



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:47 pm BST

PDB ID : 1LD9
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

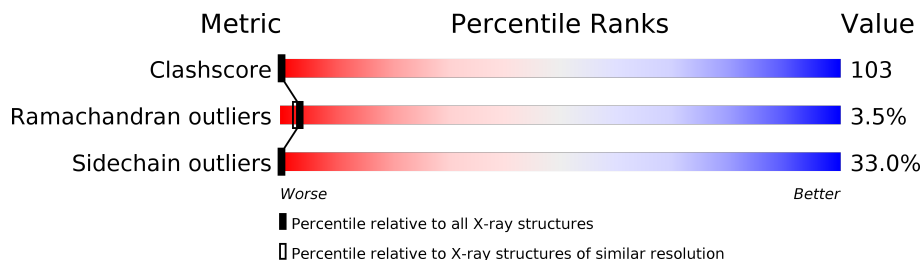
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 on 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	16% 40% 25% 19%
1	D	268	17% 40% 25% 19%
2	B	99	18% 36% 30% 15%
2	E	99	16% 37% 31% 15%
3	C	9	44% 11% 44%
3	F	9	44% 11% 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
			Total	C	N	O	S			
1	A	268	Total 2184	C 1381	N 381	O 412	S 10	0	0	0
1	D	268	Total 2184	C 1381	N 381	O 412	S 10	0	0	0

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

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

- Molecule 3 is a protein called NANO-PEPTIDE.

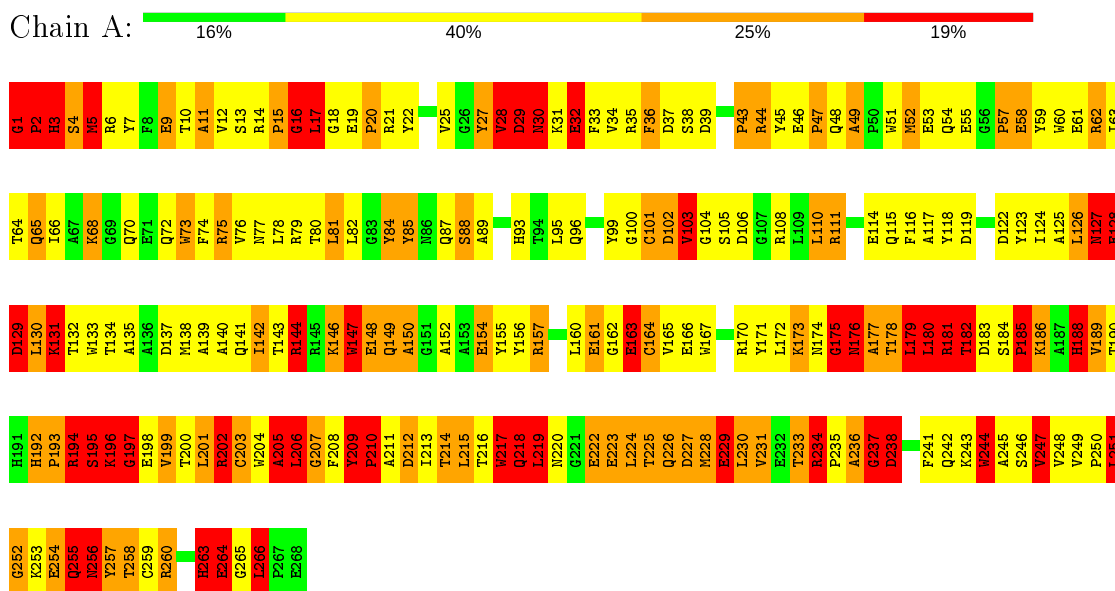
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total 80	C 52	N 14	O 14	0	0	0
3	F	9	Total 80	C 52	N 14	O 14	0	0	0

3 Residue-property plots

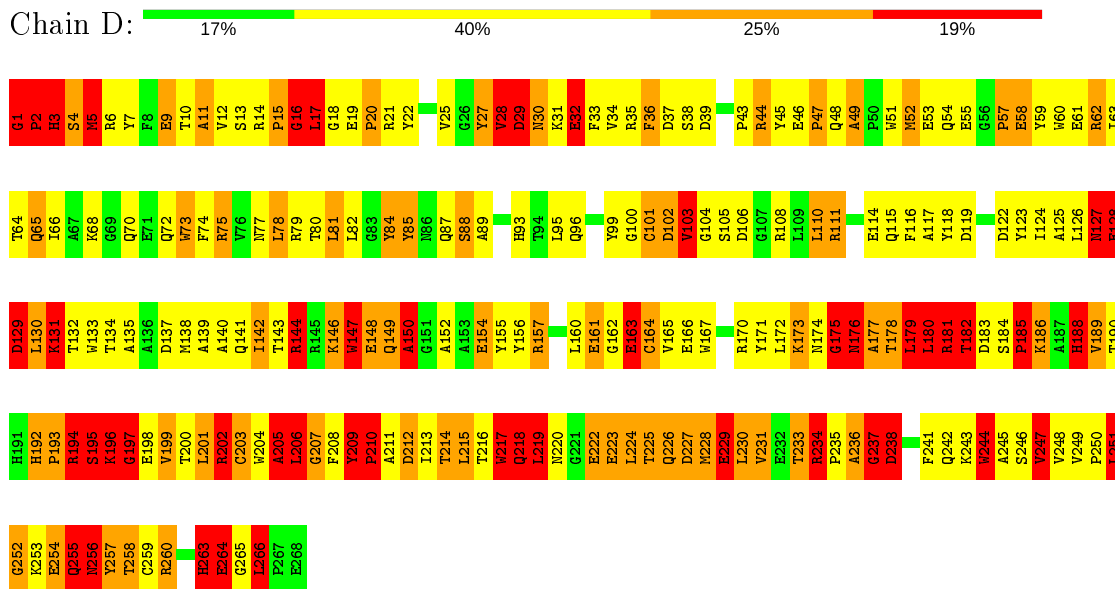
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

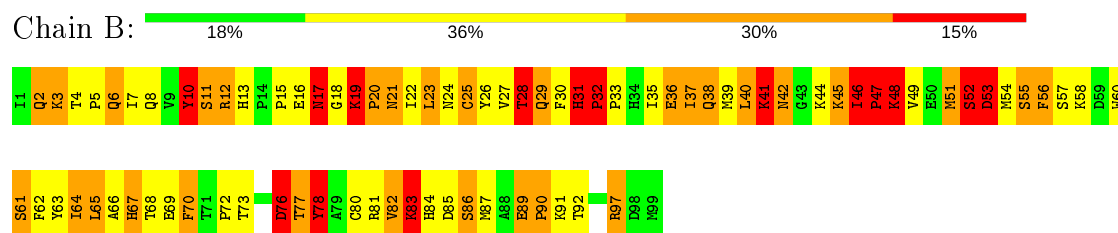
- Molecule 1: MHC CLASS I H-2LD HEAVY CHAIN



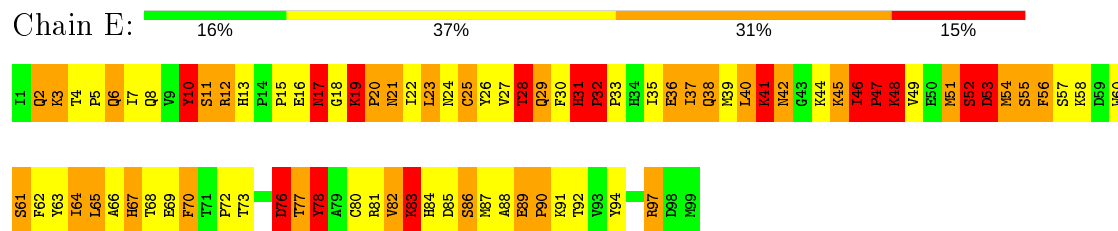
- Molecule 1: MHC CLASS I H-2LD HEAVY CHAIN



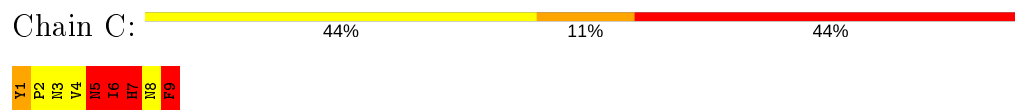
- Molecule 2: BETA-2 MICROGLOBULIN



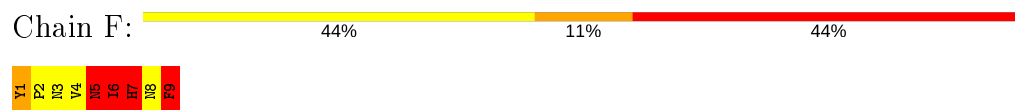
- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 3: NANO-PEPTIDE



