA	1.52	0.88
1:D:208:PHE:CZ	1:D:213:ILE:HG22	2.08	0.88
2:B:32:PRO:CD	2:B:84:HIS:HE1	1.80	0.88
2:B:46:ILE:HD12	2:B:46:ILE:H	1.39	0.88
1:D:3:HIS:CE1	1:D:105:SER:HA	2.07	0.88
1:A:21:ARG:HH12	2:B:54:MET:HE1	1.36	0.88
1:A:181:ARG:HB3	2:E:19:LYS:CE	2.01	0.88
1:D:5:MET:CG	1:D:101:CYS:N	2.37	0.87
1:A:194:ARG:HG3	1:A:200:THR:HB	1.57	0.87
1:A:5:MET:CG	1:A:101:CYS:N	2.37	0.87
1:A:237:GLY:C	1:A:238:ASP:O	2.10	0.87
2:E:46:ILE:HD12	2:E:46:ILE:H	1.39	0.87
1:D:194:ARG:HG3	1:D:200:THR:HB	1.57	0.87
1:A:208:PHE:CD1	1:A:263:HIS:CE1	2.63	0.87
1:D:33:PHE:CE1	1:D:51:TRP:CZ2	2.63	0.86
2:B:32:PRO:HD3	2:B:84:HIS:CE1	2.06	0.86
1:A:3:HIS:NE2	1:A:105:SER:HA	1.90	0.86
2:E:20:PRO:CG	2:E:20:PRO:CA	2.54	0.86
2:B:20:PRO:CG	2:B:20:PRO:CA	2.54	0.86
1:D:253:LYS:HG3	1:D:255:GLN:NE2	1.86	0.86
2:B:46:ILE:O	2:B:48:LYS:N	2.09	0.85
1:D:208:PHE:CD1	1:D:263:HIS:CE1	2.63	0.85
1:A:33:PHE:CE1	1:A:51:TRP:CZ2	2.63	0.85
1:A:75:ARG:HH12	1:A:79:ARG:HH21	1.24	0.85
1:A:219:LEU:O	1:A:257:TYR:HA	1.76	0.85
1:D:3:HIS:NE2	1:D:105:SER:HA	1.90	0.85
1:D:195:SER:OG	1:D:198:GLU:CB	2.24	0.85
1:D:139:ALA:O	1:D:142:ILE:HG13	1.78	0.84
1:D:253:LYS:HG3	1:D:255:GLN:HG3	1.56	0.84
1:A:44:ARG:HG3	1:A:64:THR:HG21	1.58	0.84
1:D:44:ARG:HG3	1:D:64:THR:HG21	1.58	0.84
1:A:195:SER:OG	1:A:198:GLU:CB	2.25	0.84
2:E:46:ILE:O	2:E:48:LYS:N	2.09	0.84
1:D:219:LEU:O	1:D:257:TYR:HA	1.76	0.84
1:A:253:LYS:HG3	1:A:255:GLN:HG3	1.56	0.84
1:D:3:HIS:CG	1:D:103:VAL:HG21	2.13	0.83
1:A:195:SER:OG	1:A:196:LYS:N	2.00	0.83
1:A:3:HIS:CG	1:A:103:VAL:HG21	2.13	0.83
2:B:40:LEU:HA	2:B:44:LYS:O	1.78	0.83
1:D:183:ASP:H	1:D:209:TYR:HB2	0.96	0.83
1:D:75:ARG:HH12	1:D:79:ARG:HH21	1.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LYS:CG	1:D:255:GLN:CD	2.52	0.83
1:D:141:GLN:HE22	1:D:144:ARG:HH21	1.26	0.83
1:A:75:ARG:HB3	1:A:75:ARG:NH1	1.94	0.83
1:A:183:ASP:H	1:A:209:TYR:HB2	0.96	0.83
1:A:141:GLN:HE22	1:A:144:ARG:HH21	1.25	0.82
1:D:5:MET:HG2	1:D:101:CYS:H	1.43	0.82
2:E:40:LEU:HA	2:E:44:LYS:O	1.78	0.82
1:A:51:TRP:HZ3	1:A:52:MET:SD	2.02	0.82
2:E:32:PRO:HD2	2:E:84:HIS:NE2	1.94	0.82
2:B:24:ASN:ND2	2:B:65:LEU:HD11	1.94	0.82
1:D:225:THR:O	1:D:225:THR:HG22	1.78	0.82
2:E:24:ASN:ND2	2:E:65:LEU:HD11	1.94	0.82
2:E:32:PRO:HD3	2:E:84:HIS:CE1	2.06	0.82
1:A:139:ALA:O	1:A:142:ILE:HG13	1.78	0.82
2:E:39:MET:C	2:E:46:ILE:HG13	2.05	0.82
1:A:253:LYS:CG	1:A:255:GLN:CD	2.52	0.82
2:B:6:GLN:HA	2:B:6:GLN:NE2	1.94	0.82
1:D:219:LEU:CD2	1:D:224:LEU:HD22	2.10	0.82
2:B:39:MET:C	2:B:46:ILE:HG13	2.05	0.82
1:D:75:ARG:NH1	1:D:75:ARG:HB3	1.94	0.81
1:A:5:MET:HG2	1:A:101:CYS:H	1.43	0.81
1:D:33:PHE:CD1	1:D:51:TRP:HH2	1.99	0.81
1:A:96:GLN:NE2	2:B:31:HIS:NE2	2.29	0.81
1:D:96:GLN:NE2	2:E:31:HIS:NE2	2.29	0.81
1:A:195:SER:HG	1:A:198:GLU:HB2	1.43	0.81
1:D:51:TRP:HZ3	1:D:52:MET:SD	2.02	0.81
1:D:33:PHE:CE1	1:D:51:TRP:HZ2	1.99	0.81
1:D:253:LYS:HD2	1:D:255:GLN:NE2	1.78	0.81
1:A:33:PHE:CE1	1:A:51:TRP:HZ2	1.99	0.80
1:A:225:THR:HG22	1:A:225:THR:O	1.79	0.80
2:B:38:GLN:HB2	2:B:83:LYS:NZ	1.96	0.80
1:D:33:PHE:HE1	1:D:51:TRP:HZ2	1.28	0.80
2:E:17:ASN:HB3	2:E:97:ARG:HH12	1.45	0.80
1:A:52:MET:O	1:A:55:GLU:HB2	1.82	0.80
1:A:216:THR:HG21	1:A:223:GLU:HB3	1.64	0.80
1:A:219:LEU:CD2	1:A:224:LEU:HD22	2.10	0.80
1:A:33:PHE:CD1	1:A:51:TRP:HH2	1.99	0.80
1:A:63:ILE:HD11	3:C:2:PRO:HD3	1.62	0.80
1:D:52:MET:O	1:D:55:GLU:HB2	1.82	0.80
1:A:237:GLY:H	2:B:12:ARG:HE	1.28	0.80
2:B:32:PRO:HD2	2:B:84:HIS:NE2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PRO:HG3	1:D:181:ARG:HH11	1.44	0.80
1:D:29:ASP:N	1:D:31:LYS:H	1.79	0.80
1:A:2:PRO:C	1:A:3:HIS:CD2	2.60	0.80
2:B:17:ASN:HB3	2:B:97:ARG:HH12	1.45	0.80
1:D:63:ILE:HD11	3:F:2:PRO:HD3	1.62	0.79
1:A:75:ARG:HB3	1:A:75:ARG:CZ	2.12	0.79
2:E:39:MET:O	2:E:46:ILE:HG13	1.83	0.79
1:D:237:GLY:H	2:E:12:ARG:HE	1.28	0.79
2:E:38:GLN:HB2	2:E:83:LYS:NZ	1.96	0.79
1:D:57:PRO:HA	1:D:60:TRP:CD1	2.18	0.79
2:B:39:MET:O	2:B:46:ILE:HG13	1.83	0.79
1:A:75:ARG:NH1	1:A:79:ARG:HH21	1.80	0.79
1:D:2:PRO:C	1:D:3:HIS:CD2	2.60	0.79
1:A:33:PHE:HE1	1:A:51:TRP:CZ2	2.01	0.79
1:D:195:SER:HG	1:D:198:GLU:HB2	1.43	0.79
1:A:3:HIS:NE2	1:A:104:GLY:O	2.16	0.79
1:A:196:LYS:O	1:A:196:LYS:CG	2.30	0.78
2:E:6:GLN:HA	2:E:6:GLN:NE2	1.94	0.78
1:A:29:ASP:N	1:A:31:LYS:H	1.79	0.78
1:D:196:LYS:O	1:D:196:LYS:HG3	1.83	0.78
1:A:33:PHE:HE1	1:A:51:TRP:HZ2	1.28	0.78
1:D:33:PHE:HE1	1:D:51:TRP:CZ2	2.01	0.78
1:D:196:LYS:O	1:D:196:LYS:CG	2.30	0.78
1:D:216:THR:HG21	1:D:223:GLU:HB3	1.64	0.78
1:D:220:ASN:OD1	1:D:256:ASN:HA	1.84	0.78
1:A:181:ARG:CZ	2:E:20:PRO:HD3	2.13	0.78
1:D:28:VAL:HG22	1:D:31:LYS:HB3	1.65	0.78
1:D:75:ARG:NH1	1:D:79:ARG:HH21	1.80	0.78
2:E:17:ASN:HA	2:E:72:PRO:HG2	1.66	0.78
1:A:57:PRO:HA	1:A:60:TRP:CD1	2.18	0.78
1:D:75:ARG:HB3	1:D:75:ARG:CZ	2.12	0.77
2:B:17:ASN:HA	2:B:72:PRO:HG2	1.66	0.77
2:B:46:ILE:HD13	2:B:47:PRO:O	1.85	0.77
2:E:46:ILE:HD13	2:E:47:PRO:O	1.85	0.77
1:D:219:LEU:HD21	1:D:224:LEU:HD22	1.67	0.77
1:A:183:ASP:CB	1:A:209:TYR:HB2	2.14	0.77
1:A:196:LYS:O	1:A:196:LYS:HG3	1.83	0.77
1:D:123:TYR:CE1	3:F:9:PHE:HE1	2.03	0.77
1:A:220:ASN:OD1	1:A:256:ASN:HA	1.84	0.76
1:D:3:HIS:NE2	1:D:104:GLY:O	2.16	0.76
2:E:66:ALA:O	2:E:67:HIS:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:OD2	1:A:179:LEU:HD13	1.86	0.76
1:A:58:GLU:HB2	1:A:62:ARG:NE	2.00	0.76
1:A:123:TYR:CE1	3:C:9:PHE:HE1	2.03	0.76
1:D:183:ASP:CB	1:D:209:TYR:HB2	2.14	0.76
2:B:66:ALA:O	2:B:67:HIS:HB3	1.86	0.76
1:D:32:GLU:O	1:D:33:PHE:CD2	2.39	0.76
1:D:84:TYR:HB3	1:D:139:ALA:HB1	1.68	0.76
1:A:32:GLU:O	1:A:33:PHE:CD2	2.39	0.76
1:A:253:LYS:HG3	1:A:255:GLN:CD	2.11	0.76
1:A:28:VAL:HG22	1:A:31:LYS:HB3	1.65	0.76
1:A:84:TYR:HB3	1:A:139:ALA:HB1	1.68	0.75
1:D:58:GLU:HB2	1:D:62:ARG:NE	2.00	0.75
1:D:229:GLU:O	1:D:246:SER:N	2.18	0.75
2:B:28:THR:CG2	2:B:29:GLN:NE2	2.50	0.75
1:D:44:ARG:HA	1:D:64:THR:CG2	2.17	0.75
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.22	0.75
1:A:59:TYR:HA	1:A:62:ARG:HD2	1.69	0.75
1:D:5:MET:HG2	1:D:101:CYS:N	2.00	0.75
1:D:29:ASP:OD2	1:D:179:LEU:HD13	1.86	0.75
1:D:59:TYR:HA	1:D:62:ARG:HD2	1.69	0.75
1:D:229:GLU:HB3	1:D:244:TRP:CZ3	2.21	0.75
1:A:5:MET:HG2	1:A:101:CYS:N	2.00	0.75
1:D:146:LYS:HG3	1:D:147:TRP:N	2.01	0.75
1:A:3:HIS:H	1:A:103:VAL:HG11	0.86	0.75
1:A:181:ARG:HB3	2:E:19:LYS:NZ	2.01	0.75
1:D:263:HIS:N	1:D:266:LEU:HD22	2.01	0.75
1:A:146:LYS:HG3	1:A:147:TRP:N	2.01	0.75
