



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:38 AM UTC

PDB ID : 1GUM / pdb_00001gum
Title : HUMAN GLUTATHIONE TRANSFERASE A4-4 WITHOUT LIGANDS
Authors : Bruns, C.M.; Hubatsch, I.; Ridderstrom, M.; Mannervik, B.; Tainer, J.A.
Deposited on : 1998-06-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

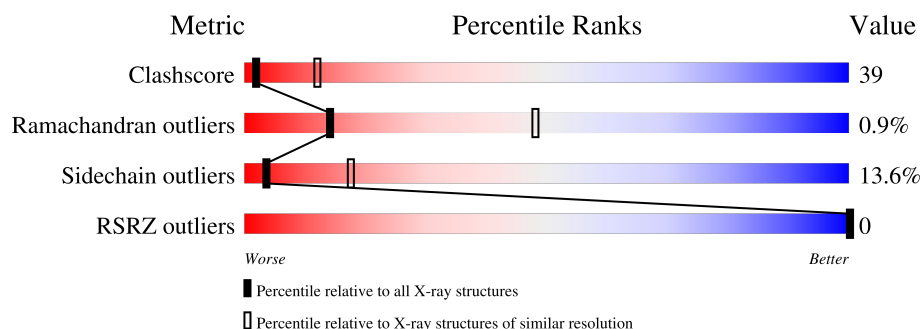
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	222	37% 43% 17% .
1	B	222	36% 43% 18% .
1	C	222	36% 44% 17% ..
1	D	222	36% 44% 17% ..
1	E	222	36% 46% 16% .
1	F	222	36% 45% 16% ..
1	G	222	36% 45% 15% .

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Mol	Chain	Length	Quality of chain
1	H	222	36% 45% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14400 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 PROTEIN (GLUTATHIONE TRANSFERASE A4-4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	B	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	C	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	D	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	E	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	F	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	G	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	H	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	23	Total	O	0	0
			23	23		
2	C	23	Total	O	0	0
			23	23		
2	D	23	Total	O	0	0
			23	23		
2	E	23	Total	O	0	0
			23	23		
2	F	23	Total	O	0	0
			23	23		

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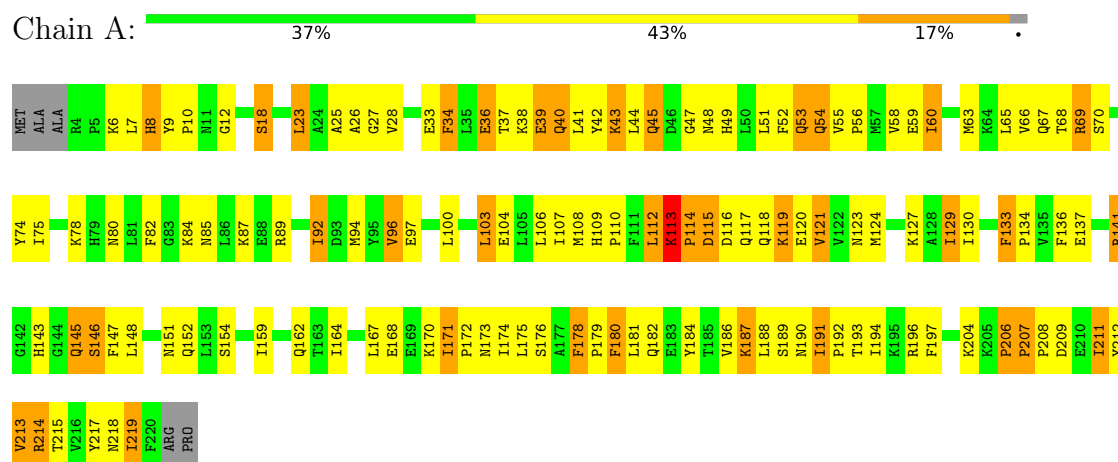
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	23	Total 23	O 23	0	0
2	H	23	Total 23	O 23	0	0