- Molecule 3: NANO-PEPTIDE



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.62	41/2248 (1.8%)	2.94	122/3056 (4.0%)
1	D	1.62	41/2248 (1.8%)	2.94	121/3056 (4.0%)
2	B	1.94	23/846 (2.7%)	2.22	34/1148 (3.0%)
2	E	1.94	22/846 (2.6%)	2.22	35/1148 (3.0%)
3	C	1.26	1/83 (1.2%)	1.74	6/112 (5.4%)
3	F	1.26	1/83 (1.2%)	1.74	6/112 (5.4%)
All	All	1.70	129/6354 (2.0%)	2.74	324/8632 (3.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	20	PRO	N-CD	20.15	1.76	1.47
2	B	20	PRO	N-CD	20.11	1.76	1.47
2	E	47	PRO	N-CD	19.59	1.75	1.47
2	B	47	PRO	N-CD	19.57	1.75	1.47
2	B	19	LYS	C-O	-18.04	0.89	1.23
2	E	19	LYS	C-O	-18.03	0.89	1.23
1	A	254	GLU	C-O	-16.04	0.92	1.23
1	D	254	GLU	C-O	-16.00	0.93	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	LYS	C-N	-12.50	1.05	1.34
1	D	131	LYS	C-N	-12.49	1.05	1.34
1	A	175	GLY	C-N	10.95	1.59	1.34
1	D	175	GLY	C-N	10.94	1.59	1.34
1	D	226	GLN	N-CA	-9.73	1.26	1.46
1	A	226	GLN	N-CA	-9.72	1.26	1.46
2	E	18	GLY	N-CA	-9.67	1.31	1.46
2	B	18	GLY	N-CA	-9.64	1.31	1.46
2	B	20	PRO	CG-CD	9.21	1.81	1.50
2	E	20	PRO	CG-CD	9.19	1.80	1.50
1	D	166	GLU	CG-CD	9.06	1.65	1.51
1	A	166	GLU	CG-CD	9.04	1.65	1.51
2	E	18	GLY	CA-C	9.02	1.66	1.51
2	B	18	GLY	CA-C	9.01	1.66	1.51
2	B	47	PRO	CG-CD	8.97	1.80	1.50
2	E	47	PRO	CG-CD	8.97	1.80	1.50
1	D	30	ASN	N-CA	-8.75	1.28	1.46
1	A	30	ASN	N-CA	-8.72	1.28	1.46
1	A	263	HIS	C-N	8.30	1.53	1.34
1	D	263	HIS	C-N	8.28	1.53	1.34
1	D	101	CYS	CB-SG	8.16	1.96	1.82
1	A	101	CYS	CB-SG	8.14	1.96	1.82
1	A	128	GLU	C-N	7.83	1.52	1.34
1	D	128	GLU	C-N	7.81	1.52	1.34
1	D	110	LEU	C-N	7.54	1.51	1.34
1	A	110	LEU	C-N	7.51	1.51	1.34
1	A	225	THR	CA-C	-7.21	1.34	1.52
1	D	225	THR	CA-C	-7.21	1.34	1.52
2	B	16	GLU	C-N	7.04	1.50	1.34
2	E	16	GLU	C-N	7.02	1.50	1.34
1	D	2	PRO	CA-C	6.84	1.66	1.52
1	A	2	PRO	CA-C	6.83	1.66	1.52
1	D	225	THR	C-N	-6.83	1.18	1.34
1	A	225	THR	C-N	-6.82	1.18	1.34
2	B	19	LYS	N-CA	6.75	1.59	1.46
2	E	19	LYS	N-CA	6.74	1.59	1.46
1	D	217	TRP	CE3-CZ3	6.66	1.49	1.38
1	A	217	TRP	CE3-CZ3	6.63	1.49	1.38
1	A	154	GLU	CG-CD	6.57	1.61	1.51
1	D	154	GLU	CG-CD	6.57	1.61	1.51
1	D	4	SER	N-CA	6.53	1.59	1.46
1	A	4	SER	N-CA	6.53	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	N-CA	6.48	1.59	1.46
1	D	229	GLU	N-CA	6.45	1.59	1.46
1	D	129	ASP	C-N	6.42	1.48	1.34
2	B	53	ASP	CB-CG	6.41	1.65	1.51
2	E	53	ASP	CB-CG	6.41	1.65	1.51
1	A	129	ASP	C-N	6.41	1.48	1.34
1	D	207	GLY	CA-C	6.37	1.62	1.51
1	A	207	GLY	CA-C	6.35	1.62	1.51
1	A	3	HIS	N-CA	6.32	1.58	1.46
1	A	29	ASP	CA-C	-6.32	1.36	1.52
1	D	29	ASP	CA-C	-6.31	1.36	1.52
1	D	210	PRO	N-CA	-6.30	1.36	1.47
1	A	210	PRO	N-CA	-6.29	1.36	1.47
1	D	3	HIS	N-CA	6.29	1.58	1.46
1	D	193	PRO	C-N	6.26	1.48	1.34
1	D	62	ARG	CB-CG	6.26	1.69	1.52
1	A	62	ARG	CB-CG	6.24	1.69	1.52
1	A	193	PRO	C-N	6.23	1.48	1.34
1	D	196	LYS	N-CA	-6.20	1.33	1.46
1	A	196	LYS	N-CA	-6.18	1.33	1.46
1	A	164	CYS	C-N	-6.11	1.20	1.34
1	A	166	GLU	CB-CG	6.11	1.63	1.52
1	D	164	CYS	C-N	-6.09	1.20	1.34
1	D	166	GLU	CB-CG	6.08	1.63	1.52
2	B	31	HIS	CA-C	-6.06	1.37	1.52
2	E	31	HIS	CA-C	-6.05	1.37	1.52
2	B	31	HIS	C-N	-6.03	1.22	1.34
2	E	31	HIS	C-N	-6.00	1.22	1.34
1	D	49	ALA	C-N	5.98	1.45	1.34
1	A	256	ASN	C-N	5.97	1.47	1.34
1	A	49	ALA	C-N	5.96	1.45	1.34
1	D	256	ASN	C-N	5.93	1.47	1.34
1	D	228	MET	N-CA	5.90	1.58	1.46
1	A	229	GLU	C-N	-5.88	1.20	1.34
1	D	229	GLU	C-N	-5.88	1.20	1.34
1	A	228	MET	N-CA	5.87	1.58	1.46
2	E	20	PRO	CB-CG	5.85	1.79	1.50
2	B	20	PRO	CB-CG	5.85	1.79	1.50
2	B	42	ASN	N-CA	-5.84	1.34	1.46
2	E	42	ASN	N-CA	-5.83	1.34	1.46
1	A	264	GLU	CG-CD	5.77	1.60	1.51
1	D	62	ARG	CG-CD	5.73	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ARG	CG-CD	5.72	1.66	1.51
1	D	264	GLU	CG-CD	5.72	1.60	1.51
2	B	46	ILE	C-N	5.68	1.45	1.34
1	D	147	TRP	CB-CG	-5.67	1.40	1.50
1	A	147	TRP	CB-CG	-5.66	1.40	1.50
2	E	46	ILE	C-N	5.66	1.45	1.34
1	D	218	GLN	C-N	-5.52	1.21	1.34
1	A	218	GLN	C-N	-5.51	1.21	1.34
2	B	25	CYS	CB-SG	5.50	1.91	1.82
2	E	25	CYS	CB-SG	5.50	1.91	1.82
1	A	195	SER	C-N	-5.50	1.21	1.34
2	E	17	ASN	CA-C	-5.49	1.38	1.52
2	B	17	ASN	CA-C	-5.47	1.38	1.52
1	D	195	SER	C-N	-5.47	1.21	1.34
2	E	82	VAL	CB-CG1	-5.43	1.41	1.52
2	B	82	VAL	CB-CG1	-5.43	1.41	1.52
2	E	31	HIS	C-O	-5.38	1.13	1.23
2	B	31	HIS	C-O	-5.36	1.13	1.23
1	A	185	PRO	C-N	-5.34	1.21	1.34
1	D	185	PRO	C-N	-5.34	1.21	1.34
2	E	17	ASN	C-N	5.31	1.42	1.33
2	B	17	ASN	C-N	5.28	1.42	1.33
1	A	217	TRP	CB-CG	-5.27	1.40	1.50
3	C	5	ASN	C-N	-5.25	1.22	1.34
2	B	47	PRO	CB-CG	5.25	1.76	1.50
1	D	217	TRP	CB-CG	-5.25	1.40	1.50
3	F	5	ASN	C-N	-5.25	1.22	1.34
2	E	47	PRO	CB-CG	5.24	1.76	1.50
2	E	83	LYS	CD-CE	5.09	1.64	1.51
2	B	83	LYS	CD-CE	5.08	1.64	1.51
1	D	227	ASP	CA-C	5.07	1.66	1.52
1	A	227	ASP	CA-C	5.06	1.66	1.52
1	D	163	GLU	CG-CD	5.04	1.59	1.51
1	D	177	ALA	C-N	5.04	1.45	1.34
1	A	163	GLU	CG-CD	5.01	1.59	1.51
1	A	177	ALA	C-N	5.01	1.45	1.34
2	B	32	PRO	N-CD	-5.00	1.40	1.47