1:A:229:GLU:O	1:A:246:SER:N	2.18	0.75
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.22	0.74
1:A:52:MET:HA	1:A:52:MET:HE3	1.68	0.74
1:A:219:LEU:HD21	1:A:224:LEU:HD22	1.67	0.74
1:D:253:LYS:CG	1:D:255:GLN:HG3	2.16	0.74
1:A:229:GLU:HB3	1:A:244:TRP:CZ3	2.21	0.74
1:A:263:HIS:N	1:A:266:LEU:HD22	2.01	0.74
1:A:2:PRO:N	1:A:3:HIS:CD2	2.52	0.74
1:D:52:MET:HE3	1:D:52:MET:HA	1.68	0.74
1:D:253:LYS:HG3	1:D:255:GLN:CD	2.10	0.74
1:A:44:ARG:HA	1:A:64:THR:CG2	2.17	0.74
1:A:126:LEU:HB2	1:A:133:TRP:CZ3	2.23	0.74
1:A:253:LYS:CG	1:A:255:GLN:HG3	2.16	0.74
1:A:33:PHE:CD1	1:A:51:TRP:CZ2	2.76	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:MET:HB2	1:D:101:CYS:O	1.88	0.73
2:E:33:PRO:HB3	2:E:62:PHE:CD2	2.24	0.73
2:E:28:THR:CG2	2:E:29:GLN:NE2	2.50	0.73
1:A:5:MET:HB2	1:A:101:CYS:O	1.88	0.73
1:D:44:ARG:CG	1:D:64:THR:HG21	2.18	0.73
1:A:28:VAL:HG23	1:A:31:LYS:HB3	1.71	0.73
1:A:181:ARG:NH2	2:E:20:PRO:HD3	2.04	0.73
1:D:253:LYS:CG	1:D:255:GLN:CG	2.67	0.73
1:D:33:PHE:CD1	1:D:51:TRP:CZ2	2.76	0.73
1:D:126:LEU:HB2	1:D:133:TRP:CZ3	2.23	0.73
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.19	0.72
1:D:202:ARG:HG3	1:D:204:TRP:HE1	1.53	0.72
1:D:28:VAL:HG23	1:D:31:LYS:HB3	1.71	0.72
1:D:208:PHE:HZ	1:D:213:ILE:HG22	1.54	0.72
1:A:44:ARG:CG	1:A:64:THR:HG21	2.18	0.72
1:A:194:ARG:HG3	1:A:200:THR:CB	2.19	0.72
2:E:35:ILE:HD11	2:E:82:VAL:CG1	2.19	0.72
2:B:33:PRO:HB3	2:B:62:PHE:CD2	2.24	0.72
1:A:237:GLY:H	2:B:12:ARG:NE	1.86	0.72
1:D:157:ARG:HH21	1:D:161:GLU:CD	1.98	0.72
1:A:202:ARG:HG3	1:A:204:TRP:HE1	1.53	0.71
1:A:208:PHE:CZ	1:A:213:ILE:CG2	2.73	0.71
2:E:51:MET:HB3	2:E:64:ILE:HD11	1.72	0.71
2:E:3:LYS:CB	2:E:30:PHE:HA	2.16	0.71
2:B:27:VAL:HG21	2:B:37:ILE:HD11	1.71	0.71
1:D:162:GLY:N	1:D:164:CYS:SG	2.63	0.71
1:D:194:ARG:HG3	1:D:200:THR:CB	2.19	0.71
1:D:237:GLY:H	2:E:12:ARG:NE	1.86	0.71
1:A:162:GLY:N	1:A:164:CYS:SG	2.63	0.71
1:A:157:ARG:HH21	1:A:161:GLU:CD	1.98	0.71
1:A:234:ARG:HH22	2:B:10:TYR:CB	2.02	0.71
1:A:253:LYS:CG	1:A:255:GLN:CG	2.67	0.71
1:D:208:PHE:CZ	1:D:213:ILE:CG2	2.73	0.71
1:D:250:PRO:HB2	1:D:253:LYS:HB3	1.71	0.71
1:D:126:LEU:HD22	1:D:133:TRP:CH2	2.26	0.71
1:D:195:SER:OG	1:D:198:GLU:N	2.24	0.71
1:A:195:SER:OG	1:A:198:GLU:N	2.24	0.70
1:A:126:LEU:HD22	1:A:133:TRP:CH2	2.26	0.70
2:E:27:VAL:HG21	2:E:37:ILE:HD11	1.71	0.70
1:A:208:PHE:HZ	1:A:213:ILE:HG22	1.54	0.70
1:D:5:MET:HB3	1:D:101:CYS:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ILE:O	1:D:66:ILE:HG22	1.92	0.70
2:E:55:SER:HB2	2:E:63:TYR:CE1	2.26	0.70
1:A:5:MET:HB3	1:A:101:CYS:H	1.56	0.70
1:D:2:PRO:N	1:D:3:HIS:CD2	2.52	0.70
1:A:263:HIS:C	1:A:265:GLY:H	2.00	0.70
1:A:209:TYR:O	1:A:263:HIS:CE1	2.45	0.70
1:D:28:VAL:O	1:D:29:ASP:OD1	2.10	0.70
1:A:57:PRO:HA	1:A:60:TRP:HD1	1.57	0.70
2:B:24:ASN:HD22	2:B:65:LEU:HD11	1.55	0.70
2:B:51:MET:HB3	2:B:64:ILE:HD11	1.72	0.70
1:D:263:HIS:C	1:D:265:GLY:H	2.00	0.70
1:D:234:ARG:HH22	2:E:10:TYR:CB	2.02	0.69
1:A:63:ILE:O	1:A:66:ILE:HG22	1.92	0.69
1:A:82:LEU:HD23	1:A:87:GLN:HB2	1.74	0.69
1:A:250:PRO:HB2	1:A:253:LYS:HB3	1.71	0.69
1:D:66:ILE:HD11	3:F:4:VAL:HG23	1.75	0.69
1:A:173:LYS:C	1:A:175:GLY:H	2.00	0.69
1:A:219:LEU:HD21	1:A:224:LEU:CD2	2.21	0.69
2:E:24:ASN:HD22	2:E:65:LEU:HD11	1.55	0.69
1:A:5:MET:CB	1:A:101:CYS:N	2.54	0.69
2:B:3:LYS:CB	2:B:30:PHE:HA	2.16	0.69
1:D:82:LEU:HD23	1:D:87:GLN:HB2	1.74	0.69
1:A:81:LEU:HD11	1:A:123:TYR:CE2	2.28	0.69
2:B:55:SER:HB2	2:B:63:TYR:CE1	2.26	0.69
1:A:28:VAL:O	1:A:29:ASP:OD1	2.10	0.69
1:A:66:ILE:HD11	3:C:4:VAL:HG23	1.75	0.69
1:D:206:LEU:HG	1:D:242:GLN:CG	2.23	0.69
1:D:209:TYR:O	1:D:263:HIS:CE1	2.45	0.69
1:D:81:LEU:HD11	1:D:123:TYR:CE2	2.28	0.68
1:D:123:TYR:HD1	1:D:124:ILE:HB	1.59	0.68
1:D:237:GLY:CA	1:D:238:ASP:O	2.41	0.68
2:B:20:PRO:HD3	1:D:181:ARG:HD3	1.73	0.68
1:A:47:PRO:HG3	1:A:53:GLU:OE1	1.93	0.68
1:D:47:PRO:HG3	1:D:53:GLU:OE1	1.93	0.68
1:D:5:MET:CB	1:D:101:CYS:N	2.54	0.68
1:A:59:TYR:CA	1:A:62:ARG:HH11	2.07	0.68
1:A:208:PHE:CE2	1:A:213:ILE:CG2	2.77	0.68
1:D:57:PRO:HA	1:D:60:TRP:HD1	1.57	0.68
1:D:135:ALA:HB2	1:D:144:ARG:HG3	1.76	0.68
1:D:208:PHE:CE2	1:D:213:ILE:HG21	2.29	0.68
1:A:202:ARG:HD2	1:A:204:TRP:CZ2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:TYR:CA	1:D:62:ARG:HH11	2.07	0.67
1:A:123:TYR:HD1	1:A:124:ILE:HB	1.59	0.67
1:A:135:ALA:HB2	1:A:144:ARG:HG3	1.76	0.67
1:A:208:PHE:CE2	1:A:213:ILE:HG21	2.29	0.67
1:D:33:PHE:CE1	1:D:51:TRP:CH2	2.82	0.67
1:A:77:ASN:HD22	3:C:9:PHE:HB2	1.60	0.67
2:B:36:GLU:O	2:B:82:VAL:HA	1.95	0.67
1:D:173:LYS:C	1:D:175:GLY:H	2.00	0.67
1:A:186:LYS:O	1:A:205:ALA:O	2.13	0.67
1:A:237:GLY:CA	1:A:238:ASP:O	2.41	0.67
1:D:186:LYS:O	1:D:205:ALA:O	2.13	0.67
2:E:41:LYS:O	2:E:78:TYR:HA	1.94	0.67
1:A:181:ARG:NH2	2:E:20:PRO:CD	2.58	0.67
1:A:266:LEU:HD23	1:A:266:LEU:O	1.95	0.67
1:D:3:HIS:HB2	1:D:103:VAL:HG21	0.73	0.67
1:A:3:HIS:HB2	1:A:103:VAL:HG21	0.73	0.67
2:E:36:GLU:O	2:E:82:VAL:HA	1.95	0.67
1:D:266:LEU:HD23	1:D:266:LEU:O	1.95	0.66
2:B:41:LYS:O	2:B:78:TYR:HA	1.94	0.66
1:D:208:PHE:CE2	1:D:213:ILE:CG2	2.77	0.66
1:A:3:HIS:C	1:A:103:VAL:HB	2.15	0.66
1:D:77:ASN:HD22	3:F:9:PHE:HB2	1.60	0.66
1:D:3:HIS:H	1:D:103:VAL:HG11	0.86	0.66
1:D:3:HIS:CB	1:D:103:VAL:CG2	2.47	0.66
1:D:202:ARG:HD2	1:D:204:TRP:CZ2	2.29	0.66
2:E:46:ILE:H	2:E:46:ILE:CD1	2.08	0.66
1:A:206:LEU:HG	1:A:242:GLN:CG	2.23	0.66
1:A:29:ASP:OD1	1:A:179:LEU:HD13	1.96	0.66
1:A:198:GLU:HB3	1:A:248:VAL:HG23	1.78	0.66
2:B:20:PRO:HG3	1:D:181:ARG:HH12	1.52	0.66
1:D:218:GLN:HA	1:D:222:GLU:O	1.96	0.66
1:D:123:TYR:CE1	3:F:9:PHE:CE1	2.84	0.65
1:D:198:GLU:HB3	1:D:248:VAL:HG23	1.78	0.65
1:D:229:GLU:O	1:D:245:ALA:HA	1.96	0.65
1:A:123:TYR:CE1	3:C:9:PHE:CE1	2.85	0.65
1:D:29:ASP:OD1	1:D:179:LEU:HD13	1.96	0.65
1:A:204:TRP:HE3	1:A:206:LEU:HD13	1.62	0.65
2:B:46:ILE:H	2:B:46:ILE:CD1	2.08	0.65
1:D:1:GLY:H2	1:D:105:SER:HA	1.62	0.65
1:A:33:PHE:CE1	1:A:51:TRP:CH2	2.82	0.65
1:D:3:HIS:CD2	1:D:104:GLY:C	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:CD2	1:A:104:GLY:C	2.75	0.65
1:A:123:TYR:CD1	1:A:124:ILE:HB	2.32	0.65
2:B:23:LEU:O	2:B:67:HIS:HB2	1.96	0.65
1:D:234:ARG:NH2	2:E:10:TYR:CG	2.65	0.65
2:E:23:LEU:O	2:E:67:HIS:HB2	1.96	0.65
1:A:218:GLN:HA	1:A:222:GLU:O	1.96	0.65
1:A:263:HIS:H	1:A:266:LEU:CD2	2.06	0.65
1:D:3:HIS:C	1:D:103:VAL:HB	2.15	0.65
1:D:59:TYR:HB2	1:D:62:ARG:NH1	2.12	0.65
1:D:224:LEU:C	1:D:226:GLN:H	2.05	0.65