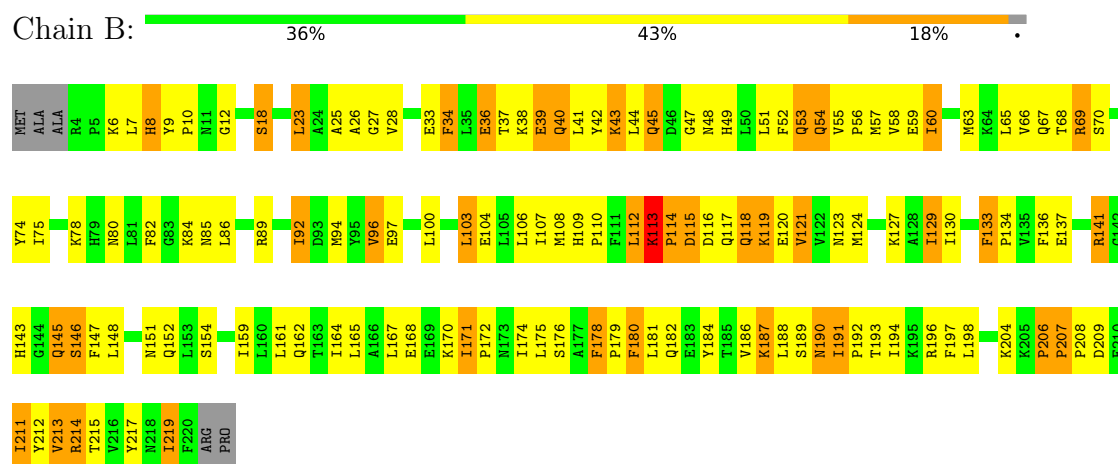
3 Residue-property plots

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

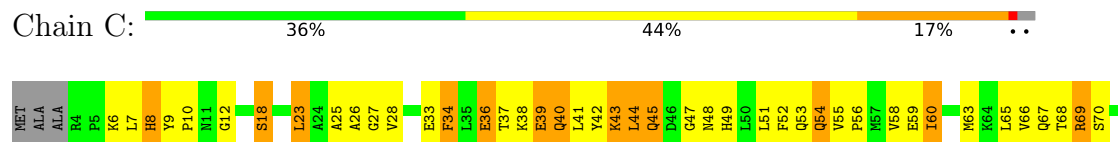
• Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

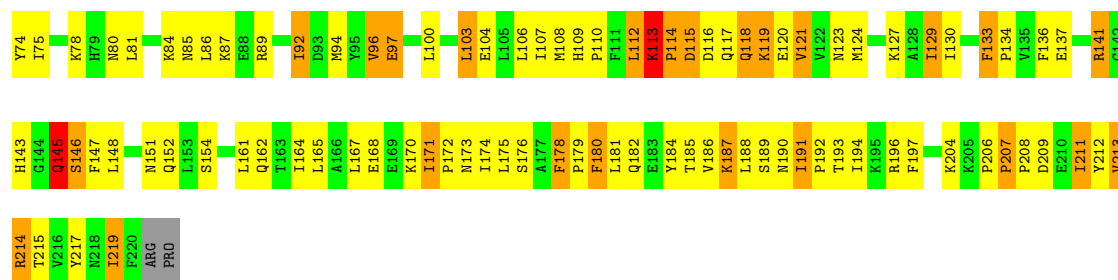


• Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)



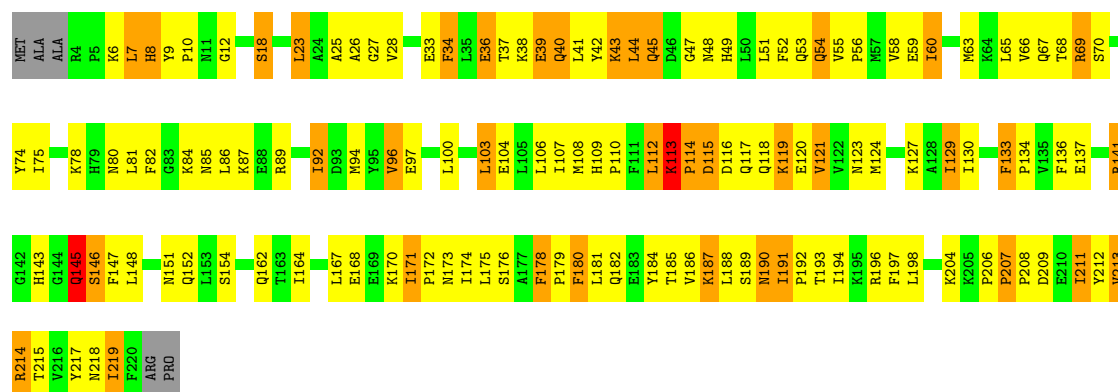
• Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)





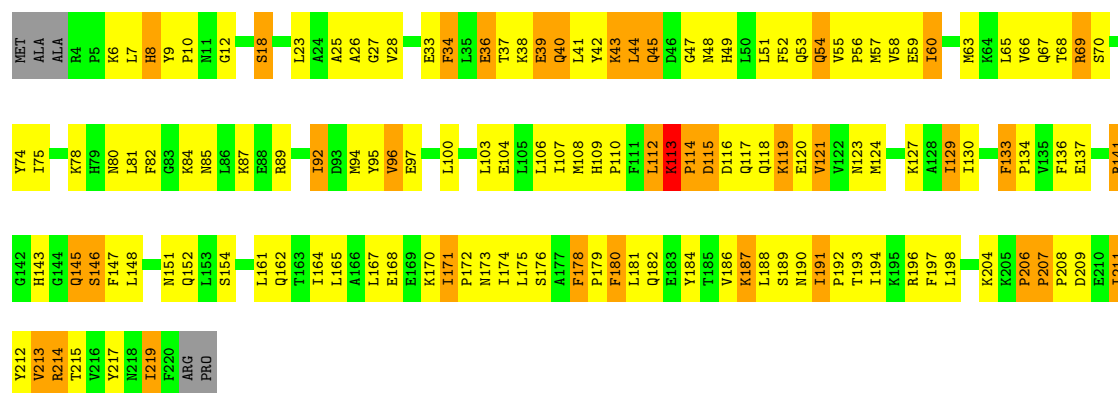
- Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

Chain D: 36% 44% 17% ..



- Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

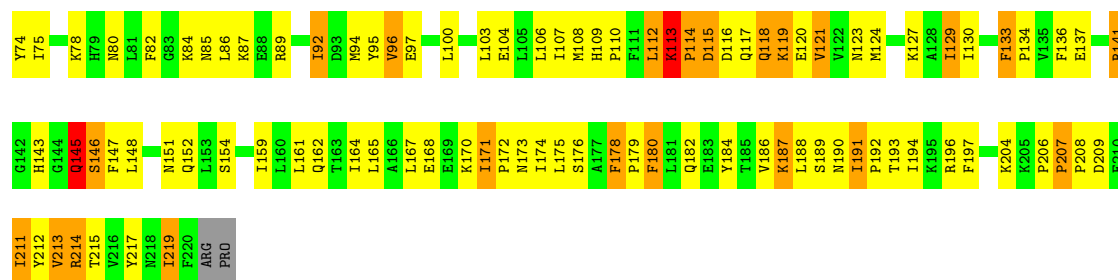
Chain E: 36% 46% 16% .



- Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

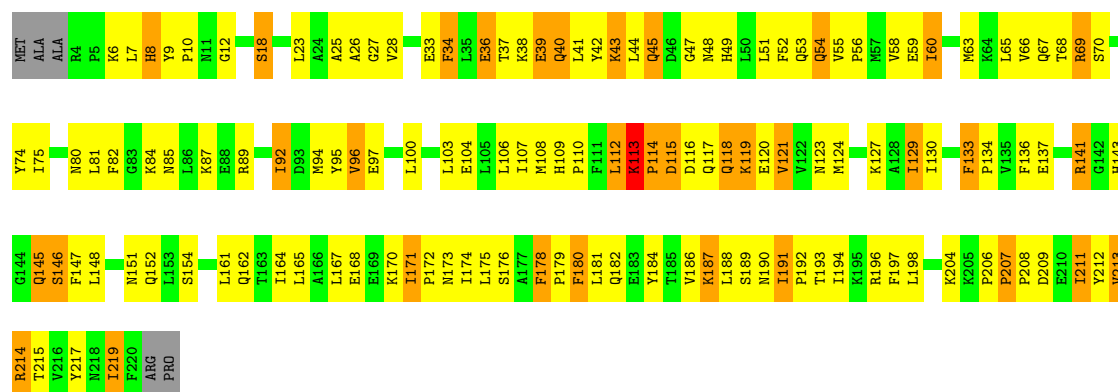
Chain F: 36% 45% 16% ..





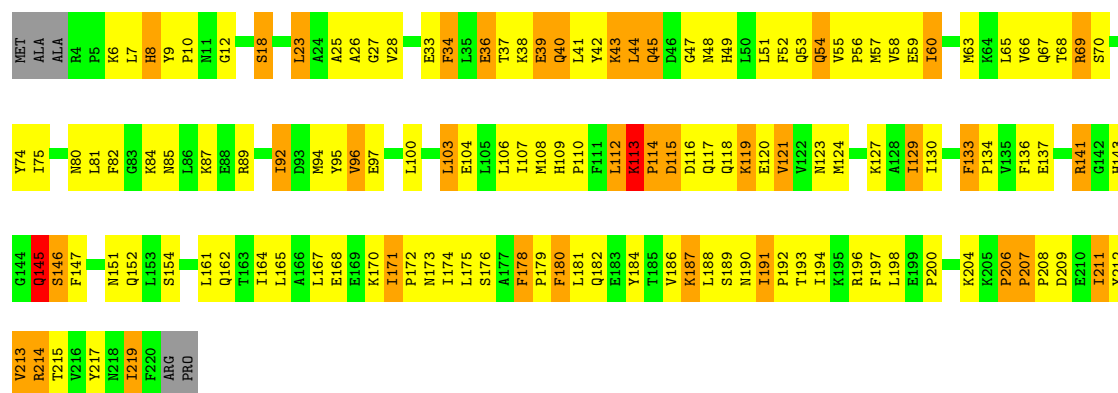
- Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

Chain G: 36% 45% 15% .



- Molecule 1: PROTEIN (GLUTATHIONE TRANSFERASE A4-4)