All (324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ALA	O-C-N	-58.63	23.52	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ALA	O-C-N	-58.62	23.55	123.20
1	D	206	LEU	O-C-N	-45.83	45.30	123.20
1	A	206	LEU	O-C-N	-45.81	45.33	123.20
1	D	264	GLU	O-C-N	-42.72	50.57	123.20
1	A	264	GLU	O-C-N	-42.71	50.59	123.20
1	A	256	ASN	O-C-N	-38.93	60.42	122.70
1	D	256	ASN	O-C-N	-38.91	60.45	122.70
1	A	236	ALA	C-N-CA	-29.67	60.00	122.30
1	D	236	ALA	C-N-CA	-29.66	60.02	122.30
1	A	28	VAL	O-C-N	-29.61	75.32	122.70
1	D	28	VAL	O-C-N	-29.61	75.32	122.70
1	A	131	LYS	O-C-N	-27.27	79.06	122.70
1	D	131	LYS	O-C-N	-27.27	79.07	122.70
2	B	46	ILE	O-C-N	-26.90	69.99	121.10
2	E	46	ILE	O-C-N	-26.90	69.99	121.10
1	D	131	LYS	CA-C-N	19.69	160.52	117.20
1	A	131	LYS	CA-C-N	19.69	160.51	117.20
1	A	206	LEU	C-N-CA	19.60	163.46	122.30
1	D	206	LEU	C-N-CA	19.58	163.42	122.30
1	A	129	ASP	O-C-N	-19.08	92.18	122.70
1	D	129	ASP	O-C-N	-19.04	92.23	122.70
2	B	52	SER	O-C-N	-18.55	93.03	122.70
2	E	52	SER	O-C-N	-18.53	93.05	122.70
1	A	196	LYS	C-N-CA	17.80	159.68	122.30
1	D	196	LYS	C-N-CA	17.80	159.68	122.30
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
1	D	17	LEU	CA-C-N	17.46	151.12	116.20
1	A	17	LEU	CA-C-N	17.42	151.05	116.20
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
2	B	53	ASP	O-C-N	-15.36	98.12	122.70
2	E	53	ASP	O-C-N	-15.35	98.13	122.70
1	A	205	ALA	O-C-N	-15.33	98.17	122.70
1	D	205	ALA	O-C-N	-15.33	98.18	122.70
1	A	211	ALA	O-C-N	15.20	147.02	122.70
1	D	211	ALA	O-C-N	15.19	147.00	122.70
1	D	1	GLY	C-N-CD	-15.00	87.59	120.60
1	A	1	GLY	C-N-CD	-14.99	87.63	120.60
2	B	20	PRO	CA-N-CD	14.78	132.39	111.70
2	E	20	PRO	CA-N-CD	14.78	132.39	111.70
1	D	197	GLY	O-C-N	-14.74	99.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLY	O-C-N	-14.73	99.12	122.70
1	A	128	GLU	CA-C-N	-14.30	85.73	117.20
1	D	128	GLU	CA-C-N	-14.30	85.74	117.20
1	D	128	GLU	O-C-N	13.96	145.03	122.70
1	A	128	GLU	O-C-N	13.95	145.01	122.70
1	D	264	GLU	CA-C-N	-13.87	88.45	116.20
1	A	264	GLU	CA-C-N	-13.87	88.46	116.20
1	D	28	VAL	CA-C-N	13.80	147.57	117.20
1	A	28	VAL	CA-C-N	13.79	147.53	117.20
1	A	127	ASN	O-C-N	-13.78	100.65	122.70
1	D	127	ASN	O-C-N	-13.78	100.66	122.70
1	A	252	GLY	O-C-N	-13.49	101.12	122.70
1	D	252	GLY	O-C-N	-13.48	101.14	122.70
1	D	1	GLY	O-C-N	-13.28	95.86	121.10
1	A	1	GLY	O-C-N	-13.28	95.87	121.10
1	A	237	GLY	O-C-N	-13.22	101.54	122.70
1	D	237	GLY	O-C-N	-13.21	101.56	122.70
1	A	28	VAL	CB-CA-C	-13.09	86.53	111.40
1	D	28	VAL	CB-CA-C	-13.08	86.55	111.40
1	D	179	LEU	O-C-N	-12.37	102.90	122.70
1	A	179	LEU	O-C-N	-12.36	102.92	122.70
1	D	254	GLU	C-N-CA	11.39	150.17	121.70
1	A	254	GLU	C-N-CA	11.38	150.15	121.70
1	A	209	TYR	C-N-CD	-11.37	95.58	120.60
1	D	209	TYR	C-N-CD	-11.37	95.59	120.60
1	D	176	ASN	O-C-N	-10.97	105.16	122.70
1	A	176	ASN	O-C-N	-10.95	105.18	122.70
1	D	211	ALA	CA-C-N	-10.74	93.58	117.20
1	A	211	ALA	CA-C-N	-10.73	93.60	117.20
1	A	205	ALA	CA-C-N	10.72	140.79	117.20
1	D	205	ALA	CA-C-N	10.71	140.76	117.20
1	D	17	LEU	O-C-N	-10.69	105.03	123.20
1	A	17	LEU	O-C-N	-10.65	105.09	123.20
2	B	48	LYS	CA-C-N	-10.65	93.77	117.20
2	E	48	LYS	CA-C-N	-10.64	93.79	117.20
1	A	127	ASN	C-N-CA	9.80	146.20	121.70
1	D	127	ASN	C-N-CA	9.79	146.16	121.70
2	B	19	LYS	C-N-CD	-9.78	99.08	120.60
2	E	19	LYS	C-N-CD	-9.78	99.08	120.60
1	D	16	GLY	O-C-N	-9.69	107.20	122.70
1	A	16	GLY	O-C-N	-9.67	107.23	122.70
2	E	18	GLY	C-N-CA	9.55	145.57	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	GLY	C-N-CA	9.54	145.56	121.70
1	D	174	ASN	C-N-CA	-9.51	102.33	122.30
1	A	174	ASN	C-N-CA	-9.51	102.33	122.30
1	D	174	ASN	O-C-N	9.49	139.33	123.20
1	A	174	ASN	O-C-N	9.48	139.32	123.20
1	A	29	ASP	CA-C-N	-9.35	96.62	117.20
1	A	236	ALA	CA-C-N	9.35	134.90	116.20
1	D	29	ASP	CA-C-N	-9.34	96.64	117.20
1	D	236	ALA	CA-C-N	9.34	134.87	116.20
1	A	229	GLU	CA-C-N	-9.29	96.75	117.20
1	D	229	GLU	CA-C-N	-9.29	96.76	117.20
1	D	174	ASN	CA-C-N	-9.14	97.92	116.20
1	A	174	ASN	CA-C-N	-9.12	97.96	116.20
1	A	227	ASP	O-C-N	-9.11	108.12	122.70
1	D	227	ASP	O-C-N	-9.10	108.14	122.70
1	A	266	LEU	O-C-N	-9.02	103.97	121.10
1	D	266	LEU	O-C-N	-9.00	104.01	121.10
1	A	144	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	D	144	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	A	5	MET	O-C-N	-8.71	108.77	122.70
1	D	5	MET	O-C-N	-8.70	108.78	122.70
1	A	237	GLY	CA-C-N	-8.64	98.20	117.20
1	D	237	GLY	CA-C-N	-8.64	98.20	117.20
2	E	42	ASN	O-C-N	8.63	137.87	123.20
2	B	42	ASN	O-C-N	8.62	137.86	123.20
1	A	175	GLY	O-C-N	-8.58	108.97	122.70
1	D	175	GLY	O-C-N	-8.57	108.99	122.70
1	A	131	LYS	C-N-CA	8.51	142.97	121.70
1	D	131	LYS	C-N-CA	8.50	142.94	121.70
2	B	46	ILE	C-N-CA	-8.42	86.62	122.00
2	E	46	ILE	C-N-CA	-8.42	86.64	122.00
1	D	17	LEU	CA-C-O	-8.37	102.52	120.10
1	A	17	LEU	CA-C-O	-8.36	102.54	120.10
2	E	42	ASN	CA-C-N	-8.29	99.62	116.20
2	B	42	ASN	CA-C-N	-8.26	99.67	116.20
1	D	181	ARG	C-N-CA	-8.24	101.09	121.70
1	A	181	ARG	C-N-CA	-8.24	101.10	121.70
1	D	256	ASN	CA-C-N	8.20	135.24	117.20
1	A	256	ASN	CA-C-N	8.19	135.21	117.20
1	A	219	LEU	O-C-N	8.14	135.73	122.70
1	D	219	LEU	O-C-N	8.13	135.72	122.70
1	D	180	LEU	O-C-N	-8.11	109.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	LEU	O-C-N	-8.09	109.76	122.70
1	D	144	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	144	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	175	GLY	C-N-CA	-7.97	101.77	121.70
2	E	42	ASN	CB-CA-C	7.97	126.34	110.40
1	D	175	GLY	C-N-CA	-7.96	101.80	121.70
2	B	42	ASN	CB-CA-C	7.96	126.32	110.40
1	D	251	LEU	O-C-N	-7.91	109.76	123.20
1	A	251	LEU	O-C-N	-7.90	109.78	123.20
1	D	27	TYR	O-C-N	7.84	135.25	122.70
1	A	27	TYR	O-C-N	7.83	135.24	122.70
1	A	129	ASP	CA-C-N	7.81	134.38	117.20
1	D	129	ASP	CA-C-N	7.80	134.35	117.20
2	B	47	PRO	CA-N-CD	7.74	122.53	111.70
1	A	18	GLY	O-C-N	7.72	135.06	122.70
1	D	18	GLY	O-C-N	7.72	135.05	122.70
2	E	47	PRO	CA-N-CD	7.70	122.48	111.70
1	A	178	THR	O-C-N	-7.67	110.42	122.70
1	A	263	HIS	C-N-CA	-7.67	102.52	121.70
1	D	178	THR	O-C-N	-7.67	110.44	122.70
1	D	263	HIS	C-N-CA	-7.67	102.53	121.70
3	F	6	ILE	O-C-N	-7.65	110.47	122.70
1	D	1	GLY	CA-C-N	7.64	138.49	117.10
3	C	6	ILE	O-C-N	-7.63	110.49	122.70
1	A	1	GLY	CA-C-N	7.62	138.45	117.10
1	D	194	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	19	LYS	O-C-N	-7.54	106.77	121.10
2	E	19	LYS	O-C-N	-7.53	106.80	121.10
1	D	255	GLN	CA-C-N	-7.51	100.68	117.20
1	A	255	GLN	CA-C-N	-7.50	100.71	117.20
1	A	194	ARG	NE-CZ-NH2	7.47	124.04	120.30
2	E	28	THR	C-N-CA	7.46	140.34	121.70
2	B	28	THR	C-N-CA	7.45	140.33	121.70
2	E	47	PRO	C-N-CA	7.45	140.32	121.70
2	B	47	PRO	C-N-CA	7.43	140.28	121.70
1	A	150	ALA	C-N-CA	-7.43	106.70	122.30