1:A:234:ARG:NH2	2:B:10:TYR:CG	2.65	0.64
2:B:12:ARG:CB	2:B:22:ILE:HB	2.27	0.64
1:D:219:LEU:HA	1:D:257:TYR:CE1	2.32	0.64
2:E:12:ARG:CB	2:E:22:ILE:HB	2.27	0.64
2:E:19:LYS:CA	2:E:20:PRO:CD	2.75	0.64
1:A:229:GLU:O	1:A:245:ALA:HA	1.96	0.64
2:B:81:ARG:HG2	2:B:83:LYS:HE2	1.79	0.64
2:B:81:ARG:HA	2:B:91:LYS:O	1.97	0.64
1:A:108:ARG:CZ	1:A:108:ARG:HB2	2.28	0.64
1:D:75:ARG:HH12	1:D:79:ARG:NH2	1.94	0.64
1:D:123:TYR:CD1	1:D:124:ILE:HB	2.32	0.64
1:D:237:GLY:HA2	1:D:238:ASP:O	1.98	0.64
1:A:6:ARG:HE	1:A:100:GLY:HA3	1.63	0.64
1:A:219:LEU:HA	1:A:257:TYR:CE1	2.32	0.64
2:E:25:CYS:HB3	2:E:66:ALA:HB3	1.80	0.64
2:E:81:ARG:HG2	2:E:83:LYS:HE2	1.79	0.64
1:A:75:ARG:HH12	1:A:79:ARG:NH2	1.94	0.64
1:A:59:TYR:HB2	1:A:62:ARG:NH1	2.12	0.64
1:A:103:VAL:HG13	1:A:104:GLY:N	2.11	0.64
1:D:32:GLU:OE2	1:D:35:ARG:NH1	2.31	0.64
1:D:204:TRP:HE3	1:D:206:LEU:HD13	1.62	0.64
1:A:237:GLY:HA2	1:A:238:ASP:O	1.98	0.64
2:B:19:LYS:CA	2:B:20:PRO:CD	2.75	0.64
3:C:4:VAL:HG11	3:C:6:ILE:HD12	1.80	0.64
1:D:229:GLU:HB3	1:D:244:TRP:HZ3	1.63	0.64
1:A:32:GLU:O	1:A:33:PHE:CG	2.51	0.64
1:D:206:LEU:CD1	1:D:242:GLN:HB3	2.28	0.64
1:D:183:ASP:HB2	1:D:209:TYR:H	0.74	0.63
1:D:219:LEU:HD21	1:D:224:LEU:CD2	2.21	0.63
1:A:36:PHE:HB2	1:A:45:TYR:CD1	2.34	0.63
1:D:103:VAL:HG13	1:D:104:GLY:N	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:HB3	1:A:244:TRP:HZ3	1.63	0.63
1:D:6:ARG:HE	1:D:100:GLY:HA3	1.63	0.63
1:D:263:HIS:H	1:D:266:LEU:CD2	2.06	0.63
1:A:1:GLY:H2	1:A:105:SER:HA	1.63	0.63
2:E:81:ARG:HA	2:E:91:LYS:O	1.97	0.63
1:A:32:GLU:OE2	1:A:35:ARG:NH1	2.31	0.63
1:D:44:ARG:HA	1:D:64:THR:HG21	1.81	0.63
1:D:189:VAL:HA	1:D:202:ARG:O	1.98	0.63
1:A:73:TRP:CD1	1:A:74:PHE:N	2.66	0.63
1:A:206:LEU:CD1	1:A:242:GLN:HB3	2.28	0.63
1:D:73:TRP:CD1	1:D:74:PHE:N	2.66	0.63
1:D:163:GLU:O	1:D:167:TRP:HD1	1.81	0.63
1:A:224:LEU:C	1:A:226:GLN:H	2.05	0.63
1:D:36:PHE:HB2	1:D:45:TYR:CD1	2.34	0.63
1:D:230:LEU:N	1:D:230:LEU:HD23	2.14	0.63
1:A:146:LYS:O	1:A:149:GLN:HG3	1.99	0.62
1:A:183:ASP:HB2	1:A:209:TYR:H	0.74	0.62
1:A:189:VAL:HA	1:A:202:ARG:O	1.99	0.62
1:D:59:TYR:HB2	1:D:62:ARG:HH11	1.64	0.62
3:F:4:VAL:HG11	3:F:6:ILE:HD12	1.80	0.62
2:B:25:CYS:HB3	2:B:66:ALA:HB3	1.80	0.62
1:D:3:HIS:NE2	1:D:104:GLY:C	2.57	0.62
1:A:230:LEU:HD23	1:A:230:LEU:N	2.14	0.62
1:D:164:CYS:SG	1:D:165:VAL:HG23	2.39	0.62
1:A:51:TRP:HZ3	1:A:52:MET:CE	2.12	0.62
1:A:164:CYS:SG	1:A:165:VAL:HG23	2.39	0.62
1:D:32:GLU:O	1:D:33:PHE:CG	2.51	0.62
1:D:108:ARG:HB2	1:D:108:ARG:CZ	2.28	0.62
1:D:59:TYR:CA	1:D:62:ARG:HD2	2.29	0.62
1:A:3:HIS:NE2	1:A:104:GLY:C	2.57	0.62
1:A:190:THR:O	1:A:201:LEU:HA	1.99	0.62
1:A:44:ARG:HA	1:A:64:THR:HG21	1.81	0.62
1:D:84:TYR:CB	1:D:139:ALA:HB1	2.30	0.62
1:D:190:THR:O	1:D:201:LEU:HA	1.99	0.62
1:D:183:ASP:CB	1:D:209:TYR:CB	2.78	0.62
1:A:84:TYR:CB	1:A:139:ALA:HB1	2.30	0.61
1:A:183:ASP:CB	1:A:209:TYR:CB	2.78	0.61
2:B:36:GLU:CB	2:B:83:LYS:HB2	2.30	0.61
1:A:3:HIS:CG	1:A:103:VAL:CG2	2.82	0.61
1:D:3:HIS:CG	1:D:103:VAL:CG2	2.82	0.61
2:E:39:MET:C	2:E:40:LEU:HG	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:O	1:A:167:TRP:HD1	1.81	0.61
2:B:39:MET:C	2:B:40:LEU:HG	2.26	0.61
1:A:104:GLY:HA3	1:A:108:ARG:O	2.00	0.61
1:D:21:ARG:HH12	2:E:54:MET:CE	2.12	0.61
1:D:51:TRP:HZ3	1:D:52:MET:CE	2.12	0.61
1:D:208:PHE:HD1	1:D:263:HIS:CE1	2.17	0.61
1:A:59:TYR:CA	1:A:62:ARG:HD2	2.29	0.61
1:A:208:PHE:HD1	1:A:263:HIS:CE1	2.17	0.61
1:A:219:LEU:HD23	1:A:257:TYR:HE1	1.66	0.61
1:D:104:GLY:HA3	1:D:108:ARG:O	2.00	0.61
1:D:146:LYS:O	1:D:149:GLN:HG3	1.99	0.61
1:D:73:TRP:HD1	1:D:74:PHE:N	1.99	0.61
1:D:234:ARG:HH22	2:E:10:TYR:HB3	1.62	0.61
1:A:73:TRP:HD1	1:A:74:PHE:N	1.99	0.61
2:B:7:ILE:HD13	2:B:91:LYS:HD3	1.82	0.61
2:E:36:GLU:CB	2:E:83:LYS:HB2	2.30	0.61
1:A:3:HIS:C	1:A:103:VAL:HG11	2.25	0.61
1:A:2:PRO:CA	1:A:3:HIS:CG	2.77	0.61
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.36	0.61
1:D:219:LEU:HD23	1:D:257:TYR:HE1	1.65	0.61
1:D:5:MET:CE	1:D:101:CYS:SG	2.89	0.60
1:A:181:ARG:CZ	2:E:20:PRO:CD	2.76	0.60
1:A:234:ARG:NH2	2:B:10:TYR:CD2	2.70	0.60
1:D:185:PRO:HD3	1:D:263:HIS:CD2	2.36	0.60
1:D:180:LEU:O	1:D:181:ARG:C	2.37	0.60
1:D:198:GLU:HB3	1:D:248:VAL:CG2	2.32	0.60
1:A:5:MET:CE	1:A:101:CYS:SG	2.89	0.60
2:B:36:GLU:HB3	2:B:83:LYS:HB2	1.81	0.60
1:D:44:ARG:HA	1:D:64:THR:HG23	1.84	0.60
1:A:16:GLY:O	1:A:17:LEU:HG	2.02	0.60
1:A:176:ASN:O	1:A:179:LEU:N	2.35	0.60
1:D:16:GLY:O	1:D:17:LEU:HG	2.02	0.60
1:D:176:ASN:O	1:D:179:LEU:N	2.35	0.60
1:D:3:HIS:C	1:D:103:VAL:HG11	2.25	0.60
1:A:21:ARG:HH12	2:B:54:MET:CE	2.12	0.60
1:A:21:ARG:NH1	2:B:54:MET:HE1	2.14	0.60
1:A:5:MET:CG	1:A:101:CYS:SG	2.83	0.60
2:B:40:LEU:O	2:B:78:TYR:HA	2.01	0.60
2:E:36:GLU:HB3	2:E:83:LYS:HB2	1.81	0.60
2:E:38:GLN:HB2	2:E:83:LYS:HZ1	1.66	0.60
1:A:59:TYR:HB2	1:A:62:ARG:HH11	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:CD2	1:D:3:HIS:N	2.70	0.60
2:E:7:ILE:HD13	2:E:91:LYS:HD3	1.82	0.60
1:A:3:HIS:CD2	1:A:3:HIS:N	2.70	0.60
1:D:217:TRP:CE3	1:D:224:LEU:HB2	2.37	0.60
1:D:234:ARG:NH2	2:E:10:TYR:CD2	2.69	0.60
1:D:124:ILE:HD11	1:D:144:ARG:HG2	1.84	0.59
1:A:124:ILE:HD11	1:A:144:ARG:HG2	1.84	0.59
1:A:5:MET:HB3	1:A:101:CYS:N	2.17	0.59
1:A:44:ARG:HA	1:A:64:THR:HG23	1.84	0.59
1:A:198:GLU:HB3	1:A:248:VAL:CG2	2.32	0.59
1:A:202:ARG:HG3	1:A:204:TRP:NE1	2.17	0.59
1:A:38:SER:O	1:A:43:PRO:HG3	2.02	0.59
1:A:138:MET:HA	1:A:141:GLN:HB3	1.84	0.59
1:A:192:HIS:HB3	1:A:193:PRO:HD2	1.84	0.59
1:D:38:SER:O	1:D:43:PRO:HG3	2.02	0.59
1:D:213:ILE:HG13	1:D:214:THR:H	1.67	0.59
1:A:208:PHE:CE1	1:A:263:HIS:CE1	2.90	0.59
1:A:217:TRP:CE3	1:A:224:LEU:HB2	2.37	0.59
1:D:5:MET:O	1:D:100:GLY:HA3	2.02	0.59
1:D:59:TYR:N	1:D:62:ARG:NH1	2.51	0.59
2:E:40:LEU:O	2:E:78:TYR:HA	2.01	0.59
1:D:66:ILE:CD1	3:F:4:VAL:HG23	2.33	0.59
1:D:77:ASN:HA	1:D:80:THR:HG22	1.83	0.59
1:A:5:MET:O	1:A:100:GLY:HA3	2.02	0.59
1:A:66:ILE:CD1	3:C:4:VAL:HG23	2.33	0.59
1:D:138:MET:HA	1:D:141:GLN:HB3	1.84	0.59
1:D:206:LEU:HD12	1:D:242:GLN:HB3	1.85	0.59
1:A:59:TYR:N	1:A:62:ARG:NH1	2.51	0.59
1:D:192:HIS:HB3	1:D:193:PRO:HD2	1.84	0.59
1:D:208:PHE:CE1	1:D:263:HIS:CE1	2.90	0.59
1:A:77:ASN:HA	1:A:80:THR:HG22	1.83	0.59
1:D:35:ARG:NH2	2:E:54:MET:O	2.36	0.58
1:A:206:LEU:HD12	1:A:242:GLN:HB3	1.85	0.58
1:A:35:ARG:NH2	2:B:54:MET:O	2.36	0.58
1:D:5:MET:HE2	1:D:101:CYS:SG	2.44	0.58
1:D:58:GLU:C	1:D:62:ARG:HD2	2.29	0.58
2:B:38:GLN:HB2	2:B:83:LYS:HZ1	1.67	0.58