Chain H: 36% 45% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.30Å 156.10Å 101.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	160.00 – 3.00 110.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (160.00-3.00) 90.8 (110.09-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.91 (at 2.90Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.253 , 0.270 0.283 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	1.2	Xtriage
Anisotropy	4.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 115.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.189 for k,h,-l	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	14400	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.57	8/1817 (0.4%)	1.90	41/2456 (1.7%)
1	B	1.57	8/1817 (0.4%)	1.90	41/2456 (1.7%)
1	C	1.57	9/1817 (0.5%)	1.90	42/2456 (1.7%)
1	D	1.57	10/1817 (0.6%)	1.90	42/2456 (1.7%)
1	E	1.57	7/1817 (0.4%)	1.90	41/2456 (1.7%)
1	F	1.57	7/1817 (0.4%)	1.90	42/2456 (1.7%)
1	G	1.57	7/1817 (0.4%)	1.90	41/2456 (1.7%)
1	H	1.57	8/1817 (0.4%)	1.90	42/2456 (1.7%)
All	All	1.57	64/14536 (0.4%)	1.90	332/19648 (1.7%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	GLN	CA-C	-6.88	1.44	1.52
1	D	53	GLN	CA-C	-6.87	1.44	1.52
1	H	53	GLN	CA-C	-6.86	1.44	1.52
1	F	53	GLN	CA-C	-6.85	1.44	1.52
1	C	53	GLN	CA-C	-6.84	1.44	1.52
1	E	53	GLN	CA-C	-6.82	1.44	1.52
1	A	53	GLN	CA-C	-6.82	1.44	1.52
1	G	53	GLN	CA-C	-6.81	1.44	1.52
1	D	97	GLU	CD-OE2	5.88	1.36	1.25
1	B	97	GLU	CD-OE2	5.87	1.36	1.25
1	H	97	GLU	CD-OE2	5.86	1.36	1.25
1	A	97	GLU	CD-OE2	5.86	1.36	1.25
1	C	97	GLU	CD-OE2	5.86	1.36	1.25
1	F	97	GLU	CD-OE2	5.85	1.36	1.25
1	G	97	GLU	CD-OE2	5.85	1.36	1.25
1	E	97	GLU	CD-OE2	5.84	1.36	1.25
1	C	121	VAL	CA-CB	-5.62	1.47	1.54
1	A	121	VAL	CA-CB	-5.58	1.47	1.54
1	F	121	VAL	CA-CB	-5.58	1.47	1.54
1	G	121	VAL	CA-CB	-5.57	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	121	VAL	CA-CB	-5.57	1.47	1.54
1	H	121	VAL	CA-CB	-5.57	1.47	1.54
1	B	121	VAL	CA-CB	-5.51	1.47	1.54
1	D	121	VAL	CA-CB	-5.48	1.47	1.54
1	C	75	ILE	CA-CB	-5.47	1.47	1.54
1	D	75	ILE	CA-CB	-5.46	1.48	1.54
1	E	75	ILE	CA-CB	-5.43	1.48	1.54
1	E	213	VAL	CA-CB	-5.43	1.48	1.54
1	F	75	ILE	CA-CB	-5.43	1.48	1.54
1	H	213	VAL	CA-CB	-5.43	1.48	1.54
1	H	75	ILE	CA-CB	-5.43	1.48	1.54
1	G	75	ILE	CA-CB	-5.42	1.48	1.54
1	D	213	VAL	CA-CB	-5.42	1.48	1.54
1	G	213	VAL	CA-CB	-5.40	1.48	1.54
1	F	213	VAL	CA-CB	-5.39	1.48	1.54
1	A	213	VAL	CA-CB	-5.39	1.48	1.54
1	B	213	VAL	CA-CB	-5.38	1.48	1.54
1	B	75	ILE	CA-CB	-5.37	1.48	1.54
1	C	213	VAL	CA-CB	-5.37	1.48	1.54
1	A	75	ILE	CA-CB	-5.36	1.48	1.54
1	A	28	VAL	CA-CB	-5.26	1.48	1.54
1	C	28	VAL	CA-CB	-5.25	1.48	1.54
1	D	28	VAL	CA-CB	-5.24	1.48	1.54
1	E	28	VAL	CA-CB	-5.24	1.48	1.54
1	B	28	VAL	CA-CB	-5.23	1.48	1.54
1	F	28	VAL	CA-CB	-5.22	1.48	1.54
1	G	28	VAL	CA-CB	-5.21	1.48	1.54
1	H	28	VAL	CA-CB	-5.16	1.48	1.54
1	G	207	PRO	CA-C	-5.12	1.47	1.52
1	C	207	PRO	CA-C	-5.11	1.47	1.52
1	D	207	PRO	CA-C	-5.10	1.47	1.52
1	H	207	PRO	CA-C	-5.09	1.47	1.52
1	B	207	PRO	CA-C	-5.07	1.47	1.52
1	C	103	LEU	C-N	-5.07	1.27	1.33
1	A	207	PRO	CA-C	-5.06	1.47	1.52
1	E	207	PRO	CA-C	-5.05	1.47	1.52
1	D	185	THR	C-N	-5.05	1.27	1.33
1	A	103	LEU	C-N	-5.05	1.27	1.33
1	H	103	LEU	C-N	-5.05	1.27	1.33
1	B	103	LEU	C-N	-5.03	1.27	1.33
1	D	103	LEU	C-N	-5.01	1.27	1.33
1	F	207	PRO	CA-C	-5.01	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	THR	C-N	-5.01	1.27	1.33
1	D	7	LEU	N-CA	-5.00	1.40	1.46