1	D	150	ALA	C-N-CA	-7.43	106.70	122.30
1	A	196	LYS	O-C-N	-7.39	110.63	123.20
1	D	196	LYS	O-C-N	-7.39	110.63	123.20
1	D	234	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	D	181	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	234	ARG	NE-CZ-NH2	7.35	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	LYS	CA-C-N	-7.33	101.53	116.20
1	A	196	LYS	CA-C-N	-7.33	101.54	116.20
1	A	181	ARG	NE-CZ-NH2	7.32	123.96	120.30
2	B	48	LYS	C-N-CA	-7.26	103.56	121.70
2	E	48	LYS	C-N-CA	-7.25	103.57	121.70
2	B	18	GLY	O-C-N	7.22	134.26	122.70
2	E	18	GLY	O-C-N	7.20	134.22	122.70
1	D	205	ALA	C-N-CA	7.15	139.58	121.70
1	A	205	ALA	C-N-CA	7.14	139.56	121.70
1	A	164	CYS	O-C-N	7.13	134.12	122.70
1	D	164	CYS	O-C-N	7.13	134.10	122.70
2	B	41	LYS	CB-CA-C	7.11	124.62	110.40
1	A	238	ASP	N-CA-C	-7.10	91.84	111.00
1	D	238	ASP	N-CA-C	-7.09	91.86	111.00
2	E	41	LYS	CB-CA-C	7.09	124.58	110.40
2	E	16	GLU	N-CA-C	-6.96	92.20	111.00
2	B	16	GLU	N-CA-C	-6.96	92.22	111.00
2	B	32	PRO	O-C-N	-6.90	107.98	121.10
2	E	32	PRO	O-C-N	-6.89	108.00	121.10
1	D	177	ALA	CA-C-N	-6.88	102.07	117.20
1	A	177	ALA	CA-C-N	-6.87	102.09	117.20
1	D	209	TYR	O-C-N	-6.87	108.06	121.10
1	A	209	TYR	O-C-N	-6.86	108.06	121.10
1	A	228	MET	O-C-N	-6.86	111.72	122.70
1	D	228	MET	O-C-N	-6.86	111.73	122.70
1	D	225	THR	O-C-N	6.75	133.51	122.70
1	A	181	ARG	CA-C-N	-6.74	102.38	117.20
1	A	225	THR	O-C-N	6.73	133.47	122.70
1	D	181	ARG	CA-C-N	-6.73	102.39	117.20
1	A	81	LEU	CA-CB-CG	-6.68	99.94	115.30
1	D	81	LEU	CA-CB-CG	-6.66	99.97	115.30
1	D	219	LEU	CA-C-N	-6.64	102.59	117.20
1	A	219	LEU	CA-C-N	-6.63	102.62	117.20
2	B	18	GLY	CA-C-N	-6.61	102.66	117.20
2	E	18	GLY	CA-C-N	-6.61	102.66	117.20
1	D	252	GLY	CA-C-N	6.58	131.68	117.20
2	E	90	PRO	N-CA-C	6.57	129.17	112.10
1	A	252	GLY	CA-C-N	6.56	131.64	117.20
2	B	90	PRO	N-CA-C	6.56	129.15	112.10
1	A	161	GLU	C-N-CA	-6.50	108.65	122.30
1	D	161	GLU	C-N-CA	-6.49	108.67	122.30
1	A	176	ASN	CA-C-N	-6.43	103.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ASN	CA-C-N	-6.42	103.08	117.20
1	D	193	PRO	C-N-CA	-6.38	105.75	121.70
1	A	193	PRO	C-N-CA	-6.37	105.77	121.70
1	A	210	PRO	O-C-N	-6.30	112.62	122.70
1	D	210	PRO	O-C-N	-6.29	112.63	122.70
2	E	52	SER	C-N-CA	-6.28	106.00	121.70
2	B	52	SER	C-N-CA	-6.28	106.01	121.70
3	C	7	HIS	N-CA-CB	6.18	121.72	110.60
1	D	215	LEU	CA-CB-CG	6.17	129.48	115.30
3	F	7	HIS	N-CA-CB	6.17	121.70	110.60
1	A	215	LEU	CA-CB-CG	6.15	129.46	115.30
1	D	5	MET	CG-SD-CE	6.14	110.02	100.20
1	D	211	ALA	C-N-CA	-6.13	106.37	121.70
1	A	5	MET	CG-SD-CE	6.13	110.01	100.20
1	A	211	ALA	C-N-CA	-6.13	106.38	121.70
2	B	10	TYR	N-CA-C	6.12	127.54	111.00
2	E	10	TYR	N-CA-C	6.11	127.51	111.00
2	E	19	LYS	CA-C-N	6.10	134.19	117.10
2	B	19	LYS	CA-C-N	6.09	134.15	117.10
1	A	197	GLY	CA-C-N	6.08	130.56	117.20
1	D	197	GLY	CA-C-N	6.06	130.53	117.20
1	A	227	ASP	CA-C-N	6.06	130.53	117.20
1	D	227	ASP	CA-C-N	6.06	130.52	117.20
1	D	150	ALA	O-C-N	-6.02	112.97	123.20
2	B	17	ASN	CA-C-N	-6.02	104.17	116.20
2	E	17	ASN	CA-C-N	-6.02	104.17	116.20
2	B	76	ASP	N-CA-C	6.00	127.22	111.00
2	E	76	ASP	N-CA-C	6.00	127.20	111.00
1	D	228	MET	CG-SD-CE	5.99	109.79	100.20
1	A	228	MET	CG-SD-CE	5.99	109.78	100.20
1	A	150	ALA	O-C-N	-5.99	113.02	123.20
1	A	103	VAL	N-CA-C	5.95	127.07	111.00
1	D	103	VAL	N-CA-C	5.95	127.06	111.00
1	A	62	ARG	CG-CD-NE	5.91	124.20	111.80
1	D	62	ARG	CG-CD-NE	5.91	124.20	111.80
3	C	5	ASN	O-C-N	-5.78	113.46	122.70
3	F	5	ASN	O-C-N	-5.76	113.48	122.70
1	A	193	PRO	O-C-N	5.71	131.84	122.70
1	D	193	PRO	O-C-N	5.71	131.83	122.70
1	A	210	PRO	C-N-CA	5.68	135.91	121.70
1	D	210	PRO	C-N-CA	5.68	135.91	121.70
1	A	58	GLU	N-CA-C	-5.64	95.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	GLU	N-CA-C	-5.63	95.79	111.00
2	E	46	ILE	CA-C-N	5.63	132.86	117.10
2	B	46	ILE	CA-C-N	5.63	132.86	117.10
1	D	260	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	C	9	PHE	N-CA-C	5.59	126.11	111.00
3	F	9	PHE	N-CA-C	5.59	126.09	111.00
1	A	62	ARG	CA-CB-CG	5.57	125.66	113.40
1	D	62	ARG	CA-CB-CG	5.57	125.65	113.40
1	A	176	ASN	N-CA-C	5.51	125.87	111.00
1	D	176	ASN	N-CA-C	5.50	125.86	111.00
1	A	181	ARG	O-C-N	5.49	131.49	122.70
1	D	181	ARG	O-C-N	5.49	131.49	122.70
1	A	178	THR	CA-C-N	5.47	129.24	117.20
1	A	260	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	260	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	178	THR	CA-C-N	5.47	129.23	117.20
1	A	27	TYR	C-N-CA	-5.46	108.04	121.70
1	D	27	TYR	C-N-CA	-5.46	108.06	121.70
1	A	202	ARG	N-CA-C	5.44	125.68	111.00
1	D	164	CYS	CA-C-N	-5.44	105.24	117.20
1	D	202	ARG	N-CA-C	5.44	125.68	111.00
1	A	164	CYS	CA-C-N	-5.43	105.25	117.20
1	A	182	THR	O-C-N	-5.42	114.03	122.70
1	D	182	THR	O-C-N	-5.41	114.05	122.70
1	A	27	TYR	CA-C-N	-5.39	105.34	117.20
1	A	260	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	27	TYR	CA-C-N	-5.38	105.36	117.20
1	D	127	ASN	CA-C-N	5.36	129.00	117.20
1	A	127	ASN	CA-C-N	5.36	128.99	117.20
1	A	251	LEU	C-N-CA	-5.35	111.06	122.30
1	A	192	HIS	O-C-N	5.35	131.26	121.10
1	D	251	LEU	C-N-CA	-5.34	111.08	122.30
1	A	244	TRP	CA-CB-CG	5.34	123.85	113.70
1	D	5	MET	CA-C-N	5.34	128.95	117.20
1	A	5	MET	CA-C-N	5.34	128.95	117.20
1	D	193	PRO	CA-C-N	-5.34	105.45	117.20
1	D	244	TRP	CA-CB-CG	5.34	123.84	113.70
2	E	89	GLU	CB-CA-C	5.33	121.07	110.40
1	A	193	PRO	CA-C-N	-5.33	105.47	117.20
2	B	89	GLU	CB-CA-C	5.33	121.06	110.40
1	D	192	HIS	O-C-N	5.32	131.22	121.10
1	D	11	ALA	N-CA-C	-5.32	96.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLU	CB-CA-C	5.31	121.03	110.40
1	A	11	ALA	N-CA-C	-5.31	96.66	111.00
1	A	225	THR	CA-C-N	-5.30	105.55	117.20
1	D	1	GLY	C-N-CA	5.30	144.24	122.00
1	D	225	THR	CA-C-N	-5.30	105.55	117.20
1	A	1	GLY	C-N-CA	5.29	144.22	122.00
1	D	222	GLU	CB-CA-C	5.29	120.98	110.40
1	A	166	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	D	166	GLU	OE1-CD-OE2	-5.25	117.00	123.30
2	E	19	LYS	CA-C-O	-5.22	109.14	120.10
1	A	5	MET	C-N-CA	-5.21	108.68	121.70
1	D	5	MET	C-N-CA	-5.20	108.70	121.70
1	D	247	VAL	CB-CA-C	-5.20	101.52	111.40
2	B	19	LYS	CA-C-O	-5.20	109.18	120.10
1	A	247	VAL	CB-CA-C	-5.19	101.54	111.40
1	D	95	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	95	LEU	CA-CB-CG	5.13	127.10	115.30
1	D	122	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	122	ASP	CB-CG-OD1	5.11	122.90	118.30
2	B	47	PRO	CA-C-N	-5.09	105.99	117.20
3	C	5	ASN	N-CA-CB	-5.07	101.47	110.60
2	E	47	PRO	CA-C-N	-5.07	106.04	117.20
3	F	5	ASN	N-CA-CB	-5.07	101.48	110.60
3	F	6	ILE	N-CA-C	5.06	124.66	111.00
3	C	6	ILE	N-CA-C	5.04	124.60	111.00
1	A	126	LEU	CB-CG-CD2	-5.01	102.49	111.00
2	B	32	PRO	CA-C-N	5.01	131.12	117.10
2	E	54	MET	CB-CG-SD	-5.00	97.38	112.40
2	E	32	PRO	CA-C-N	5.00	131.10	117.10