1:D:192:HIS:CB	1:D:193:PRO:HD2	2.33	0.58
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.04	0.58
1:D:216:THR:O	1:D:259:CYS:HA	2.04	0.58
1:D:233:THR:OG1	1:D:243:LYS:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:C	1:A:62:ARG:HD2	2.28	0.58
1:D:213:ILE:HG13	1:D:214:THR:N	2.19	0.58
1:A:213:ILE:HG13	1:A:214:THR:H	1.67	0.58
2:B:3:LYS:CG	2:B:31:HIS:HB2	2.34	0.58
1:A:59:TYR:N	1:A:62:ARG:HH11	2.02	0.58
1:A:180:LEU:O	1:A:182:THR:HG23	1.93	0.58
1:A:1:GLY:H2	1:A:105:SER:CA	2.17	0.58
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.86	0.58
1:A:213:ILE:HG13	1:A:214:THR:N	2.19	0.57
1:A:81:LEU:HD21	1:A:123:TYR:HE2	1.68	0.57
1:A:5:MET:HE2	1:A:101:CYS:SG	2.44	0.57
1:A:192:HIS:CB	1:A:193:PRO:HD2	2.33	0.57
1:A:234:ARG:HH22	2:B:10:TYR:HB3	1.62	0.57
2:B:26:TYR:HD1	2:B:65:LEU:HD23	1.68	0.57
1:D:59:TYR:N	1:D:62:ARG:HH11	2.02	0.57
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.86	0.57
1:D:234:ARG:HH21	2:E:10:TYR:HB3	1.66	0.57
2:E:3:LYS:CG	2:E:31:HIS:HB2	2.34	0.57
1:A:114:GLU:HB3	1:A:126:LEU:HB3	1.87	0.57
1:D:81:LEU:HD21	1:D:123:TYR:HE2	1.68	0.57
2:E:3:LYS:HG2	2:E:31:HIS:HB2	1.87	0.57
2:E:26:TYR:HD1	2:E:65:LEU:HD23	1.69	0.57
1:A:3:HIS:HD2	1:A:103:VAL:HG13	1.70	0.57
1:D:114:GLU:HB3	1:D:126:LEU:HB3	1.87	0.57
1:A:216:THR:O	1:A:259:CYS:HA	2.04	0.57
1:A:5:MET:O	1:A:6:ARG:CD	2.52	0.57
1:A:22:TYR:CD1	1:A:36:PHE:HE1	2.23	0.57
1:D:1:GLY:H2	1:D:105:SER:CA	2.18	0.57
1:D:5:MET:O	1:D:6:ARG:CD	2.52	0.57
1:A:99:TYR:HB3	1:A:114:GLU:OE1	2.05	0.57
1:A:3:HIS:CB	1:A:103:VAL:CG2	2.47	0.56
1:A:5:MET:O	1:A:6:ARG:CG	2.53	0.56
1:A:32:GLU:OE1	1:A:48:GLN:HG3	2.05	0.56
1:A:63:ILE:HD11	3:C:2:PRO:CD	2.32	0.56
1:A:213:ILE:HD12	1:A:263:HIS:HB2	1.87	0.56
1:D:21:ARG:NH1	2:E:54:MET:HE1	2.14	0.56
1:D:219:LEU:HA	1:D:257:TYR:CD1	2.41	0.56
1:A:29:ASP:H	1:A:31:LYS:N	1.85	0.56
1:A:180:LEU:O	1:A:181:ARG:C	2.37	0.56
2:B:35:ILE:CD1	2:B:84:HIS:HB2	2.34	0.56
1:D:22:TYR:CD1	1:D:36:PHE:HE1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ALA:O	1:D:52:MET:HB2	2.06	0.56
1:D:99:TYR:HB3	1:D:114:GLU:OE1	2.05	0.56
1:D:202:ARG:HG3	1:D:204:TRP:NE1	2.18	0.56
2:E:35:ILE:CD1	2:E:84:HIS:HB2	2.34	0.56
1:D:3:HIS:C	1:D:103:VAL:CG1	2.79	0.56
1:D:5:MET:CG	1:D:101:CYS:SG	2.83	0.56
1:D:5:MET:O	1:D:6:ARG:CG	2.53	0.56
1:D:63:ILE:HD11	3:F:2:PRO:CD	2.32	0.56
1:A:14:ARG:NE	1:A:19:GLU:O	2.39	0.56
1:A:225:THR:O	1:A:225:THR:CG2	2.45	0.56
1:D:29:ASP:H	1:D:31:LYS:N	1.85	0.56
1:A:59:TYR:CB	1:A:62:ARG:HH11	2.19	0.56
1:A:183:ASP:HB2	1:A:209:TYR:CB	2.36	0.56
1:A:234:ARG:HH21	2:B:10:TYR:HB3	1.66	0.56
1:D:5:MET:HB3	1:D:101:CYS:N	2.17	0.56
1:D:14:ARG:NE	1:D:19:GLU:O	2.39	0.56
1:D:213:ILE:HD12	1:D:263:HIS:HB2	1.87	0.56
1:A:38:SER:O	1:A:43:PRO:CG	2.53	0.56
1:A:49:ALA:O	1:A:52:MET:HB2	2.06	0.56
1:D:3:HIS:HD2	1:D:103:VAL:HG13	1.70	0.56
1:D:38:SER:O	1:D:43:PRO:CG	2.53	0.56
1:D:72:GLN:HE22	1:D:75:ARG:HH21	1.54	0.56
1:A:219:LEU:HA	1:A:257:TYR:CD1	2.40	0.56
1:D:32:GLU:OE1	1:D:48:GLN:HG3	2.05	0.56
1:A:72:GLN:HE22	1:A:75:ARG:HH21	1.54	0.56
1:D:225:THR:O	1:D:225:THR:CG2	2.45	0.56
2:B:3:LYS:HG2	2:B:31:HIS:HB2	1.87	0.55
1:D:2:PRO:CA	1:D:3:HIS:CG	2.77	0.55
1:D:59:TYR:CB	1:D:62:ARG:HH11	2.19	0.55
1:A:3:HIS:C	1:A:103:VAL:CG1	2.79	0.55
2:B:35:ILE:HD11	2:B:82:VAL:HG12	1.88	0.55
2:E:35:ILE:HD11	2:E:82:VAL:HG12	1.88	0.55
1:D:7:TYR:HB3	1:D:9:GLU:OE1	2.07	0.55
1:D:253:LYS:HG2	1:D:255:GLN:NE2	2.16	0.55
1:D:183:ASP:HB2	1:D:209:TYR:CB	2.36	0.55
1:A:7:TYR:HB3	1:A:9:GLU:OE1	2.07	0.55
1:A:208:PHE:C	1:A:209:TYR:O	2.49	0.55
1:D:6:ARG:HA	1:D:99:TYR:O	2.07	0.55
1:D:72:GLN:HE22	1:D:75:ARG:NH2	2.05	0.55
1:A:6:ARG:HA	1:A:99:TYR:O	2.07	0.55
2:E:47:PRO:O	2:E:49:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HE22	1:A:75:ARG:NH2	2.05	0.54
1:A:82:LEU:HD22	1:A:88:SER:O	2.06	0.54
1:A:5:MET:HG2	1:A:101:CYS:CB	2.38	0.54
1:A:182:THR:C	1:A:209:TYR:CB	2.80	0.54
1:A:103:VAL:HG22	1:A:104:GLY:N	2.23	0.54
1:D:5:MET:HG2	1:D:101:CYS:CB	2.37	0.54
1:D:164:CYS:SG	1:D:165:VAL:N	2.80	0.54
2:B:20:PRO:HG3	1:D:181:ARG:CZ	2.28	0.54
2:B:47:PRO:O	2:B:49:VAL:HG13	2.07	0.54
1:D:130:LEU:N	1:D:130:LEU:HD23	2.22	0.54
1:D:217:TRP:O	1:D:223:GLU:HA	2.08	0.54
1:D:231:VAL:O	1:D:243:LYS:HE3	2.08	0.54
2:E:3:LYS:CG	2:E:31:HIS:N	2.71	0.54
1:A:217:TRP:O	1:A:223:GLU:HA	2.08	0.54
1:D:182:THR:C	1:D:209:TYR:CB	2.80	0.54
2:E:6:GLN:NE2	2:E:6:GLN:CA	2.70	0.54
1:A:231:VAL:O	1:A:243:LYS:HE3	2.08	0.54
1:D:47:PRO:HB2	1:D:52:MET:HB3	1.90	0.54
1:D:82:LEU:HD22	1:D:88:SER:O	2.06	0.54
1:A:61:GLU:O	1:A:62:ARG:C	2.51	0.53
1:D:5:MET:CG	1:D:100:GLY:CA	2.82	0.53
1:A:130:LEU:N	1:A:130:LEU:HD23	2.22	0.53
1:D:141:GLN:NE2	1:D:144:ARG:HH21	2.02	0.53
1:A:77:ASN:HD21	3:C:8:ASN:HD22	1.57	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:A:259:CYS:C	1:A:260:ARG:HD2	2.33	0.53
2:B:3:LYS:CG	2:B:31:HIS:N	2.71	0.53
1:D:237:GLY:N	2:E:12:ARG:HE	2.03	0.53
2:E:81:ARG:HD3	2:E:83:LYS:HZ3	1.74	0.53
1:A:36:PHE:CB	1:A:45:TYR:CD1	2.91	0.53
1:A:184:SER:O	1:A:186:LYS:HD3	2.08	0.53
1:A:210:PRO:O	1:A:212:ASP:N	2.41	0.53
1:D:77:ASN:HD21	3:F:8:ASN:HD22	1.57	0.53
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.44	0.53
1:A:47:PRO:HB2	1:A:52:MET:HB3	1.90	0.53
1:A:15:PRO:HD2	1:A:16:GLY:H	1.74	0.53
1:D:255:GLN:C	1:D:256:ASN:CG	2.76	0.53
2:E:33:PRO:HB3	2:E:62:PHE:CE2	2.44	0.53
1:A:22:TYR:CE1	1:A:36:PHE:CE1	2.97	0.53
1:A:202:ARG:HH11	1:A:202:ARG:HB3	1.74	0.53
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:PHE:CB	1:D:45:TYR:CD1	2.91	0.53
1:D:103:VAL:HG22	1:D:104:GLY:N	2.23	0.53
1:D:184:SER:O	1:D:186:LYS:HD3	2.08	0.53
1:D:22:TYR:CE1	1:D:36:PHE:CE1	2.97	0.53
1:A:3:HIS:C	1:A:103:VAL:CB	2.79	0.52
1:D:259:CYS:C	1:D:260:ARG:HD2	2.33	0.52
1:A:249:VAL:HG22	1:A:257:TYR:CD2	2.44	0.52
1:D:116:PHE:HB2	1:D:124:ILE:HG22	1.92	0.52
1:D:188:HIS:O	1:D:203:CYS:HA	2.10	0.52
1:D:208:PHE:C	1:D:209:TYR:O	2.49	0.52
1:A:197:GLY:O	1:A:198:GLU:HG3	2.10	0.52
1:A:213:ILE:CG1	1:A:214:THR:N	2.72	0.52
1:A:36:PHE:CD1	1:A:36:PHE:C	2.88	0.52
1:D:210:PRO:O	1:D:212:ASP:N	2.41	0.52
1:D:213:ILE:CG1	1:D:214:THR:N	2.72	0.52
1:A:188:HIS:O	1:A:203:CYS:HA	2.10	0.52
1:A:216:THR:CG2	1:A:217:TRP:N	2.73	0.52
1:A:228:MET:O	1:A:230:LEU:HD22	2.09	0.52
1:D:61:GLU:O	1:D:62:ARG:C	2.51	0.52
1:A:66:ILE:HG21	3:C:2:PRO:HG2	1.92	0.52
1:A:255:GLN:C	1:A:256:ASN:CG	2.76	0.52
2:B:7:ILE:CD1	2:B:91:LYS:HD3	2.39	0.52