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	PHE	CA-CB-CG	-8.83	104.97	113.80
1	H	147	PHE	CA-CB-CG	-8.82	104.98	113.80
1	G	147	PHE	CA-CB-CG	-8.81	104.99	113.80
1	B	147	PHE	CA-CB-CG	-8.81	104.99	113.80
1	F	147	PHE	CA-CB-CG	-8.80	105.00	113.80
1	D	147	PHE	CA-CB-CG	-8.79	105.01	113.80
1	E	147	PHE	CA-CB-CG	-8.79	105.01	113.80
1	C	147	PHE	CA-CB-CG	-8.76	105.04	113.80
1	E	180	PHE	CA-CB-CG	-8.60	105.20	113.80
1	B	180	PHE	CA-CB-CG	-8.54	105.26	113.80
1	G	180	PHE	CA-CB-CG	-8.54	105.25	113.80
1	H	180	PHE	CA-CB-CG	-8.54	105.27	113.80
1	A	180	PHE	CA-CB-CG	-8.53	105.28	113.80
1	D	180	PHE	CA-CB-CG	-8.52	105.28	113.80
1	F	180	PHE	CA-CB-CG	-8.52	105.28	113.80
1	C	180	PHE	CA-CB-CG	-8.51	105.29	113.80
1	D	171	ILE	CA-C-N	7.42	128.08	119.47
1	D	171	ILE	C-N-CA	7.42	128.08	119.47
1	F	171	ILE	CA-C-N	7.41	128.06	119.47
1	F	171	ILE	C-N-CA	7.41	128.06	119.47
1	H	171	ILE	CA-C-N	7.39	128.05	119.47
1	H	171	ILE	C-N-CA	7.39	128.05	119.47
1	B	171	ILE	CA-C-N	7.39	128.04	119.47
1	B	171	ILE	C-N-CA	7.39	128.04	119.47
1	E	171	ILE	CA-C-N	7.38	128.03	119.47
1	E	171	ILE	C-N-CA	7.38	128.03	119.47
1	A	171	ILE	CA-C-N	7.37	128.02	119.47
1	A	171	ILE	C-N-CA	7.37	128.02	119.47
1	G	171	ILE	CA-C-N	7.37	128.01	119.47
1	G	171	ILE	C-N-CA	7.37	128.01	119.47
1	C	171	ILE	CA-C-N	7.32	127.96	119.47
1	C	171	ILE	C-N-CA	7.32	127.96	119.47
1	D	178	PHE	CA-C-N	7.21	128.86	119.84
1	D	178	PHE	C-N-CA	7.21	128.86	119.84
1	B	178	PHE	CA-C-N	7.20	128.84	119.84
1	B	178	PHE	C-N-CA	7.20	128.84	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	PHE	CA-C-N	7.20	128.84	119.84
1	E	178	PHE	C-N-CA	7.20	128.84	119.84
1	F	178	PHE	CA-C-N	7.19	128.82	119.84
1	F	178	PHE	C-N-CA	7.19	128.82	119.84
1	G	178	PHE	CA-C-N	7.18	128.82	119.84
1	G	178	PHE	C-N-CA	7.18	128.82	119.84
1	C	178	PHE	CA-C-N	7.16	128.79	119.84
1	C	178	PHE	C-N-CA	7.16	128.79	119.84
1	H	178	PHE	CA-C-N	7.16	128.79	119.84
1	H	178	PHE	C-N-CA	7.16	128.79	119.84
1	A	178	PHE	CA-C-N	7.15	128.78	119.84
1	A	178	PHE	C-N-CA	7.15	128.78	119.84
1	C	113	LYS	C-N-CD	-7.12	95.81	125.00
1	G	113	LYS	C-N-CD	-7.12	95.82	125.00
1	D	113	LYS	C-N-CD	-7.11	95.83	125.00
1	F	113	LYS	C-N-CD	-7.11	95.84	125.00
1	B	113	LYS	C-N-CD	-7.11	95.85	125.00
1	H	113	LYS	C-N-CD	-7.11	95.85	125.00
1	E	113	LYS	C-N-CD	-7.11	95.86	125.00
1	A	113	LYS	C-N-CD	-7.11	95.86	125.00
1	G	113	LYS	CA-C-N	6.92	128.49	119.84
1	G	113	LYS	C-N-CA	6.92	128.49	119.84
1	H	190	ASN	N-CA-CB	6.92	121.68	110.40
1	C	190	ASN	N-CA-CB	6.91	121.66	110.40
1	F	190	ASN	N-CA-CB	6.91	121.66	110.40
1	E	190	ASN	N-CA-CB	6.90	121.64	110.40
1	G	190	ASN	N-CA-CB	6.90	121.64	110.40
1	A	190	ASN	N-CA-CB	6.89	121.64	110.40
1	H	113	LYS	CA-C-N	6.89	128.45	119.84
1	H	113	LYS	C-N-CA	6.89	128.45	119.84
1	D	190	ASN	N-CA-CB	6.88	121.62	110.40
1	A	113	LYS	CA-C-N	6.88	128.44	119.84
1	A	113	LYS	C-N-CA	6.88	128.44	119.84
1	B	190	ASN	N-CA-CB	6.88	121.61	110.40
1	B	113	LYS	CA-C-N	6.88	128.44	119.84
1	B	113	LYS	C-N-CA	6.88	128.44	119.84
1	D	113	LYS	CA-C-N	6.87	128.43	119.84
1	D	113	LYS	C-N-CA	6.87	128.43	119.84
1	E	113	LYS	CA-C-N	6.87	128.43	119.84
1	E	113	LYS	C-N-CA	6.87	128.43	119.84
1	F	113	LYS	CA-C-N	6.87	128.42	119.84