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	2039	503	14
1	D	2184	0	2041	486	17
2	B	820	0	795	141	0
2	E	820	0	795	147	2
3	C	80	0	72	23	2
3	F	80	0	72	23	2
All	All	6168	0	5814	1229	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 103.

All (1229) 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:CG	2:E:47:PRO:CB	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
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:N	2:E:47:PRO:CD	1.75	1.48
2:E:20:PRO:N	2:E:20:PRO:CD	1.76	1.46
2:B:47:PRO:CD	2:B:47:PRO:N	1.75	1.46
2:B:20:PRO:N	2:B:20:PRO:CD	1.76	1.44
2:B:51:MET:SD	2:B:51:MET:CE	2.04	1.44
2:E:51:MET:CE	2:E:51:MET:SD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:237:GLY:O	1:A:238:ASP:O	1.63	1.15
1:A:3:HIS:H	1:A:103:VAL:CG1	1.60	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:D:195:SER:HB3	1:D:198:GLU:O	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HD2	1:A:255:GLN:HE21	1.17	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
2:E:32:PRO:CD	2:E:84:HIS:CE1	2.37	1.07
1:D:5:MET:HG3	1:D:100:GLY:HA2	1.35	1.07
1:A:28:VAL:CG2	1:A:28:VAL:O	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:D:183:ASP:H	1:D:209:TYR:CB	1.69	1.05
1:A:181:ARG:HH12	2:E:20:PRO:HD2	0.93	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:N	2:E:47:PRO:CG	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:A:5:MET:CB	1:A:101:CYS:H	1.72	1.01
2:E:20:PRO:N	2:E:20:PRO:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PRO:HB2	1:D:253:LYS:HB2	1.42	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: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
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: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:D:237:GLY:O	1:D:238:ASP:C	1.94	0.97
1:D:33:PHE:CD1	1:D:51:TRP:CH2	2.52	0.97
1:A:181:ARG:HB3	2:E:19:LYS:HE2	1.45	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: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:D:29:ASP:CG	1:D:179:LEU:HD13	1.87	0.95
1:D:195:SER:CB	1:D:198:GLU:HB2	1.96	0.95
1:D:58:GLU:HB2	1:D:62:ARG:CZ	1.97	0.95
1:A:207:GLY:HA2	1:A:241:PHE:O	1.66	0.94
1:A:29:ASP:CG	1:A:179:LEU:HD13	1.87	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: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:237:GLY:O	1:A:238:ASP:C	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:2:PRO:CA	1:D:3:HIS:NE2	2.02	0.92
2:B:19:LYS:C	2:B:20:PRO:CD	2.38	0.92
2:E:19:LYS:C	2:E:20:PRO:CD	2.38	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
1:D:4:SER:OG	1:D:28:VAL:C	2.09	0.91
2:E:6:GLN:HE21	2:E:6:GLN:HA	1.35	0.91
1:A:253:LYS:HG3	1:A:255:GLN:NE2	1.86	0.91
1:A:79:ARG:HA	1:A:82:LEU:HD12	1.51	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:4:SER:OG	1:A:28:VAL:C	2.09	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:220:ASN:OD1	1:D:256:ASN:C	2.10	0.90
2:E:47:PRO:CA	2:E:47:PRO:CG	2.49	0.90
1:A:253:LYS:HD2	1:A:255:GLN:NE2	1.78	0.90
1:A:3:HIS:O	1:A:103:VAL:CG1	2.18	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:CA	2:B:47:PRO:CG	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:220:ASN:OD1	1:A:256:ASN:C	2.10	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
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: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
2:E:46:ILE:H	2:E:46:ILE:HD12	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:237:GLY:C	1:D:238:ASP:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:141:GLN:HE22	1:D:144:ARG:HH21	1.26	0.83
1:A:183:ASP:H	1:A:209:TYR:HB2	0.96	0.83
1:A:75:ARG:NH1	1:A:75:ARG:HB3	1.94	0.83
1:D:225:THR:O	1:D:225:THR:HG22	1.78	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
1:A:237:GLY:C	1:A:238:ASP:O	2.10	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
2:E:32:PRO:HD3	2:E:84:HIS:CE1	2.06	0.82
2:E:24:ASN:ND2	2:E:65:LEU:HD11	1.94	0.82
1:A:139:ALA:O	1:A:142:ILE:HG13	1.78	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
1:D:75:ARG:HB3	1:D:75:ARG:NH1	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:21:ARG:HH12	2:B:54:MET:HE1	1.44	0.81
1:D:51:TRP:HZ3	1:D:52:MET:SD	2.02	0.81
1:D:21:ARG:HH12	2:E:54:MET:HE1	1.43	0.81
1:D:253:LYS:HD2	1:D:255:GLN:NE2	1.78	0.81
1:D:33:PHE:CE1	1:D:51:TRP:HZ2	1.99	0.81
1:A:225:THR:HG22	1:A:225:THR:O	1.79	0.80
1:A:33:PHE:CE1	1:A:51:TRP:HZ2	1.99	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:219:LEU:CD2	1:A:224:LEU:HD22	2.10	0.80
1:A:216:THR:HG21	1:A:223:GLU:HB3	1.64	0.80
1:A:52:MET:O	1:A:55:GLU:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:CZ	1:A:75:ARG:HB3	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:A:33:PHE:HE1	1:A:51:TRP:CZ2	2.01	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:NE2	2:E:6:GLN:HA	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:196:LYS:O	1:D:196:LYS:CG	2.30	0.78
1:D:220:ASN:OD1	1:D:256:ASN:HA	1.84	0.78
1:D:216:THR:HG21	1:D:223:GLU:HB3	1.64	0.78
1:D:253:LYS:CG	1:D:255:GLN:CD	2.52	0.78
1:D:33:PHE:HE1	1:D:51:TRP:CZ2	2.01	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
1:A:181:ARG:CZ	2:E:20:PRO:HD3	2.13	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
2:E:39:MET:C	2:E:46:ILE:HG13	2.05	0.77
1:A:253:LYS:CG	1:A:255:GLN:CD	2.52	0.77
2:B:39:MET:C	2:B:46:ILE:HG13	2.05	0.77
1:D:219:LEU:HD21	1:D:224:LEU:HD22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:CB	1:A:209:TYR:HB2	2.14	0.77
1:A:196:LYS:HG3	1:A:196:LYS:O	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
1:A:29:ASP:OD2	1:A:179:LEU:HD13	1.86	0.76
1:A:123:TYR:CE1	3:C:9:PHE:HE1	2.03	0.76
1:A:58:GLU:HB2	1:A:62:ARG:NE	2.00	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: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:229:GLU:O	1:D:246:SER:N	2.18	0.75
1:D:58:GLU:HB2	1:D:62:ARG:NE	2.00	0.75
2:B:28:THR:CG2	2:B:29:GLN:NE2	2.50	0.75
1:D:195:SER:HG	1:D:198:GLU:HB2	1.47	0.75
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.22	0.75
1:D:44:ARG:HA	1:D:64:THR:CG2	2.17	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:229:GLU:HB3	1:D:244:TRP:CZ3	2.21	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: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:A:2:PRO:C	1:A:3:HIS:CD2	2.60	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: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:195:SER:HG	1:A:198:GLU:HB2	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PRO:C	1:D:3:HIS:CD2	2.60	0.74
1:A:2:PRO:N	1:A:3:HIS:CD2	2.52	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:44:ARG:HA	1:A:64:THR:CG2	2.17	0.74
1:A:33:PHE:CD1	1:A:51:TRP:CZ2	2.76	0.74
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:D:253:LYS:CG	1:D:255:GLN:CG	2.67	0.73
1:A:181:ARG:NH2	2:E:20:PRO:HD3	2.04	0.73
1:D:126:LEU:HB2	1:D:133:TRP:CZ3	2.23	0.73
1:D:33:PHE:CD1	1:D:51:TRP:CZ2	2.76	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:208:PHE:HZ	1:D:213:ILE:HG22	1.54	0.72
1:D:28:VAL:HG23	1:D:31:LYS:HB3	1.71	0.72
1:A:194:ARG:HG3	1:A:200:THR:CB	2.19	0.72
1:A:44:ARG:CG	1:A:64:THR:HG21	2.18	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: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:234:ARG:HH22	2:B:10:TYR:CB	2.02	0.71
1:A:253:LYS:HG3	1:A:255:GLN:CD	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:250:PRO:HB2	1:A:253:LYS:HB3	1.71	0.69
1:A:82:LEU:HD23	1:A:87:GLN:HB2	1.74	0.69
1:D:253:LYS:HG3	1:D:255:GLN:CD	2.10	0.69
1:D:66:ILE:HD11	3:F:4:VAL:HG23	1.75	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:135:ALA:HB2	1:D:144:ARG:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PHE:CE2	1:D:213:ILE:HG21	2.29	0.68
1:D:57:PRO:HA	1:D:60:TRP:HD1	1.57	0.68
1:A:202:ARG:HD2	1:A:204:TRP:CZ2	2.29	0.67
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
1:D:157:ARG:HH21	1:D:161:GLU:CD	1.98	0.67
2:B:36:GLU:O	2:B:82:VAL:HA	1.95	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:O	1:D:266:LEU:HD23	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:157:ARG:HH21	1:A:161:GLU:CD	1.98	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:198:GLU:HB3	1:A:248:VAL:HG23	1.78	0.66