1:D:59:TYR:N	1:D:62:ARG:HD2	2.24	0.52
1:D:249:VAL:HG22	1:D:257:TYR:CD2	2.44	0.52
1:A:160:LEU:O	1:A:164:CYS:SG	2.67	0.52
1:A:59:TYR:N	1:A:62:ARG:HD2	2.24	0.52
1:D:202:ARG:HB3	1:D:202:ARG:HH11	1.74	0.52
1:D:253:LYS:HG2	1:D:255:GLN:CD	2.34	0.52
2:B:3:LYS:HG3	2:B:30:PHE:C	2.35	0.52
1:D:15:PRO:HD2	1:D:16:GLY:H	1.74	0.52
1:D:228:MET:O	1:D:230:LEU:HD22	2.09	0.52
1:A:116:PHE:HB2	1:A:124:ILE:HG22	1.92	0.51
1:D:73:TRP:CZ3	3:F:7:HIS:O	2.63	0.51
2:E:46:ILE:C	2:E:47:PRO:O	2.50	0.51
1:A:73:TRP:CZ3	3:C:7:HIS:O	2.63	0.51
1:A:164:CYS:SG	1:A:165:VAL:N	2.80	0.51
1:D:216:THR:CG2	1:D:217:TRP:N	2.73	0.51
1:A:28:VAL:O	1:A:29:ASP:CG	2.53	0.51
1:A:218:GLN:HB2	1:A:258:THR:HG23	1.92	0.51
1:A:224:LEU:O	1:A:226:GLN:N	2.43	0.51
1:D:2:PRO:C	1:D:3:HIS:CG	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:PHE:CD1	1:D:36:PHE:C	2.88	0.51
1:D:73:TRP:HZ3	3:F:7:HIS:C	2.18	0.51
1:D:224:LEU:O	1:D:226:GLN:N	2.43	0.51
2:E:7:ILE:HG22	2:E:8:GLN:N	2.26	0.51
1:A:2:PRO:C	1:A:3:HIS:CG	2.88	0.51
2:B:7:ILE:HG22	2:B:8:GLN:N	2.26	0.51
2:E:7:ILE:CD1	2:E:91:LYS:HD3	2.39	0.51
1:D:192:HIS:HB3	1:D:193:PRO:CD	2.40	0.51
1:D:196:LYS:HG2	1:D:197:GLY:N	2.25	0.51
1:D:197:GLY:O	1:D:198:GLU:HG3	2.09	0.51
1:D:217:TRP:HB3	1:D:258:THR:O	2.11	0.51
1:A:102:ASP:HB2	1:A:111:ARG:O	2.11	0.51
1:A:183:ASP:HB2	1:A:209:TYR:CA	2.36	0.51
2:E:3:LYS:HG3	2:E:30:PHE:C	2.35	0.51
3:C:4:VAL:HG12	3:C:6:ILE:HB	1.93	0.51
1:D:66:ILE:HG21	3:F:2:PRO:HG2	1.92	0.51
2:E:38:GLN:HB2	2:E:83:LYS:HZ2	1.74	0.51
1:A:73:TRP:HZ3	3:C:7:HIS:C	2.18	0.51
1:D:218:GLN:HB2	1:D:258:THR:HG23	1.92	0.51
2:B:6:GLN:NE2	2:B:6:GLN:CA	2.70	0.51
1:A:202:ARG:O	1:A:204:TRP:HD1	1.94	0.50
2:B:38:GLN:HB2	2:B:83:LYS:HZ2	1.72	0.50
1:D:155:TYR:CZ	3:F:6:ILE:HG22	2.46	0.50
1:A:22:TYR:HD1	1:A:36:PHE:HE1	1.59	0.50
1:A:102:ASP:HB2	1:A:111:ARG:HB3	1.93	0.50
1:A:155:TYR:CZ	3:C:6:ILE:HG22	2.46	0.50
1:A:194:ARG:HB3	1:A:198:GLU:O	2.11	0.50
1:D:102:ASP:HB2	1:D:111:ARG:O	2.11	0.50
3:F:4:VAL:HG12	3:F:6:ILE:HB	1.93	0.50
1:D:22:TYR:HD1	1:D:36:PHE:HE1	1.59	0.50
1:A:196:LYS:HG2	1:A:197:GLY:N	2.25	0.50
1:A:259:CYS:O	1:A:260:ARG:HD2	2.12	0.50
1:D:29:ASP:OD1	1:D:179:LEU:CD1	2.59	0.50
1:D:183:ASP:HB2	1:D:209:TYR:CA	2.36	0.50
1:A:141:GLN:NE2	1:A:144:ARG:HH21	2.02	0.50
1:A:192:HIS:HB3	1:A:193:PRO:CD	2.40	0.50
1:A:217:TRP:HB3	1:A:258:THR:O	2.11	0.50
1:D:102:ASP:HB2	1:D:111:ARG:HB3	1.93	0.50
1:D:259:CYS:O	1:D:260:ARG:HD2	2.12	0.50
1:A:81:LEU:HD21	1:A:123:TYR:CE2	2.46	0.50
2:B:35:ILE:HD13	2:B:84:HIS:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:SER:CB	1:D:198:GLU:CB	2.82	0.50
2:E:35:ILE:HG13	2:E:37:ILE:HD12	1.93	0.50
1:A:5:MET:CG	1:A:100:GLY:CA	2.82	0.50
1:A:77:ASN:ND2	3:C:9:PHE:HB2	2.26	0.50
1:A:237:GLY:N	2:B:12:ARG:HE	2.03	0.50
2:E:12:ARG:HB2	2:E:22:ILE:HB	1.93	0.50
1:A:75:ARG:NH1	1:A:79:ARG:HE	2.10	0.50
1:A:146:LYS:CG	1:A:147:TRP:N	2.72	0.50
2:B:5:PRO:O	2:B:91:LYS:NZ	2.45	0.50
1:D:146:LYS:CG	1:D:147:TRP:N	2.72	0.50
1:A:253:LYS:HG2	1:A:255:GLN:CD	2.34	0.50
2:B:35:ILE:HG13	2:B:37:ILE:HD12	1.93	0.50
1:D:75:ARG:NH1	1:D:79:ARG:HE	2.10	0.50
1:A:202:ARG:HD2	1:A:204:TRP:CE2	2.46	0.49
2:B:26:TYR:CD1	2:B:65:LEU:HD23	2.47	0.49
2:B:56:PHE:CE1	2:B:60:TRP:HA	2.47	0.49
1:D:202:ARG:HD2	1:D:204:TRP:CE2	2.46	0.49
2:B:12:ARG:HB2	2:B:22:ILE:HB	1.93	0.49
2:B:56:PHE:CD1	2:B:60:TRP:HA	2.47	0.49
1:D:249:VAL:HG13	1:D:253:LYS:O	2.12	0.49
1:D:250:PRO:CB	1:D:253:LYS:HB3	2.40	0.49
2:E:7:ILE:N	2:E:7:ILE:HD12	2.27	0.49
2:E:64:ILE:HG13	2:E:65:LEU:N	2.27	0.49
1:A:229:GLU:O	1:A:245:ALA:CA	2.61	0.49
2:B:20:PRO:CG	1:D:181:ARG:NH1	2.36	0.49
1:D:194:ARG:HB3	1:D:198:GLU:O	2.11	0.49
2:E:26:TYR:CD1	2:E:65:LEU:HD23	2.47	0.49
1:A:146:LYS:HG3	1:A:147:TRP:H	1.75	0.49
1:D:229:GLU:O	1:D:245:ALA:CA	2.61	0.49
1:A:144:ARG:HD2	1:A:148:GLU:OE1	2.13	0.49
1:A:234:ARG:HH22	2:B:10:TYR:HB2	1.76	0.49
1:D:133:TRP:O	1:D:144:ARG:NH1	2.45	0.49
2:E:56:PHE:CD1	2:E:60:TRP:HA	2.47	0.49
1:A:161:GLU:C	1:A:164:CYS:SG	2.96	0.49
1:A:230:LEU:N	1:A:230:LEU:CD2	2.76	0.49
2:B:7:ILE:N	2:B:7:ILE:HD12	2.27	0.49
2:E:35:ILE:HD13	2:E:84:HIS:HD2	1.77	0.49
1:A:133:TRP:O	1:A:144:ARG:NH1	2.45	0.49
1:A:250:PRO:CB	1:A:253:LYS:HB3	2.40	0.49
1:D:202:ARG:O	1:D:204:TRP:HD1	1.95	0.49
1:A:29:ASP:OD1	1:A:179:LEU:CD1	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:NE2	2:B:60:TRP:HB3	2.28	0.49
2:B:47:PRO:CD	2:B:47:PRO:CA	2.81	0.49
2:B:81:ARG:HD3	2:B:83:LYS:HZ3	1.77	0.49
2:B:87:MET:SD	2:B:91:LYS:HD2	2.53	0.49
1:A:163:GLU:O	1:A:167:TRP:CD1	2.64	0.49
2:B:46:ILE:C	2:B:47:PRO:O	2.50	0.49
1:D:14:ARG:CZ	1:D:19:GLU:O	2.61	0.49
2:E:5:PRO:O	2:E:91:LYS:NZ	2.45	0.49
2:E:7:ILE:HD13	2:E:91:LYS:HE2	1.95	0.49
2:B:7:ILE:HD13	2:B:91:LYS:HE2	1.95	0.48
1:D:161:GLU:C	1:D:164:CYS:SG	2.96	0.48
1:A:79:ARG:O	1:A:82:LEU:HB2	2.13	0.48
1:A:249:VAL:HG13	1:A:253:LYS:O	2.12	0.48
1:D:123:TYR:HD1	1:D:124:ILE:CB	2.25	0.48
2:E:56:PHE:CE1	2:E:60:TRP:HA	2.47	0.48
1:A:61:GLU:O	1:A:65:GLN:HB2	2.13	0.48
1:A:224:LEU:CD1	1:A:247:VAL:HG11	2.43	0.48
2:B:22:ILE:HD12	2:B:22:ILE:N	2.28	0.48
1:D:61:GLU:O	1:D:65:GLN:HB2	2.13	0.48
1:A:51:TRP:CZ3	1:A:52:MET:CE	2.95	0.48
2:B:70:PHE:HB2	2:B:78:TYR:OH	2.12	0.48
1:D:96:GLN:NE2	2:E:60:TRP:HB3	2.28	0.48
2:E:2:GLN:HG2	2:E:31:HIS:O	2.13	0.48
1:A:173:LYS:C	1:A:175:GLY:N	2.66	0.48
2:B:64:ILE:HG13	2:B:65:LEU:N	2.27	0.48
1:D:77:ASN:ND2	3:F:9:PHE:HB2	2.26	0.48
1:D:163:GLU:O	1:D:167:TRP:CD1	2.64	0.48
1:D:180:LEU:O	1:D:182:THR:HG23	1.93	0.48
2:E:70:PHE:HB2	2:E:78:TYR:OH	2.12	0.48
1:D:81:LEU:HD21	1:D:123:TYR:CE2	2.46	0.48
1:D:123:TYR:CD1	3:F:9:PHE:HE1	2.32	0.48
1:D:230:LEU:N	1:D:230:LEU:CD2	2.76	0.48
1:A:73:TRP:CD1	1:A:73:TRP:C	2.92	0.48
1:A:160:LEU:C	1:A:164:CYS:SG	2.97	0.48
2:B:13:HIS:O	2:B:21:ASN:OD1	2.31	0.48
3:C:5:ASN:O	3:C:7:HIS:N	2.47	0.48
1:D:79:ARG:O	1:D:82:LEU:HB2	2.14	0.48
2:E:51:MET:CB	2:E:64:ILE:HD11	2.43	0.48
1:A:4:SER:OG	1:A:29:ASP:N	2.47	0.48
1:D:5:MET:CB	1:D:101:CYS:O	2.59	0.48
1:D:73:TRP:CD1	1:D:73:TRP:C	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:CD1	1:D:247:VAL:HG11	2.43	0.48
1:A:14:ARG:CZ	1:A:19:GLU:O	2.61	0.48
1:A:47:PRO:O	1:A:47:PRO:HG2	2.13	0.48
1:A:123:TYR:HD1	1:A:124:ILE:CB	2.25	0.48
1:D:84:TYR:HB3	1:D:139:ALA:CB	2.42	0.48
1:D:103:VAL:HG22	1:D:104:GLY:O	2.14	0.48
1:D:127:ASN:HB2	1:D:132:THR:O	2.14	0.48
2:E:87:MET:SD	2:E:91:LYS:HD2	2.53	0.48