1	F	113	LYS	C-N-CA	6.87	128.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	LYS	CA-C-N	6.86	128.41	119.84
1	C	113	LYS	C-N-CA	6.86	128.41	119.84
1	D	133	PHE	CA-CB-CG	-6.85	106.95	113.80
1	B	133	PHE	CA-CB-CG	-6.83	106.97	113.80
1	G	133	PHE	CA-CB-CG	-6.83	106.97	113.80
1	F	133	PHE	CA-CB-CG	-6.81	106.99	113.80
1	E	133	PHE	CA-CB-CG	-6.80	107.00	113.80
1	H	133	PHE	CA-CB-CG	-6.79	107.00	113.80
1	A	133	PHE	CA-CB-CG	-6.79	107.01	113.80
1	C	133	PHE	CA-CB-CG	-6.79	107.01	113.80
1	A	34	PHE	CA-C-N	-6.63	111.94	121.42
1	A	34	PHE	C-N-CA	-6.63	111.94	121.42
1	H	34	PHE	CA-C-N	-6.61	111.96	121.42
1	H	34	PHE	C-N-CA	-6.61	111.96	121.42
1	E	34	PHE	CA-C-N	-6.60	111.98	121.42
1	E	34	PHE	C-N-CA	-6.60	111.98	121.42
1	G	34	PHE	CA-C-N	-6.59	111.99	121.42
1	G	34	PHE	C-N-CA	-6.59	111.99	121.42
1	F	34	PHE	CA-C-N	-6.59	112.00	121.42
1	F	34	PHE	C-N-CA	-6.59	112.00	121.42
1	B	34	PHE	CA-C-N	-6.58	112.01	121.42
1	B	34	PHE	C-N-CA	-6.58	112.01	121.42
1	D	34	PHE	CA-C-N	-6.57	112.03	121.42
1	D	34	PHE	C-N-CA	-6.57	112.03	121.42
1	C	34	PHE	CA-C-N	-6.55	112.05	121.42
1	C	34	PHE	C-N-CA	-6.55	112.05	121.42
1	G	120	GLU	CA-CB-CG	-6.50	101.09	114.10
1	E	34	PHE	N-CA-C	6.50	120.10	109.76
1	E	120	GLU	CA-CB-CG	-6.49	101.11	114.10
1	A	120	GLU	CA-CB-CG	-6.49	101.13	114.10
1	D	120	GLU	CA-CB-CG	-6.49	101.12	114.10
1	C	120	GLU	CA-CB-CG	-6.49	101.13	114.10
1	C	34	PHE	N-CA-C	6.48	120.07	109.76
1	H	120	GLU	CA-CB-CG	-6.48	101.14	114.10
1	F	34	PHE	N-CA-C	6.48	120.06	109.76
1	F	120	GLU	CA-CB-CG	-6.48	101.14	114.10
1	B	120	GLU	CA-CB-CG	-6.48	101.14	114.10
1	D	34	PHE	N-CA-C	6.47	120.06	109.76
1	H	34	PHE	N-CA-C	6.47	120.05	109.76
1	A	34	PHE	N-CA-C	6.46	120.03	109.76
1	G	34	PHE	N-CA-C	6.45	120.02	109.76
1	B	34	PHE	N-CA-C	6.45	120.02	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	HIS	CA-CB-CG	-6.09	107.71	113.80
1	C	8	HIS	CA-CB-CG	-6.07	107.73	113.80
1	G	8	HIS	CA-CB-CG	-6.05	107.75	113.80
1	D	8	HIS	CA-CB-CG	-6.05	107.75	113.80
1	D	207	PRO	CA-C-N	6.04	125.99	119.76
1	D	207	PRO	C-N-CA	6.04	125.99	119.76
1	B	36	GLU	N-CA-CB	6.04	119.04	111.00
1	G	207	PRO	CA-C-N	6.04	125.98	119.76
1	G	207	PRO	C-N-CA	6.04	125.98	119.76
1	A	36	GLU	N-CA-CB	6.04	119.03	111.00
1	F	36	GLU	N-CA-CB	6.03	119.02	111.00
1	H	8	HIS	CA-CB-CG	-6.02	107.78	113.80
1	H	36	GLU	N-CA-CB	6.02	119.01	111.00
1	D	36	GLU	N-CA-CB	6.02	119.00	111.00
1	F	8	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	8	HIS	CA-CB-CG	-6.01	107.79	113.80
1	C	36	GLU	N-CA-CB	6.01	118.99	111.00
1	H	207	PRO	CA-C-N	6.00	125.94	119.76
1	H	207	PRO	C-N-CA	6.00	125.94	119.76
1	G	36	GLU	N-CA-CB	6.00	118.98	111.00
1	B	207	PRO	CA-C-N	6.00	125.94	119.76
1	B	207	PRO	C-N-CA	6.00	125.94	119.76
1	F	207	PRO	CA-C-N	5.99	125.93	119.76
1	F	207	PRO	C-N-CA	5.99	125.93	119.76
1	B	8	HIS	CA-CB-CG	-5.99	107.81	113.80
1	E	36	GLU	N-CA-CB	5.99	118.97	111.00
1	E	207	PRO	CA-C-N	5.98	125.92	119.76
1	E	207	PRO	C-N-CA	5.98	125.92	119.76
1	A	207	PRO	CA-C-N	5.98	125.92	119.76
1	A	207	PRO	C-N-CA	5.98	125.92	119.76
1	C	207	PRO	CA-C-N	5.96	125.89	119.76
1	C	207	PRO	C-N-CA	5.96	125.89	119.76
1	B	136	PHE	CA-CB-CG	-5.93	107.87	113.80
1	G	136	PHE	CA-CB-CG	-5.92	107.88	113.80