1:A:29:ASP:OD1	1:A:179:LEU:HD13	1.96	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:229:GLU:O	1:D:245:ALA:HA	1.96	0.65
1:D:198:GLU:HB3	1:D:248:VAL:HG23	1.78	0.65
1:D:123:TYR:CE1	3:F:9:PHE:CE1	2.84	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:CD1	2:B:46:ILE:H	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:GLY:H2	1:D:105:SER:HA	1.62	0.65
1:A:263:HIS:C	1:A:265:GLY:H	2.00	0.65
1:A:33:PHE:CE1	1:A:51:TRP:CH2	2.82	0.65
1:D:263:HIS:C	1:D:265:GLY:H	2.00	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:59:TYR:HB2	1:D:62:ARG:NH1	2.12	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:HB2	1:A:108:ARG:CZ	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:219:LEU:HA	1:A:257:TYR:CE1	2.32	0.64
1:A:6:ARG:HE	1:A:100:GLY:HA3	1.63	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:D:173:LYS:C	1:D:175:GLY:H	2.00	0.64
1:A:103:VAL:HG13	1:A:104:GLY:N	2.11	0.64
1:A:59:TYR:HB2	1:A:62:ARG:NH1	2.12	0.64
1:D:204:TRP:HE3	1:D:206:LEU:HD13	1.62	0.64
1:D:32:GLU:OE2	1:D:35:ARG:NH1	2.31	0.64
1:A:1:GLY:H2	1:A:105:SER:HA	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:173:LYS:C	1:A:175:GLY:H	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:189:VAL:HA	1:D:202:ARG:O	1.98	0.63
1:D:44:ARG:HA	1:D:64:THR:HG21	1.81	0.63
1:A:206:LEU:CD1	1:A:242:GLN:HB3	2.28	0.63
1:A:73:TRP:CD1	1:A:74:PHE:N	2.66	0.63
1:D:163:GLU:O	1:D:167:TRP:HD1	1.81	0.63
1:D:73:TRP:CD1	1:D:74:PHE:N	2.66	0.63
1:A:51:TRP:HZ3	1:A:52:MET:HE1	1.63	0.63
1:D:230:LEU:HD23	1:D:230:LEU:N	2.14	0.63
1:D:36:PHE:HB2	1:D:45:TYR:CD1	2.34	0.63
1:A:146:LYS:O	1:A:149:GLN:HG3	1.99	0.62
1:A:189:VAL:HA	1:A:202:ARG:O	1.99	0.62
1:A:183:ASP:HB2	1:A:209:TYR:H	0.74	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:51:TRP:HZ3	1:D:52:MET:HE1	1.63	0.62
1:A:230:LEU:N	1:A:230:LEU:HD23	2.14	0.62
1:D:164:CYS:SG	1:D:165:VAL:HG23	2.39	0.62
1:A:164:CYS:SG	1:A:165:VAL:HG23	2.39	0.62
1:A:51:TRP:HZ3	1:A:52:MET:CE	2.12	0.62
1:D:108:ARG:HB2	1:D:108:ARG:CZ	2.28	0.62
1:D:32:GLU:O	1:D:33:PHE:CG	2.51	0.62
1:D:59:TYR:CA	1:D:62:ARG:HD2	2.29	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:183:ASP:CB	1:A:209:TYR:CB	2.78	0.61
1:A:84:TYR:CB	1:A:139:ALA:HB1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:CG	1:D:103:VAL:CG2	2.82	0.61
1:A:163:GLU:O	1:A:167:TRP:HD1	1.81	0.61
1:A:52:MET:HA	1:A:52:MET:HE3	1.81	0.61
1:A:104:GLY:HA3	1:A:108:ARG:O	2.00	0.61
1:D:208:PHE:HD1	1:D:263:HIS:CE1	2.17	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:A:219:LEU:HD23	1:A:257:TYR:HE1	1.66	0.61
1:A:208:PHE:HD1	1:A:263:HIS:CE1	2.17	0.61
1:A:59:TYR:CA	1:A:62:ARG:HD2	2.29	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:185:PRO:HD3	1:A:263:HIS:CD2	2.36	0.61
1:A:2:PRO:CA	1:A:3:HIS:CG	2.77	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: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:A:181:ARG:CZ	2:E:20:PRO:CD	2.76	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:3:HIS:CD2	1:D:104:GLY:C	2.75	0.60
1:D:44:ARG:HA	1:D:64:THR:HG23	1.84	0.60
1:A:3:HIS:CD2	1:A:104:GLY:C	2.75	0.60
1:A:176:ASN:O	1:A:179:LEU:N	2.35	0.60
1:A:16:GLY:O	1:A:17:LEU:HG	2.02	0.60
1:D:176:ASN:O	1:D:179:LEU:N	2.35	0.60
1:D:16:GLY:O	1:D:17:LEU:HG	2.02	0.60
1:A:21:ARG:HH12	2:B:54:MET:CE	2.12	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
1:A:59:TYR:HB2	1:A:62:ARG:HH11	1.64	0.60
1:D:3:HIS:N	1:D:3:HIS:CD2	2.70	0.60
2:E:7:ILE:HD13	2:E:91:LYS:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:HB3	2:E:19:LYS:HZ3	1.67	0.60
1:A:3:HIS:N	1:A:3:HIS:CD2	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: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: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: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:A:38:SER:O	1:A:43:PRO:HG3	2.02	0.59
1:D:213:ILE:HG13	1:D:214:THR:H	1.67	0.59
1:D:38:SER:O	1:D:43:PRO:HG3	2.02	0.59
1:D:52:MET:HA	1:D:52:MET:HE3	1.83	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:59:TYR:N	1:D:62:ARG:NH1	2.51	0.59
1:D:5:MET:O	1:D:100:GLY:HA3	2.02	0.59
2:E:40:LEU:O	2:E:78:TYR:HA	2.01	0.59
1:D:77:ASN:HA	1:D:80:THR:HG22	1.83	0.59
1:D:66:ILE:CD1	3:F:4:VAL:HG23	2.33	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
2:E:38:GLN:HB2	2:E:83:LYS:HZ2	1.68	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: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:233:THR:OG1	1:D:243:LYS:HD2	2.04	0.58
1:D:216:THR:O	1:D:259:CYS:HA	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:LYS:CG	2:B:31:HIS:HB2	2.34	0.58
1:A:180:LEU:O	1:A:182:THR:HG23	1.93	0.58
1:A:59:TYR:N	1:A:62:ARG:HH11	2.02	0.58
1:D:3:HIS:NE2	1:D:104:GLY:C	2.57	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:192:HIS:CB	1:A:193:PRO:HD2	2.33	0.57
1:A:3:HIS:NE2	1:A:104:GLY:C	2.57	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:93:HIS:HD2	1:D:119:ASP:OD2	1.86	0.57
1:D:59:TYR:N	1:D:62:ARG:HH11	2.02	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:26:TYR:HD1	2:E:65:LEU:HD23	1.69	0.57
2:E:3:LYS:HG2	2:E:31:HIS:HB2	1.87	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:22:TYR:CD1	1:A:36:PHE:HE1	2.23	0.57
1:A:5:MET:O	1:A:6:ARG:CD	2.52	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:213:ILE:HD12	1:A:263:HIS:HB2	1.87	0.56
1:A:32:GLU:OE1	1:A:48:GLN:HG3	2.05	0.56
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:63:ILE:HD11	3:C:2:PRO:CD	2.32	0.56
2:B:39:MET:C	2:B:40:LEU:HG	2.26	0.56
1:D:219:LEU:HA	1:D:257:TYR:CD1	2.41	0.56
2:E:39:MET:C	2:E:40:LEU:HG	2.26	0.56
2:B:35:ILE:CD1	2:B:84:HIS:HB2	2.34	0.56
2:B:38:GLN:HB2	2:B:83:LYS:HZ1	1.69	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
1:A:29:ASP:H	1:A:31:LYS:N	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:TYR:CD1	1:D:36:PHE:HE1	2.23	0.56
1:D:49:ALA:O	1:D:52:MET:HB2	2.06	0.56
2:E:35:ILE:CD1	2:E:84:HIS:HB2	2.34	0.56
1:D:5:MET:CG	1:D:101:CYS:SG	2.83	0.56
1:A:3:HIS:C	1:A:103:VAL:HG11	2.25	0.56
1:D:63:ILE:HD11	3:F:2:PRO:CD	2.32	0.56
1:D:5:MET:O	1:D:6:ARG:CG	2.53	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:183:ASP:HB2	1:A:209:TYR:CB	2.36	0.56
1:A:59:TYR:CB	1:A:62:ARG:HH11	2.19	0.56
1:A:234:ARG:HH21	2:B:10:TYR:HB3	1.66	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:D:5:MET:HB3	1:D:101:CYS:N	2.17	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:3:HIS:C	1:D:103:VAL:HG11	2.25	0.55
1:D:59:TYR:CB	1:D:62:ARG:HH11	2.19	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:253:LYS:HG2	1:D:255:GLN:NE2	2.16	0.55
1:D:7:TYR:HB3	1:D:9:GLU:OE1	2.07	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: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
1:A:164:CYS:SG	1:A:165:VAL:N	2.80	0.54
1:A:72:GLN:HE22	1:A:75:ARG:NH2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:51:TRP:CZ3	1:D:52:MET:HE1	2.41	0.54
1:A:103:VAL:HG22	1:A:104:GLY:N	2.23	0.54
1:D:164:CYS:SG	1:D:165:VAL:N	2.80	0.54
1:D:5:MET:HG2	1:D:101:CYS:CB	2.37	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:HD23	1:D:130:LEU:N	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
1:D:5:MET:HE2	1:D:101:CYS:SG	2.48	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
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:D:58:GLU:C	1:D:62:ARG:HD2	2.29	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:A:58:GLU:C	1:A:62:ARG:HD2	2.28	0.53
1:D:141:GLN:NE2	1:D:144:ARG:HH21	2.02	0.53
2:B:3:LYS:CG	2:B:31:HIS:N	2.71	0.53
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:A:77:ASN:HD21	3:C:8:ASN:HD22	1.57	0.53
1:D:237:GLY:N	2:E:12:ARG:HE	2.03	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:A:36:PHE:CB	1:A:45:TYR:CD1	2.91	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:A:51:TRP:CZ3	1:A:52:MET:HE1	2.42	0.53
2:E:33:PRO:HB3	2:E:62:PHE:CE2	2.44	0.53
1:A:202:ARG:HB3	1:A:202:ARG:HH11	1.74	0.53
1:A:22:TYR:CE1	1:A:36:PHE:CE1	2.97	0.53
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.44	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