1:A:5:MET:CB	1:A:101:CYS:O	2.59	0.47
1:D:144:ARG:HD2	1:D:148:GLU:OE1	2.13	0.47
2:E:22:ILE:N	2:E:22:ILE:HD12	2.28	0.47
1:A:123:TYR:CD1	3:C:9:PHE:HE1	2.32	0.47
1:D:47:PRO:O	1:D:47:PRO:HG2	2.13	0.47
1:D:160:LEU:C	1:D:164:CYS:SG	2.97	0.47
3:F:4:VAL:CG1	3:F:6:ILE:HD12	2.44	0.47
3:C:4:VAL:CG1	3:C:6:ILE:HD12	2.44	0.47
1:D:5:MET:HE2	1:D:164:CYS:O	2.14	0.47
2:E:13:HIS:O	2:E:21:ASN:OD1	2.31	0.47
1:D:126:LEU:HD12	1:D:132:THR:O	2.15	0.47
1:D:234:ARG:HH22	2:E:10:TYR:HB2	1.76	0.47
1:D:75:ARG:CZ	1:D:75:ARG:CB	2.89	0.47
1:D:141:GLN:HE22	1:D:144:ARG:NH2	2.03	0.47
2:E:39:MET:H	2:E:46:ILE:HD11	1.80	0.47
3:F:5:ASN:O	3:F:7:HIS:N	2.47	0.47
1:A:53:GLU:C	1:A:55:GLU:H	2.23	0.47
1:A:84:TYR:HB3	1:A:139:ALA:CB	2.42	0.47
1:A:84:TYR:CD1	1:A:142:ILE:HD11	2.50	0.47
2:B:2:GLN:HG2	2:B:31:HIS:O	2.13	0.47
1:D:13:SER:OG	1:D:93:HIS:N	2.47	0.47
1:D:22:TYR:HE1	1:D:36:PHE:CE1	2.33	0.47
1:D:75:ARG:NH1	1:D:79:ARG:NH2	2.57	0.47
1:A:13:SER:OG	1:A:93:HIS:N	2.47	0.47
1:A:195:SER:CB	1:A:198:GLU:CB	2.82	0.47
2:B:35:ILE:HD12	2:B:84:HIS:HB2	1.97	0.47
2:B:39:MET:H	2:B:46:ILE:HD11	1.80	0.47
2:B:81:ARG:HD3	2:B:83:LYS:NZ	2.30	0.47
1:D:146:LYS:HG3	1:D:147:TRP:H	1.75	0.47
1:D:255:GLN:HB2	1:D:256:ASN:ND2	2.30	0.47
2:E:35:ILE:HD12	2:E:84:HIS:HB2	1.97	0.47
2:E:47:PRO:CD	2:E:47:PRO:CA	2.81	0.47
1:A:126:LEU:HD12	1:A:132:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:HE22	1:A:144:ARG:NH2	2.03	0.47
1:A:148:GLU:O	1:A:149:GLN:C	2.58	0.47
2:E:81:ARG:HD3	2:E:83:LYS:NZ	2.30	0.47
1:A:202:ARG:O	1:A:204:TRP:CD1	2.68	0.47
1:A:81:LEU:HD22	1:A:85:TYR:CD2	2.50	0.46
1:A:143:THR:O	1:A:147:TRP:HB2	2.15	0.46
1:D:143:THR:O	1:D:147:TRP:HB2	2.15	0.46
1:D:202:ARG:O	1:D:204:TRP:CD1	2.68	0.46
1:A:5:MET:HE2	1:A:164:CYS:O	2.14	0.46
1:A:125:ALA:C	1:A:133:TRP:HE3	2.23	0.46
1:D:125:ALA:C	1:D:133:TRP:HE3	2.23	0.46
1:A:229:GLU:OE1	1:A:244:TRP:HH2	1.99	0.46
2:B:36:GLU:HB2	2:B:83:LYS:HB2	1.98	0.46
1:D:4:SER:OG	1:D:29:ASP:N	2.47	0.46
1:D:28:VAL:O	1:D:29:ASP:CG	2.53	0.46
2:E:81:ARG:HG2	2:E:83:LYS:CE	2.45	0.46
1:A:218:GLN:O	1:A:219:LEU:C	2.58	0.46
1:D:84:TYR:CD1	1:D:142:ILE:HD11	2.50	0.46
1:D:20:PRO:HG2	1:D:75:ARG:HG2	1.98	0.46
1:A:103:VAL:HG22	1:A:104:GLY:O	2.14	0.46
2:B:66:ALA:O	2:B:67:HIS:CB	2.59	0.46
1:D:53:GLU:C	1:D:55:GLU:H	2.23	0.46
1:A:3:HIS:HD2	1:A:103:VAL:CG1	2.29	0.46
1:A:22:TYR:HE1	1:A:36:PHE:CE1	2.33	0.46
1:A:196:LYS:O	1:A:196:LYS:HG2	2.16	0.46
1:A:255:GLN:HB2	1:A:256:ASN:ND2	2.30	0.46
2:B:80:CYS:O	2:B:92:THR:HA	2.15	0.46
1:D:229:GLU:OE1	1:D:244:TRP:HH2	1.99	0.46
2:E:80:CYS:O	2:E:92:THR:HA	2.15	0.46
1:D:27:TYR:HA	1:D:31:LYS:O	2.16	0.46
1:D:148:GLU:O	1:D:149:GLN:C	2.58	0.46
1:A:209:TYR:CB	1:A:210:PRO:CD	2.55	0.46
1:A:217:TRP:N	1:A:217:TRP:CD2	2.84	0.46
1:A:249:VAL:HG12	1:A:250:PRO:O	2.16	0.46
1:D:81:LEU:HD23	1:D:84:TYR:CD2	2.51	0.46
1:A:11:ALA:CB	1:A:74:PHE:HB3	2.46	0.45
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.97	0.45
1:A:81:LEU:HD23	1:A:84:TYR:CD2	2.51	0.45
1:A:127:ASN:HB2	1:A:132:THR:O	2.14	0.45
2:B:23:LEU:HD12	2:B:70:PHE:CZ	2.52	0.45
1:D:77:ASN:HA	1:D:80:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:VAL:HG12	1:D:250:PRO:O	2.16	0.45
1:D:81:LEU:HD22	1:D:85:TYR:CD2	2.50	0.45
1:D:160:LEU:O	1:D:164:CYS:SG	2.67	0.45
2:E:3:LYS:HG2	2:E:31:HIS:CB	2.47	0.45
1:D:229:GLU:HB3	1:D:244:TRP:CH2	2.51	0.45
1:A:224:LEU:C	1:A:226:GLN:N	2.70	0.45
1:A:27:TYR:HA	1:A:31:LYS:O	2.16	0.45
1:D:195:SER:OG	1:D:198:GLU:CA	2.65	0.45
1:D:230:LEU:HA	1:D:244:TRP:O	2.16	0.45
1:A:199:VAL:HG22	1:A:251:LEU:CD2	2.46	0.45
1:A:208:PHE:CD1	1:A:208:PHE:C	2.95	0.45
1:A:253:LYS:HG2	1:A:255:GLN:NE2	2.16	0.45
2:B:3:LYS:HG2	2:B:31:HIS:CB	2.47	0.45
2:B:24:ASN:HD22	2:B:65:LEU:CD1	2.28	0.45
1:D:3:HIS:HD2	1:D:103:VAL:CG1	2.29	0.45
1:D:5:MET:HB3	1:D:6:ARG:HH21	1.81	0.45
1:D:114:GLU:HB3	1:D:126:LEU:CB	2.47	0.45
1:D:199:VAL:HG22	1:D:251:LEU:CD2	2.46	0.45
1:D:208:PHE:CD1	1:D:208:PHE:C	2.95	0.45
1:A:266:LEU:HD23	1:A:266:LEU:C	2.42	0.45
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.99	0.45
2:B:81:ARG:HG2	2:B:83:LYS:CE	2.46	0.45
1:D:51:TRP:CZ3	1:D:52:MET:CE	2.95	0.45
1:D:192:HIS:HD2	1:D:200:THR:HG22	1.81	0.45
1:D:255:GLN:CB	1:D:256:ASN:ND2	2.80	0.45
1:A:70:GLN:HE22	3:C:5:ASN:HB3	1.82	0.45
1:D:152:ALA:HB1	1:D:156:TYR:HE2	1.81	0.45
1:D:183:ASP:HB2	1:D:209:TYR:HB2	1.90	0.45
1:D:266:LEU:HD23	1:D:266:LEU:C	2.42	0.45
1:A:146:LYS:CG	1:A:147:TRP:H	2.30	0.45
1:A:186:LYS:C	1:A:205:ALA:O	2.60	0.45
1:A:230:LEU:HA	1:A:244:TRP:O	2.16	0.45
1:A:230:LEU:CA	1:A:245:ALA:HA	2.36	0.45
1:A:40:ALA:O	1:A:41:GLU:C	2.60	0.45
1:A:192:HIS:HD2	1:A:200:THR:HG22	1.81	0.45
1:D:36:PHE:HB2	1:D:45:TYR:HA	1.99	0.45
1:D:129:ASP:O	1:D:131:LYS:N	2.50	0.45
1:D:183:ASP:N	1:D:209:TYR:CG	2.84	0.45
1:D:201:LEU:HD23	1:D:201:LEU:H	1.82	0.45
1:D:217:TRP:N	1:D:217:TRP:CD2	2.84	0.45
2:E:36:GLU:HB2	2:E:83:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:HA2	1:A:2:PRO:HD3	1.39	0.44
1:A:255:GLN:CB	1:A:256:ASN:ND2	2.80	0.44
1:D:1:GLY:HA2	1:D:2:PRO:HD3	1.39	0.44
2:E:21:ASN:C	2:E:22:ILE:HD12	2.43	0.44
2:E:24:ASN:HD22	2:E:65:LEU:CD1	2.28	0.44
1:A:182:THR:HA	1:A:209:TYR:HB3	1.99	0.44
1:D:3:HIS:C	1:D:103:VAL:CB	2.79	0.44
1:D:11:ALA:CB	1:D:74:PHE:HB3	2.46	0.44
1:D:46:GLU:HB3	1:D:47:PRO:HD2	1.99	0.44
1:A:46:GLU:HB3	1:A:47:PRO:HD2	1.99	0.44
1:A:77:ASN:HA	1:A:80:THR:CG2	2.46	0.44
1:D:144:ARG:O	1:D:148:GLU:HB2	2.18	0.44
1:D:208:PHE:CE2	1:D:213:ILE:HG22	2.47	0.44
2:E:23:LEU:HD12	2:E:70:PHE:CZ	2.51	0.44
1:A:152:ALA:HB1	1:A:156:TYR:HE2	1.82	0.44
1:A:218:GLN:HE21	1:A:260:ARG:HG2	1.82	0.44
1:D:25:VAL:HG22	1:D:27:TYR:CZ	2.53	0.44
1:D:40:ALA:O	1:D:41:GLU:C	2.60	0.44
1:A:195:SER:OG	1:A:198:GLU:CA	2.65	0.44
2:B:21:ASN:C	2:B:22:ILE:HD12	2.43	0.44
2:B:51:MET:CB	2:B:64:ILE:HD11	2.43	0.44
2:B:54:MET:HB2	2:B:54:MET:HE3	1.43	0.44
1:D:81:LEU:HD23	1:D:81:LEU:HA	1.71	0.44
1:A:129:ASP:O	1:A:131:LYS:N	2.50	0.44
1:D:126:LEU:HD22	1:D:133:TRP:CZ2	2.52	0.44
1:D:137:ASP:O	1:D:141:GLN:N	2.46	0.44
1:D:218:GLN:HE21	1:D:260:ARG:HG2	1.82	0.44
1:A:5:MET:HB3	1:A:6:ARG:HH21	1.81	0.44
2:B:51:MET:CE	2:B:51:MET:CG	2.91	0.44
2:B:68:THR:HG23	2:B:69:GLU:N	2.33	0.44
1:D:182:THR:HA	1:D:209:TYR:HB3	1.99	0.44
1:D:186:LYS:C	1:D:205:ALA:O	2.60	0.44
1:A:126:LEU:HD22	1:A:133:TRP:CZ2	2.52	0.44
2:E:68:THR:HG23	2:E:69:GLU:N	2.33	0.44
1:A:114:GLU:HB3	1:A:126:LEU:CB	2.47	0.44