1	F	136	PHE	CA-CB-CG	-5.91	107.89	113.80
1	D	136	PHE	CA-CB-CG	-5.89	107.91	113.80
1	H	136	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	136	PHE	CA-CB-CG	-5.88	107.92	113.80
1	C	136	PHE	CA-CB-CG	-5.87	107.93	113.80
1	E	136	PHE	CA-CB-CG	-5.87	107.93	113.80
1	F	186	VAL	CB-CA-C	-5.77	104.59	111.81
1	D	130	ILE	N-CA-C	5.76	116.81	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	186	VAL	CB-CA-C	-5.76	104.61	111.81
1	E	130	ILE	N-CA-C	5.75	116.80	111.45
1	H	186	VAL	CB-CA-C	-5.74	104.63	111.81
1	C	186	VAL	CB-CA-C	-5.74	104.64	111.81
1	A	130	ILE	N-CA-C	5.73	116.78	111.45
1	B	186	VAL	CB-CA-C	-5.73	104.65	111.81
1	G	130	ILE	N-CA-C	5.72	116.77	111.45
1	D	186	VAL	CB-CA-C	-5.71	104.67	111.81
1	B	130	ILE	N-CA-C	5.71	116.75	111.45
1	F	130	ILE	N-CA-C	5.71	116.76	111.45
1	A	186	VAL	CB-CA-C	-5.70	104.68	111.81
1	H	130	ILE	N-CA-C	5.70	116.75	111.45
1	C	130	ILE	N-CA-C	5.70	116.75	111.45
1	F	129	ILE	CB-CA-C	-5.70	104.36	112.22
1	E	129	ILE	CB-CA-C	-5.69	104.37	112.22
1	E	186	VAL	CB-CA-C	-5.69	104.70	111.81
1	F	206	PRO	CB-CA-C	-5.68	103.99	110.92
1	B	206	PRO	CB-CA-C	-5.68	103.99	110.92
1	D	129	ILE	CB-CA-C	-5.68	104.39	112.22
1	D	206	PRO	CB-CA-C	-5.67	104.00	110.92
1	H	206	PRO	CB-CA-C	-5.67	104.00	110.92
1	G	129	ILE	CB-CA-C	-5.67	104.40	112.22
1	A	129	ILE	CB-CA-C	-5.67	104.40	112.22
1	H	129	ILE	CB-CA-C	-5.66	104.41	112.22
1	B	129	ILE	CB-CA-C	-5.66	104.42	112.22
1	E	206	PRO	CB-CA-C	-5.66	104.02	110.92
1	G	206	PRO	CB-CA-C	-5.66	104.02	110.92
1	C	206	PRO	CB-CA-C	-5.65	104.03	110.92
1	G	118	GLN	N-CA-CB	5.65	118.27	110.07
1	C	129	ILE	CB-CA-C	-5.65	104.42	112.22
1	C	118	GLN	N-CA-CB	5.64	118.25	110.07
1	E	118	GLN	N-CA-CB	5.63	118.23	110.07
1	A	118	GLN	N-CA-CB	5.62	118.23	110.07
1	A	206	PRO	CB-CA-C	-5.62	104.06	110.92
1	D	118	GLN	N-CA-CB	5.62	118.22	110.07
1	H	118	GLN	N-CA-CB	5.61	118.21	110.07
1	D	49	HIS	CA-CB-CG	-5.61	108.19	113.80
1	G	49	HIS	CA-CB-CG	-5.60	108.20	113.80
1	F	118	GLN	N-CA-CB	5.60	118.19	110.07
1	B	118	GLN	N-CA-CB	5.58	118.17	110.07
1	H	49	HIS	CA-CB-CG	-5.56	108.24	113.80
1	B	49	HIS	CA-CB-CG	-5.56	108.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	HIS	CA-CB-CG	-5.55	108.25	113.80
1	E	49	HIS	CA-CB-CG	-5.55	108.25	113.80
1	C	191	ILE	CA-C-N	5.54	126.77	119.84
1	C	191	ILE	C-N-CA	5.54	126.77	119.84
1	A	49	HIS	CA-CB-CG	-5.54	108.26	113.80
1	F	49	HIS	CA-CB-CG	-5.53	108.27	113.80
1	G	8	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	D	8	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	A	8	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	C	8	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	A	191	ILE	CA-C-N	5.51	126.73	119.84
1	A	191	ILE	C-N-CA	5.51	126.73	119.84
1	D	191	ILE	CA-C-N	5.51	126.73	119.84
1	D	191	ILE	C-N-CA	5.51	126.73	119.84
1	F	8	HIS	ND1-CE1-NE2	5.51	113.91	108.40
1	F	191	ILE	CA-C-N	5.50	126.72	119.84
1	F	191	ILE	C-N-CA	5.50	126.72	119.84
1	B	8	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	H	191	ILE	CA-C-N	5.50	126.71	119.84
1	H	191	ILE	C-N-CA	5.50	126.71	119.84
1	E	191	ILE	CA-C-N	5.49	126.71	119.84
1	E	191	ILE	C-N-CA	5.49	126.71	119.84
1	H	8	HIS	ND1-CE1-NE2	5.49	113.89	108.40