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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
2:B:38:GLN:HB2	2:B:83:LYS:HZ2	1.71	0.53
1:D:22:TYR:CE1	1:D:36:PHE:CE1	2.97	0.53
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: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: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
2:B:7:ILE:CD1	2:B:91:LYS:HD3	2.39	0.52
1:A:66:ILE:HG21	3:C:2:PRO:HG2	1.92	0.52
1:D:249:VAL:HG22	1:D:257:TYR:CD2	2.44	0.52
1:D:59:TYR:N	1:D:62:ARG:HD2	2.24	0.52
1:A:3:HIS:C	1:A:103:VAL:HB	2.15	0.52
1:A:160:LEU:O	1:A:164:CYS:SG	2.67	0.52
2:E:38:GLN:HB2	2:E:83:LYS:HZ1	1.72	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:A:180:LEU:O	1:A:181:ARG:C	2.37	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
1:A:73:TRP:CZ3	3:C:7:HIS:O	2.63	0.51
1:D:3:HIS:C	1:D:103:VAL:CG1	2.79	0.51
1:D:216:THR:CG2	1:D:217:TRP:N	2.73	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:HB2	1:A:209:TYR:CA	2.36	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
1:D:218:GLN:HB2	1:D:258:THR:HG23	1.92	0.51
1:A:3:HIS:C	1:A:103:VAL:CG1	2.79	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
1:D:155:TYR:CZ	3:F:6:ILE:HG22	2.46	0.50
1:A:102:ASP:HB2	1:A:111:ARG:HB3	1.93	0.50
1:A:194:ARG:HB3	1:A:198:GLU:O	2.11	0.50
1:A:22:TYR:HD1	1:A:36:PHE:HE1	1.59	0.50
1:A:155:TYR:CZ	3:C:6:ILE:HG22	2.46	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:208:PHE:C	1:A:209:TYR:O	2.49	0.50
1:A:259:CYS:O	1:A:260:ARG:HD2	2.12	0.50
1:D:183:ASP:HB2	1:D:209:TYR:CA	2.36	0.50
1:D:29:ASP:OD1	1:D:179:LEU:CD1	2.59	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
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:237:GLY:N	2:B:12:ARG:HE	2.03	0.50
1:A:77:ASN:ND2	3:C:9:PHE:HB2	2.26	0.50
2:E:12:ARG:HB2	2:E:22:ILE:HB	1.93	0.50
1:A:146:LYS:CG	1:A:147:TRP:N	2.72	0.50
1:A:5:MET:HE2	1:A:164:CYS:O	2.11	0.50
1:A:75:ARG:NH1	1:A:79:ARG:HE	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:ILE:C	2:B:47:PRO:O	2.50	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:5:MET:HE2	1:D:164:CYS:O	2.12	0.49
1:D:250:PRO:CB	1:D:253:LYS:HB3	2.40	0.49
2:E:64:ILE:HG13	2:E:65:LEU:N	2.27	0.49
2:E:7:ILE:HD12	2:E:7:ILE: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:230:LEU:N	1:A:230:LEU:CD2	2.76	0.49
1:A:253:LYS:HG2	1:A:255:GLN:NE2	2.16	0.49
2:B:7:ILE:N	2:B:7:ILE:HD12	2.27	0.49
1:D:182:THR:C	1:D:209:TYR:CB	2.80	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
1:A:96:GLN:NE2	2:B:60:TRP:HB3	2.28	0.49
2:B:47:PRO:CA	2:B:47:PRO:CD	2.81	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
1:A:61:GLU:O	1:A:62:ARG:C	2.51	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:A:249:VAL:HG13	1:A:253:LYS:O	2.12	0.48
1:A:79:ARG:O	1:A:82:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TYR:HD1	1:D:124:ILE:CB	2.25	0.48
1:D:52:MET:HA	1:D:52:MET:CE	2.44	0.48
2:E:56:PHE:CE1	2:E:60:TRP:HA	2.47	0.48
1:A:224:LEU:CD1	1:A:247:VAL:HG11	2.43	0.48
1:A:61:GLU:O	1:A:65:GLN:HB2	2.13	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
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:259:CYS:C	1:A:260:ARG:HD2	2.33	0.48
2:B:64:ILE:HG13	2:B:65:LEU:N	2.27	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:77:ASN:ND2	3:F:9:PHE:HB2	2.26	0.48
1:D:81:LEU:HD21	1:D:123:TYR:CE2	2.46	0.48
1:D:230:LEU:CD2	1:D:230:LEU:N	2.76	0.48
1:D:259:CYS:C	1:D:260:ARG:HD2	2.33	0.48
2:E:46:ILE:C	2:E:47:PRO:O	2.50	0.48
1:D:123:TYR:CD1	3:F:9:PHE:HE1	2.32	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:208:PHE:C	1:D:209:TYR:O	2.49	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:A:5:MET:HE2	1:A:101:CYS:SG	2.53	0.48
1:D:5:MET:CB	1:D:101:CYS:O	2.59	0.48
1:D:224:LEU:CD1	1:D:247:VAL:HG11	2.43	0.48
1:A:123:TYR:HD1	1:A:124:ILE:CB	2.25	0.48
1:A:14:ARG:CZ	1:A:19:GLU:O	2.61	0.48
1:A:47:PRO:HG2	1:A:47:PRO:O	2.13	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
1:D:84:TYR:HB3	1:D:139:ALA:CB	2.42	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:52:MET:HA	1:A:52:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:CD1	3:C:9:PHE:HE1	2.32	0.47
1:D:47:PRO:HG2	1:D:47:PRO:O	2.13	0.47
3:F:4:VAL:CG1	3:F:6:ILE:HD12	2.44	0.47
1:A:36:PHE:CD1	1:A:36:PHE:C	2.88	0.47
3:C:4:VAL:CG1	3:C:6:ILE:HD12	2.44	0.47
1:D:61:GLU:O	1:D:62:ARG:C	2.51	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:141:GLN:HE22	1:D:144:ARG:NH2	2.03	0.47
1:D:75:ARG:CB	1:D:75:ARG:CZ	2.89	0.47
1:D:253:LYS:HG2	1:D:255:GLN:CD	2.34	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: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:75:ARG:NH1	1:D:79:ARG:NH2	2.57	0.47
1:A:84:TYR:HB3	1:A:139:ALA:CB	2.42	0.47
1:D:22:TYR:HE1	1:D:36:PHE:CE1	2.33	0.47
1:D:13:SER:OG	1:D:93:HIS:N	2.47	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:3:LYS:HG3	2:B:30:PHE:C	2.35	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:47:PRO:CA	2:E:47:PRO:CD	2.81	0.47
2:E:35:ILE:HD12	2:E:84:HIS:HB2	1.97	0.47
1:A:126:LEU:HD12	1:A:132:THR:O	2.15	0.47
1:A:141:GLN:HE22	1:A:144:ARG:NH2	2.03	0.47
1:D:2:PRO:C	1:D:3:HIS:CG	2.88	0.47
2:E:81:ARG:HD3	2:E:83:LYS:NZ	2.30	0.47
1:D:73:TRP:HZ3	3:F:7:HIS:C	2.18	0.47
1:A:202:ARG:O	1:A:204:TRP:CD1	2.68	0.47
1:A:28:VAL:O	1:A:29:ASP:CG	2.53	0.47
1:A:2:PRO:C	1:A:3:HIS:CG	2.88	0.46
1:D:36:PHE:C	1:D:36:PHE:CD1	2.88	0.46
1:A:143:THR:O	1:A:147:TRP:HB2	2.15	0.46
1:A:81:LEU:HD22	1:A:85:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:C	1:D:103:VAL:HB	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
2:E:3:LYS:HG3	2:E:30:PHE:C	2.35	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
2:B:81:ARG:HD3	2:B:83:LYS:HZ3	1.80	0.46
1:D:4:SER:OG	1:D:29:ASP:N	2.47	0.46
2:E:81:ARG:HG2	2:E:83:LYS:CE	2.45	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:A:73:TRP:HZ3	3:C:7:HIS:C	2.18	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
1:A:22:TYR:HE1	1:A:36:PHE:CE1	2.33	0.46
1:A:3:HIS:HD2	1:A:103:VAL:CG1	2.29	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:A:253:LYS:HG2	1:A:255:GLN:CD	2.34	0.46
1:D:27:TYR:HA	1:D:31:LYS:O	2.16	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:127:ASN:HB2	1:A:132:THR:O	2.14	0.45
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
2:B:23:LEU:HD12	2:B:70:PHE:CZ	2.52	0.45
1:D:249:VAL:HG12	1:D:250:PRO:O	2.16	0.45
1:D:77:ASN:HA	1:D:80:THR:CG2	2.46	0.45
1:A:182:THR:C	1:A:209:TYR:CB	2.80	0.45
1:D:160:LEU:O	1:D:164:CYS:SG	2.67	0.45
1:D:81:LEU:HD22	1:D:85:TYR:CD2	2.50	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:3:HIS:C	1:A:103:VAL:CB	2.79	0.45
1:A:27:TYR:HA	1:A:31:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:24:ASN:HD22	2:B:65:LEU:CD1	2.28	0.45
2:B:3:LYS:HG2	2:B:31:HIS:CB	2.47	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: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
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: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:D:51:TRP:CZ3	1:D:52:MET:CE	2.95	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:A:146:LYS:CG	1:A:147:TRP:H	2.30	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:192:HIS:HD2	1:A:200:THR:HG22	1.81	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:H	1:D:201:LEU:HD23	1.82	0.45
1:D:217:TRP:N	1:D:217:TRP:CD2	2.84	0.45
1:D:36:PHE:HB2	1:D:45:TYR:HA	1.99	0.45
2:E:36:GLU:HB2	2:E:83:LYS:HB2	1.98	0.45
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: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:46:GLU:HB3	1:D:47:PRO:HD2	1.99	0.44
1:D:11:ALA:CB	1:D:74:PHE:HB3	2.46	0.44
1:A:161:GLU:C	1:A:164:CYS:SG	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:195:SER:OG	1:A:198:GLU:CA	2.65	0.44
1:A:51:TRP:CZ3	1:A:52:MET:CE	2.95	0.44
2:B:51:MET:CB	2:B:64:ILE:HD11	2.43	0.44
1:D:81:LEU:HA	1:D:81:LEU:HD23	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:CG	2:B:51:MET:CE	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: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:A:255:GLN:C	1:A:256:ASN:CG	2.76	0.44
1:D:161:GLU:C	1:D:164:CYS:SG	2.96	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
2:B:3:LYS:HG2	2:B:31:HIS:N	2.33	0.43
1:A:230:LEU:HA	1:A:245:ALA:CA	2.35	0.43
1:A:218:GLN:O	1:A:257:TYR:HA	2.18	0.43
1:A:25:VAL:HG22	1:A:27:TYR:CZ	2.53	0.43
2:B:84:HIS:ND1	2:B:86:SER:OG	2.51	0.43
3:C:5:ASN:OD1	3:C:5:ASN:N	2.46	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:D:70:GLN:HE22	3:F:5:ASN:HB3	1.82	0.43
1:A:3:HIS:CD2	1:A:103:VAL:CG2	3.01	0.43
1:A:201:LEU:HD23	1:A:201:LEU:H	1.82	0.43
1:A:36:PHE:HB2	1:A:45:TYR:HA	1.99	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:160:LEU:C	1:A:164:CYS:SG	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.53	0.43
1:A:73:TRP:CD1	1:A:73:TRP:C	2.92	0.43
1:D:198:GLU:HA	1:D:249:VAL:O	2.19	0.43
1:D:255:GLN:C	1:D:256:ASN:CG	2.76	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:A:58:GLU:O	1:A:62:ARG:HG3	2.18	0.43
1:A:7:TYR:HB2	1:A:99:TYR:CE1	2.54	0.43
1:A:81:LEU:CD2	1:A:84:TYR:CD2	3.01	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:D:73:TRP:CD1	1:D:73:TRP:C	2.92	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:D:160:LEU:C	1:D:164:CYS:SG	2.97	0.43
1:A:155:TYR:CE2	3:C:6:ILE:HG22	2.54	0.43
1:A:173:LYS:C	1:A:175:GLY:N	2.66	0.43
1:A:88:SER:OG	1:A:89:ALA:N	2.52	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
1:D:218:GLN:O	1:D:257:TYR:HA	2.18	0.43
1:A:183:ASP:N	1:A:209:TYR:CG	2.84	0.42
1:A:10:THR:O	1:A:22:TYR:HA	2.19	0.42
1:D:22:TYR:CD1	1:D:36:PHE:CE1	3.06	0.42
1:A:137:ASP:O	1:A:141:GLN:N	2.46	0.42
1:A:133:TRP:HB2	1:A:144:ARG:HD3	2.00	0.42
1:A:167:TRP:O	1:A:171:TYR:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HB3	2:B:20:PRO:CD	2.49	0.42
1:D:230:LEU:CA	1:D:245:ALA:HA	2.36	0.42
1:D:155:TYR:CE2	3:F:6:ILE:HG22	2.54	0.42
1:A:192:HIS:O	1:A:194:ARG:HB2	2.18	0.42
1:A:25:VAL:HG22	1:A:27:TYR:CE2	2.55	0.42
1:D:34:VAL:HA	1:D:48:GLN:HG2	2.01	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:251:LEU:HD22	1:A:251:LEU:HA	1.37	0.42
1:A:34:VAL:HA	1:A:48:GLN:HG2	2.02	0.42
1:A:3:HIS:CA	1:A:103:VAL:CG1	2.83	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:146:LYS:CG	1:D:147:TRP:H	2.30	0.42
1:D:78:LEU:HA	1:D:78:LEU:HD12	1.87	0.42
1:D:7:TYR:HB2	1:D:99:TYR:CE1	2.54	0.42
2:E:51:MET:CE	2:E:51:MET:CG	2.91	0.42
1:A:53:GLU:C	1:A:55:GLU:H	2.23	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
1:A:5:MET:HE3	1:A:101:CYS:SG	2.60	0.42
1:A:148:GLU:O	1:A:149:GLN:C	2.58	0.42
2:B:27:VAL:HG21	2:B:37:ILE:CD1	2.45	0.42
1:D:182:THR:HA	1:D:209:TYR:CG	2.55	0.42
1:D:88:SER:OG	1:D:89:ALA:N	2.52	0.42
1:D:133:TRP:HB2	1:D:144:ARG:HD3	2.00	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:A:181:ARG:HE	2:E:19:LYS:HG2	1.34	0.42
1:A:181:ARG:NH1	2:E:19:LYS:CD	2.77	0.42
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.71	0.42
2:B:29:GLN:HA	2:B:61:SER:OG	2.20	0.42
1:D:167:TRP:O	1:D:171:TYR:CD2	2.72	0.42
1:D:3:HIS:CA	1:D:103:VAL:CG1	2.83	0.42
1:A:125:ALA:C	1:A:133:TRP:HE3	2.23	0.41
1:A:196:LYS:NZ	1:A:196:LYS:HB2	2.35	0.41
1:A:63:ILE:HD11	3:C:1:TYR:HA	2.01	0.41
1:D:85:TYR:HD2	1:D:118:TYR:CE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:C	1:D:133:TRP:HE3	2.23	0.41
1:D:25:VAL:HG22	1:D:27:TYR:CE2	2.55	0.41
1:D:28:VAL:O	1:D:29:ASP:CG	2.53	0.41
1:A:218:GLN:O	1:A:219:LEU:C	2.58	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:A:14:ARG:HA	1:A:15:PRO:HD3	1.81	0.41
1:A:182:THR:HA	1:A:209:TYR:CG	2.55	0.41
1:A:73:TRP:HZ3	3:C:7:HIS:O	2.03	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
1:D:53:GLU:C	1:D:55:GLU:H	2.23	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:148:GLU:O	1:D:149:GLN:C	2.58	0.41
1:D:176:ASN:O	1:D:178:THR:N	2.54	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: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: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
1:A:22:TYR:CD1	1:A:36:PHE:CE1	3.06	0.41
2:B:12:ARG:HG3	2:B:22:ILE:CG2	2.51	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
2:E:81:ARG:HD3	2:E:83:LYS:HZ3	1.86	0.41
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:102:ASP:HB2	1:D:111:ARG:CB	2.51	0.40
1:D:218:GLN:O	1:D:219:LEU:C	2.58	0.40
1:A:123:TYR:HE1	1:A:143:THR:HG21	1.86	0.40
1:A:208:PHE:C	1:A:208:PHE:CD1	2.95	0.40
2:B:37:ILE:HG21	2:B:66:ALA:HB1	2.03	0.40
1:D:208:PHE:CD1	1:D:208:PHE:C	2.95	0.40
2:E:24:ASN:HD21	2:E:65:LEU:HD11	1.81	0.40
1:A:266:LEU:HD23	1:A:266:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:5:ASN:N	3:F:5:ASN:OD1	2.46	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
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	3
1	D	266/268 (99%)	204 (77%)	53 (20%)	9 (3%)	3	3
2	B	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	2
2	E	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	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	3