1:A:144:ARG:O	1:A:148:GLU:HB2	2.18	0.44
1:A:167:TRP:O	1:A:170:ARG:HB3	2.18	0.44
1:A:229:GLU:HB3	1:A:244:TRP:CH2	2.51	0.44
1:D:81:LEU:CD2	1:D:84:TYR:CD2	3.01	0.44
2:E:45:LYS:CD	2:E:45:LYS:H	2.31	0.44
2:E:84:HIS:ND1	2:E:86:SER:OG	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:LYS:HG2	2:B:31:HIS:N	2.33	0.43
1:A:25:VAL:HG22	1:A:27:TYR:CZ	2.53	0.43
1:A:181:ARG:HB3	2:E:19:LYS:HZ3	1.82	0.43
1:A:218:GLN:O	1:A:257:TYR:HA	2.18	0.43
1:A:230:LEU:HA	1:A:245:ALA:CA	2.35	0.43
2:B:84:HIS:ND1	2:B:86:SER:OG	2.51	0.43
1:D:70:GLN:HE22	3:F:5:ASN:HB3	1.82	0.43
1:D:85:TYR:CD2	1:D:118:TYR:CE2	3.06	0.43
2:E:70:PHE:HB2	2:E:78:TYR:CZ	2.53	0.43
1:A:3:HIS:CD2	1:A:103:VAL:CG2	3.01	0.43
1:A:36:PHE:HB2	1:A:45:TYR:HA	1.99	0.43
1:A:201:LEU:HD23	1:A:201:LEU:H	1.82	0.43
2:B:70:PHE:HB2	2:B:78:TYR:CZ	2.52	0.43
1:D:3:HIS:CD2	1:D:103:VAL:CG2	3.01	0.43
1:D:192:HIS:O	1:D:194:ARG:HB2	2.18	0.43
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.53	0.43
1:D:198:GLU:HA	1:D:249:VAL:O	2.19	0.43
1:A:7:TYR:HB2	1:A:99:TYR:CE1	2.54	0.43
1:A:58:GLU:O	1:A:62:ARG:HG3	2.18	0.43
1:A:81:LEU:CD2	1:A:84:TYR:CD2	3.01	0.43
1:A:217:TRP:CZ3	1:A:224:LEU:HB2	2.53	0.43
1:A:263:HIS:O	1:A:263:HIS:CG	2.71	0.43
1:D:3:HIS:NE2	1:D:105:SER:CA	2.74	0.43
1:D:84:TYR:CE1	1:D:142:ILE:HD11	2.54	0.43
1:A:198:GLU:HA	1:A:249:VAL:O	2.19	0.43
2:B:76:ASP:HB2	2:B:78:TYR:CE1	2.53	0.43
1:D:123:TYR:CE2	1:D:140:ALA:HA	2.54	0.43
1:A:3:HIS:CD2	1:A:103:VAL:CG1	3.02	0.43
1:A:75:ARG:CZ	1:A:75:ARG:CB	2.89	0.43
1:A:85:TYR:CD2	1:A:118:TYR:CE2	3.06	0.43
1:D:3:HIS:CD2	1:D:103:VAL:CG1	3.02	0.43
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.53	0.43
2:E:3:LYS:HG2	2:E:31:HIS:N	2.33	0.43
1:A:84:TYR:CE1	1:A:142:ILE:HD11	2.54	0.43
1:D:217:TRP:CZ3	1:D:224:LEU:HB2	2.53	0.43
2:B:45:LYS:CD	2:B:45:LYS:H	2.31	0.43
1:A:88:SER:OG	1:A:89:ALA:N	2.52	0.43
1:A:155:TYR:CE2	3:C:6:ILE:HG22	2.54	0.43
1:D:10:THR:O	1:D:22:TYR:HA	2.19	0.43
1:D:111:ARG:HD2	1:D:128:GLU:CG	2.49	0.43
1:D:167:TRP:O	1:D:170:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLN:O	1:D:257:TYR:HA	2.18	0.43
2:E:39:MET:HE3	2:E:39:MET:HB2	1.88	0.43
1:A:10:THR:O	1:A:22:TYR:HA	2.19	0.42
1:A:183:ASP:N	1:A:209:TYR:CG	2.84	0.42
1:D:22:TYR:CD1	1:D:36:PHE:CE1	3.06	0.42
1:A:30:ASN:HD22	1:A:30:ASN:HA	1.69	0.42
1:A:38:SER:O	1:A:43:PRO:HG2	2.19	0.42
1:A:85:TYR:CE2	1:A:118:TYR:HD2	2.37	0.42
1:A:133:TRP:HB2	1:A:144:ARG:HD3	2.00	0.42
1:A:137:ASP:O	1:A:141:GLN:N	2.46	0.42
1:A:167:TRP:O	1:A:171:TYR:CD2	2.72	0.42
2:B:19:LYS:HB3	2:B:20:PRO:CD	2.49	0.42
1:D:155:TYR:CE2	3:F:6:ILE:HG22	2.54	0.42
1:D:230:LEU:CA	1:D:245:ALA:HA	2.36	0.42
1:A:25:VAL:HG22	1:A:27:TYR:CE2	2.55	0.42
1:A:192:HIS:O	1:A:194:ARG:HB2	2.18	0.42
1:D:34:VAL:HA	1:D:48:GLN:HG2	2.01	0.42
1:D:52:MET:HA	1:D:52:MET:CE	2.44	0.42
1:D:58:GLU:O	1:D:62:ARG:HG3	2.18	0.42
1:D:85:TYR:CE2	1:D:118:TYR:HD2	2.37	0.42
1:A:3:HIS:CA	1:A:103:VAL:CG1	2.83	0.42
1:A:34:VAL:HA	1:A:48:GLN:HG2	2.02	0.42
1:A:251:LEU:HA	1:A:251:LEU:HD22	1.37	0.42
2:B:39:MET:CA	2:B:46:ILE:HG13	2.49	0.42
2:B:62:PHE:O	2:B:63:TYR:HB3	2.19	0.42
1:D:7:TYR:HB2	1:D:99:TYR:CE1	2.54	0.42
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.87	0.42
1:D:146:LYS:CG	1:D:147:TRP:H	2.30	0.42
1:D:218:GLN:O	1:D:219:LEU:C	2.58	0.42
2:E:51:MET:CE	2:E:51:MET:CG	2.91	0.42
1:D:148:GLU:HB3	1:D:149:GLN:H	1.64	0.42
2:E:76:ASP:HB2	2:E:78:TYR:CE1	2.53	0.42
1:A:111:ARG:HD2	1:A:128:GLU:CG	2.49	0.42
1:A:123:TYR:CE2	1:A:140:ALA:HA	2.54	0.42
1:D:5:MET:HG3	1:D:101:CYS:N	2.32	0.42
2:B:27:VAL:HG21	2:B:37:ILE:CD1	2.45	0.42
1:D:88:SER:OG	1:D:89:ALA:N	2.52	0.42
1:D:182:THR:HA	1:D:209:TYR:CG	2.55	0.42
1:D:38:SER:O	1:D:43:PRO:HG2	2.19	0.42
1:D:63:ILE:HD11	3:F:1:TYR:HA	2.01	0.42
1:D:133:TRP:HB2	1:D:144:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.71	0.42
1:A:181:ARG:NH1	2:E:19:LYS:CD	2.77	0.42
1:A:181:ARG:HE	2:E:19:LYS:HG2	1.34	0.42
2:B:29:GLN:HA	2:B:61:SER:OG	2.20	0.42
1:D:3:HIS:CA	1:D:103:VAL:CG1	2.83	0.42
1:D:167:TRP:O	1:D:171:TYR:CD2	2.72	0.42
1:A:63:ILE:HD11	3:C:1:TYR:HA	2.01	0.41
1:A:196:LYS:NZ	1:A:196:LYS:HB2	2.35	0.41
1:D:25:VAL:HG22	1:D:27:TYR:CE2	2.55	0.41
1:D:85:TYR:HD2	1:D:118:TYR:CE2	2.38	0.41
1:D:146:LYS:O	1:D:147:TRP:C	2.64	0.41
1:D:157:ARG:NH2	1:D:161:GLU:CD	2.74	0.41
1:A:29:ASP:CG	1:A:179:LEU:CD1	2.77	0.41
1:A:81:LEU:HD22	1:A:85:TYR:CE2	2.55	0.41
2:B:35:ILE:HD11	2:B:82:VAL:HG11	2.01	0.41
1:D:29:ASP:CG	1:D:179:LEU:CD1	2.77	0.41
1:A:14:ARG:HA	1:A:15:PRO:HD3	1.81	0.41
1:A:73:TRP:HZ3	3:C:7:HIS:O	2.03	0.41
1:A:182:THR:HA	1:A:209:TYR:CG	2.55	0.41
1:D:58:GLU:C	1:D:62:ARG:CD	2.93	0.41
1:D:251:LEU:HD22	1:D:251:LEU:HA	1.37	0.41
1:D:263:HIS:O	1:D:263:HIS:CG	2.71	0.41
2:E:62:PHE:O	2:E:63:TYR:HB3	2.19	0.41
2:E:29:GLN:HA	2:E:61:SER:OG	2.20	0.41
1:A:250:PRO:CB	1:A:253:LYS:CB	2.82	0.41
1:D:49:ALA:HB1	1:D:51:TRP:CE2	2.55	0.41
1:D:66:ILE:CG2	3:F:2:PRO:HG2	2.51	0.41
1:D:176:ASN:O	1:D:178:THR:N	2.54	0.41
1:D:81:LEU:HD22	1:D:85:TYR:CE2	2.55	0.41
2:E:39:MET:CA	2:E:46:ILE:HG13	2.50	0.41
1:A:22:TYR:CD1	1:A:36:PHE:CE1	3.06	0.41
1:A:58:GLU:C	1:A:62:ARG:CD	2.93	0.41
1:A:93:HIS:CD2	1:A:119:ASP:OD2	2.71	0.41
1:A:176:ASN:O	1:A:178:THR:N	2.54	0.41
2:B:11:SER:CB	2:B:15:PRO:HD3	2.51	0.41
2:B:12:ARG:HG3	2:B:22:ILE:CG2	2.51	0.41
1:D:170:ARG:O	1:D:171:TYR:C	2.64	0.41
2:E:12:ARG:HG3	2:E:22:ILE:CG2	2.51	0.41
1:A:49:ALA:HB1	1:A:51:TRP:CE2	2.55	0.41
1:A:85:TYR:HD2	1:A:118:TYR:CE2	2.38	0.41
1:D:196:LYS:HB2	1:D:196:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:HB2	1:A:111:ARG:CB	2.51	0.40
2:B:35:ILE:HD13	2:B:84:HIS:CD2	2.56	0.40
1:D:263:HIS:C	1:D:265:GLY:N	2.66	0.40
1:D:102:ASP:HB2	1:D:111:ARG:CB	2.51	0.40
1:A:123:TYR:HE1	1:A:143:THR:HG21	1.86	0.40
1:A:146:LYS:O	1:A:147:TRP:C	2.64	0.40
2:B:37:ILE:HG21	2:B:66:ALA:HB1	2.03	0.40
2:E:24:ASN:HD21	2:E:65:LEU:HD11	1.81	0.40
2:E:54:MET:HE3	2:E:54:MET:HB2	1.43	0.40
3:F:5:ASN:OD1	3:F:5:ASN:N	2.46	0.40
1:D:52:MET:HE1	1:D:171:TYR:HD1	1.87	0.40
1:D:100:GLY:O	1:D:160:LEU:HD22	2.22	0.40
2:E:11:SER:CB	2:E:15:PRO:HD3	2.51	0.40

All (29) 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:D:105:SER:C	1:D:264:GLU:OE2[2_565]	0.57	1.63
1:D:106:ASP:CA	1:D:264:GLU:OE1[2_565]	0.91	1.29
1:A:106:ASP:CA	1:A:264:GLU:OE1[2_555]	1.04	1.16
1:D:105:SER:O	1:D:264:GLU:OE2[2_565]	1.09	1.11
1:A:76:VAL:CG1	1:D:149:GLN:NE2[3_546]	1.14	1.06
1:A:106:ASP:N	1:A:264:GLU:OE1[2_555]	1.38	0.82
1:D:106:ASP:N	1:D:264:GLU:OE2[2_565]	1.46	0.74
1:D:106:ASP:C	1:D:264:GLU:OE1[2_565]	1.55	0.65
1:A:65:GLN:NE2	3:F:5:ASN:ND2[3_546]	1.56	0.64
1:A:105:SER:C	1:A:264:GLU:OE2[2_555]	1.60	0.60
1:D:106:ASP:CA	1:D:264:GLU:CD[2_565]	1.69	0.51
1:D:105:SER:O	1:D:264:GLU:CD[2_565]	1.71	0.49
1:A:106:ASP:CB	1:A:264:GLU:OE1[2_555]	1.72	0.48
1:A:105:SER:CB	1:A:264:GLU:OE2[2_555]	1.73	0.47
1:D:106:ASP:N	1:D:264:GLU:CD[2_565]	1.76	0.44
1:D:105:SER:C	1:D:264:GLU:CD[2_565]	1.80	0.40
1:D:106:ASP:N	1:D:264:GLU:OE1[2_565]	1.89	0.31
1:A:106:ASP:N	1:A:264:GLU:CD[2_555]	1.90	0.30
1:A:105:SER:C	1:A:264:GLU:CD[2_555]	2.01	0.19
1:A:105:SER:CA	1:A:264:GLU:OE2[2_555]	2.02	0.18
1:A:138:MET:SD	2:E:88:ALA:O[1_554]	2.02	0.18
1:D:105:SER:CA	1:D:264:GLU:OE2[2_565]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:N	1:A:264:GLU:OE2[2_555]	2.04	0.16
3:C:8:ASN:OD1	1:D:149:GLN:OE1[3_546]	2.10	0.10
1:D:106:ASP:O	1:D:264:GLU:OE1[2_565]	2.11	0.09
1:D:251:LEU:O	2:E:94:TYR:OH[2_555]	2.12	0.08
1:A:68:LYS:CB	3:F:6:ILE:CD1[3_546]	2.16	0.04
1:A:75:ARG:NH2	1:D:150:ALA:O[3_546]	2.17	0.03
3:C:8:ASN:CG	1:D:149:GLN:OE1[3_546]	2.19	0.01

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	266/268 (99%)	204 (77%)	53 (20%)	9 (3%)	3	2
1	D	266/268 (99%)	204 (77%)	53 (20%)	9 (3%)	3	2
2	B	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	2	2
2	E	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	2	2
3	C	7/9 (78%)	3 (43%)	4 (57%)	0	100	100
3	F	7/9 (78%)	3 (43%)	4 (57%)	0	100	100
All	All	740/752 (98%)	572 (77%)	142 (19%)	26 (4%)	3	2

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	148	GLU
2	B	41	LYS
1	D	103	VAL
1	D	148	GLU
2	E	41	LYS
1	A	2	PRO
1	A	181	ARG

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Mol	Chain	Res	Type
1	A	188	HIS
1	D	2	PRO
1	D	181	ARG
1	D	188	HIS
1	A	15	PRO
2	B	32	PRO
1	D	15	PRO
2	E	32	PRO
1	A	32	GLU
2	B	58	LYS
1	D	32	GLU
2	E	58	LYS
1	A	219	LEU
2	B	67	HIS
1	D	219	LEU
2	E	67	HIS
1	A	235	PRO
1	D	235	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/223 (100%)	157 (70%)	66 (30%)	0	0
1	D	223/223 (100%)	157 (70%)	66 (30%)	0	0
2	B	94/94 (100%)	52 (55%)	42 (45%)	0	0
2	E	94/94 (100%)	52 (55%)	42 (45%)	0	0
3	C	9/9 (100%)	4 (44%)	5 (56%)	0	0
3	F	9/9 (100%)	4 (44%)	5 (56%)	0	0
All	All	652/652 (100%)	426 (65%)	226 (35%)	0	0

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	5	MET
1	A	9	GLU
1	A	12	VAL
1	A	25	VAL
1	A	32	GLU
1	A	36	PHE
1	A	39	ASP
1	A	43	PRO
1	A	44	ARG
1	A	47	PRO
1	A	54	GLN
1	A	55	GLU
1	A	57	PRO
1	A	63	ILE
1	A	65	GLN
1	A	66	ILE
1	A	68	LYS
1	A	73	TRP
1	A	75	ARG
1	A	78	LEU
1	A	84	TYR
1	A	88	SER
1	A	98	MET
1	A	102	ASP
1	A	105	SER
1	A	110	LEU
1	A	111	ARG
1	A	115	GLN
1	A	130	LEU
1	A	134	THR
1	A	142	ILE
1	A	144	ARG
1	A	146	LYS
1	A	149	GLN
1	A	154	GLU
1	A	157	ARG
1	A	163	GLU
1	A	176	ASN
1	A	180	LEU
1	A	185	PRO
1	A	188	HIS
1	A	189	VAL

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Mol	Chain	Res	Type
1	A	194	ARG
1	A	195	SER
1	A	196	LYS
1	A	199	VAL
1	A	200	THR
1	A	202	ARG
1	A	206	LEU
1	A	212	ASP
1	A	214	THR
1	A	215	LEU
1	A	217	TRP
1	A	223	GLU
1	A	230	LEU
1	A	231	VAL
1	A	234	ARG
1	A	238	ASP
1	A	244	TRP
1	A	247	VAL
1	A	251	LEU
1	A	257	TYR
1	A	258	THR
1	A	264	GLU
1	A	266	LEU
2	B	2	GLN
2	B	3	LYS
2	B	4	THR
2	B	6	GLN
2	B	7	ILE
2	B	11	SER
2	B	12	ARG
2	B	17	ASN
2	B	21	ASN
2	B	27	VAL
2	B	28	THR
2	B	29	GLN
2	B	31	HIS
2	B	36	GLU
2	B	37	ILE
2	B	38	GLN
2	B	40	LEU
2	B	41	LYS
2	B	42	ASN

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Mol	Chain	Res	Type
2	B	45	LYS
2	B	46	ILE
2	B	51	MET
2	B	52	SER
2	B	53	ASP
2	B	54	MET
2	B	55	SER
2	B	57	SER
2	B	61	SER
2	B	64	ILE
2	B	65	LEU
2	B	68	THR
2	B	73	THR
2	B	75	THR
2	B	76	ASP
2	B	77	THR
2	B	78	TYR
2	B	83	LYS
2	B	85	ASP
2	B	86	SER
2	B	89	GLU
2	B	90	PRO
2	B	93	VAL
3	C	3	ASN
3	C	5	ASN
3	C	6	ILE
3	C	7	HIS
3	C	9	PHE
1	D	3	HIS
1	D	5	MET
1	D	9	GLU
1	D	12	VAL
1	D	25	VAL
1	D	32	GLU
1	D	36	PHE
1	D	39	ASP
1	D	43	PRO
1	D	44	ARG
1	D	47	PRO
1	D	54	GLN
1	D	55	GLU
1	D	57	PRO

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Mol	Chain	Res	Type
1	D	63	ILE
1	D	65	GLN
1	D	66	ILE
1	D	68	LYS
1	D	73	TRP
1	D	75	ARG
1	D	78	LEU
1	D	84	TYR
1	D	88	SER
1	D	98	MET
1	D	102	ASP
1	D	105	SER
1	D	110	LEU
1	D	111	ARG
1	D	115	GLN
1	D	130	LEU
1	D	134	THR
1	D	142	ILE
1	D	144	ARG
1	D	146	LYS
1	D	149	GLN
1	D	154	GLU
1	D	157	ARG
1	D	163	GLU
1	D	176	ASN
1	D	180	LEU
1	D	185	PRO
1	D	188	HIS
1	D	189	VAL
1	D	194	ARG
1	D	195	SER
1	D	196	LYS
1	D	199	VAL
1	D	200	THR
1	D	202	ARG
1	D	206	LEU
1	D	212	ASP
1	D	214	THR
1	D	215	LEU
1	D	217	TRP
1	D	223	GLU
1	D	230	LEU

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Mol	Chain	Res	Type
1	D	231	VAL
1	D	234	ARG
1	D	238	ASP
1	D	244	TRP
1	D	247	VAL
1	D	251	LEU
1	D	257	TYR
1	D	258	THR
1	D	264	GLU
1	D	266	LEU
2	E	2	GLN
2	E	3	LYS
2	E	4	THR
2	E	6	GLN
2	E	7	ILE
2	E	11	SER
2	E	12	ARG
2	E	17	ASN
2	E	21	ASN
2	E	27	VAL
2	E	28	THR
2	E	29	GLN
2	E	31	HIS
2	E	36	GLU
2	E	37	ILE
2	E	38	GLN
2	E	40	LEU
2	E	41	LYS
2	E	42	ASN
2	E	45	LYS
2	E	46	ILE
2	E	51	MET
2	E	52	SER
2	E	53	ASP
2	E	54	MET
2	E	55	SER
2	E	57	SER
2	E	61	SER
2	E	64	ILE
2	E	65	LEU
2	E	68	THR
2	E	73	THR

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Mol	Chain	Res	Type
2	E	75	THR
2	E	76	ASP
2	E	77	THR
2	E	78	TYR
2	E	83	LYS
2	E	85	ASP
2	E	86	SER
2	E	89	GLU
2	E	90	PRO
2	E	93	VAL
3	F	3	ASN
3	F	5	ASN
3	F	6	ILE
3	F	7	HIS
3	F	9	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	30	ASN
1	A	70	GLN
1	A	72	GLN
1	A	77	ASN
1	A	93	HIS
1	A	96	GLN
1	A	141	GLN
1	A	226	GLN
1	A	255	GLN
1	A	256	ASN
1	A	263	HIS
2	B	6	GLN
2	B	8	GLN
2	B	21	ASN
2	B	29	GLN
2	B	38	GLN
2	B	67	HIS
3	C	7	HIS
1	D	3	HIS
1	D	30	ASN
1	D	70	GLN
1	D	72	GLN

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Mol	Chain	Res	Type
1	D	77	ASN
1	D	86	ASN
1	D	93	HIS
1	D	96	GLN
1	D	141	GLN
1	D	226	GLN
1	D	255	GLN
1	D	256	ASN
1	D	263	HIS
2	E	6	GLN
2	E	8	GLN
2	E	21	ASN
2	E	29	GLN
2	E	38	GLN
2	E	67	HIS
3	F	7	HIS

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	164:CYS	C	165:VAL	N	1.20
1	D	164:CYS	C	165:VAL	N	1.20
1	A	225:THR	C	226:GLN	N	1.18
1	D	225:THR	C	226:GLN	N	1.18
1	A	131:LYS	C	132:THR	N	1.05
1	D	131:LYS	C	132:THR	N	1.05

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.