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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/223 (100%)	161 (72%)	62 (28%)	0	0
1	D	223/223 (100%)	162 (73%)	61 (27%)	0	0
2	B	94/94 (100%)	54 (57%)	40 (43%)	0	0
2	E	94/94 (100%)	54 (57%)	40 (43%)	0	0
3	C	9/9 (100%)	3 (33%)	6 (67%)	0	0
3	F	9/9 (100%)	3 (33%)	6 (67%)	0	0
All	All	652/652 (100%)	437 (67%)	215 (33%)	0	0

All (215) 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	20	PRO
1	A	32	GLU
1	A	36	PHE
1	A	37	ASP
1	A	39	ASP
1	A	43	PRO
1	A	44	ARG
1	A	47	PRO

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Mol	Chain	Res	Type
1	A	52	MET
1	A	54	GLN
1	A	57	PRO
1	A	65	GLN
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	102	ASP
1	A	110	LEU
1	A	111	ARG
1	A	115	GLN
1	A	134	THR
1	A	142	ILE
1	A	144	ARG
1	A	146	LYS
1	A	147	TRP
1	A	149	GLN
1	A	154	GLU
1	A	157	ARG
1	A	163	GLU
1	A	176	ASN
1	A	185	PRO
1	A	186	LYS
1	A	188	HIS
1	A	189	VAL
1	A	194	ARG
1	A	195	SER
1	A	196	LYS
1	A	199	VAL
1	A	201	LEU
1	A	202	ARG
1	A	203	CYS
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

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Mol	Chain	Res	Type
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	266	LEU
2	B	2	GLN
2	B	3	LYS
2	B	4	THR
2	B	6	GLN
2	B	11	SER
2	B	12	ARG
2	B	17	ASN
2	B	21	ASN
2	B	23	LEU
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
2	B	45	LYS
2	B	46	ILE
2	B	51	MET
2	B	52	SER
2	B	53	ASP
2	B	55	SER
2	B	56	PHE
2	B	57	SER
2	B	61	SER
2	B	64	ILE
2	B	65	LEU
2	B	70	PHE
2	B	73	THR
2	B	76	ASP
2	B	77	THR
2	B	78	TYR

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Mol	Chain	Res	Type
2	B	83	LYS
2	B	85	ASP
2	B	86	SER
2	B	89	GLU
2	B	90	PRO
2	B	97	ARG
3	C	1	TYR
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	20	PRO
1	D	32	GLU
1	D	36	PHE
1	D	37	ASP
1	D	39	ASP
1	D	44	ARG
1	D	47	PRO
1	D	52	MET
1	D	54	GLN
1	D	57	PRO
1	D	65	GLN
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	102	ASP
1	D	110	LEU
1	D	111	ARG
1	D	115	GLN
1	D	134	THR
1	D	142	ILE
1	D	144	ARG
1	D	146	LYS
1	D	147	TRP

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Mol	Chain	Res	Type
1	D	149	GLN
1	D	154	GLU
1	D	157	ARG
1	D	163	GLU
1	D	176	ASN
1	D	185	PRO
1	D	186	LYS
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	201	LEU
1	D	202	ARG
1	D	203	CYS
1	D	212	ASP
1	D	214	THR
1	D	215	LEU
1	D	217	TRP
1	D	223	GLU
1	D	230	LEU
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	266	LEU
2	E	2	GLN
2	E	3	LYS
2	E	4	THR
2	E	6	GLN
2	E	11	SER
2	E	12	ARG
2	E	17	ASN
2	E	21	ASN
2	E	23	LEU
2	E	28	THR
2	E	29	GLN

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Mol	Chain	Res	Type
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	55	SER
2	E	56	PHE
2	E	57	SER
2	E	61	SER
2	E	64	ILE
2	E	65	LEU
2	E	70	PHE
2	E	73	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	97	ARG
3	F	1	TYR
3	F	3	ASN
3	F	5	ASN
3	F	6	ILE
3	F	7	HIS
3	F	9	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	30	ASN
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	72	GLN
1	A	77	ASN
1	A	86	ASN
1	A	93	HIS
1	A	96	GLN
1	A	127	ASN
1	A	141	GLN
1	A	149	GLN
1	A	255	GLN
1	A	256	ASN
1	A	263	HIS
2	B	6	GLN
2	B	29	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
1	D	77	ASN
1	D	86	ASN
1	D	93	HIS
1	D	96	GLN
1	D	127	ASN
1	D	141	GLN
1	D	149	GLN
1	D	255	GLN
1	D	256	ASN
1	D	263	HIS
2	E	6	GLN
2	E	29	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.