1	E	8	HIS	ND1-CE1-NE2	5.48	113.88	108.40
1	G	191	ILE	CA-C-N	5.48	126.69	119.84
1	G	191	ILE	C-N-CA	5.48	126.69	119.84
1	B	191	ILE	CA-C-N	5.47	126.68	119.84
1	B	191	ILE	C-N-CA	5.47	126.68	119.84
1	B	124	MET	CB-CA-C	-5.45	102.33	110.88
1	D	124	MET	CB-CA-C	-5.44	102.34	110.88
1	C	124	MET	CB-CA-C	-5.43	102.36	110.88
1	F	124	MET	CB-CA-C	-5.43	102.36	110.88
1	E	124	MET	CB-CA-C	-5.43	102.36	110.88
1	G	124	MET	CB-CA-C	-5.41	102.38	110.88
1	H	124	MET	CB-CA-C	-5.41	102.39	110.88
1	A	124	MET	CB-CA-C	-5.41	102.39	110.88
1	B	26	ALA	N-CA-C	-5.34	106.84	113.19
1	F	26	ALA	N-CA-C	-5.31	106.87	113.19
1	A	26	ALA	N-CA-C	-5.31	106.88	113.19
1	H	26	ALA	N-CA-C	-5.30	106.88	113.19
1	C	26	ALA	N-CA-C	-5.30	106.88	113.19
1	G	207	PRO	N-CA-C	-5.29	104.24	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ALA	N-CA-C	-5.29	106.90	113.19
1	D	207	PRO	N-CA-C	-5.29	104.25	110.70
1	E	26	ALA	N-CA-C	-5.29	106.90	113.19
1	H	207	PRO	N-CA-C	-5.29	104.25	110.70
1	G	26	ALA	N-CA-C	-5.28	106.91	113.19
1	A	207	PRO	N-CA-C	-5.27	104.27	110.70
1	B	118	GLN	N-CA-C	5.27	116.83	111.14
1	F	207	PRO	N-CA-C	-5.27	104.27	110.70
1	E	207	PRO	N-CA-C	-5.26	104.28	110.70
1	C	207	PRO	N-CA-C	-5.26	104.28	110.70
1	F	118	GLN	N-CA-C	5.26	116.82	111.14
1	B	207	PRO	N-CA-C	-5.25	104.30	110.70
1	A	178	PHE	O-C-N	5.24	126.04	121.17
1	D	118	GLN	N-CA-C	5.24	116.80	111.14
1	B	44	LEU	N-CA-CB	-5.24	102.48	110.07
1	H	118	GLN	N-CA-C	5.23	116.79	111.14
1	A	118	GLN	N-CA-C	5.23	116.79	111.14
1	G	44	LEU	N-CA-CB	-5.23	102.49	110.07
1	C	44	LEU	N-CA-CB	-5.22	102.50	110.07
1	G	118	GLN	N-CA-C	5.22	116.78	111.14
1	H	44	LEU	N-CA-CB	-5.22	102.50	110.07
1	E	44	LEU	N-CA-CB	-5.21	102.51	110.07
1	D	44	LEU	N-CA-CB	-5.21	102.52	110.07
1	A	44	LEU	N-CA-CB	-5.21	102.52	110.07
1	F	44	LEU	N-CA-CB	-5.21	102.52	110.07
1	C	118	GLN	N-CA-C	5.20	116.76	111.14
1	E	118	GLN	N-CA-C	5.20	116.76	111.14
1	H	178	PHE	O-C-N	5.20	126.00	121.17
1	E	96	VAL	N-CA-C	5.20	115.41	110.42
1	E	211	ILE	CB-CA-C	-5.20	105.32	111.81
1	C	211	ILE	CB-CA-C	-5.19	105.32	111.81
1	B	178	PHE	O-C-N	5.18	125.99	121.17
1	F	211	ILE	CB-CA-C	-5.18	105.34	111.81
1	G	178	PHE	O-C-N	5.18	125.99	121.17
1	H	211	ILE	CB-CA-C	-5.18	105.34	111.81
1	A	23	LEU	O-C-N	5.17	127.47	122.09
1	B	211	ILE	CB-CA-C	-5.17	105.34	111.81
1	C	23	LEU	O-C-N	5.17	127.47	122.09
1	A	211	ILE	CB-CA-C	-5.17	105.34	111.81
1	D	178	PHE	O-C-N	5.17	125.97	121.17
1	D	211	ILE	CB-CA-C	-5.17	105.35	111.81
1	C	96	VAL	N-CA-C	5.17	115.38	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	PHE	O-C-N	5.16	125.97	121.17
1	D	23	LEU	O-C-N	5.16	127.45	122.09
1	H	23	LEU	O-C-N	5.16	127.45	122.09
1	C	178	PHE	O-C-N	5.15	125.96	121.17
1	G	43	LYS	CA-C-O	5.15	125.89	119.97
1	G	211	ILE	CB-CA-C	-5.15	105.37	111.81
1	B	23	LEU	O-C-N	5.15	127.44	122.09
1	H	43	LYS	CA-C-O	5.15	125.89	119.97
1	A	43	LYS	CA-C-O	5.15	125.89	119.97
1	G	96	VAL	N-CA-C	5.15	115.36	110.42
1	B	43	LYS	CA-C-O	5.14	125.88	119.97
1	F	96	VAL	N-CA-C	5.14	115.36	110.42
1	G	23	LEU	O-C-N	5.14	127.44	122.09
1	A	96	VAL	N-CA-C	5.14	115.35	110.42
1	D	96	VAL	N-CA-C	5.14	115.35	110.42
1	E	23	LEU	O-C-N	5.14	127.43	122.09
1	F	43	LYS	CA-C-O	5.13	125.86	119.97
1	F	23	LEU	O-C-N	5.12	127.42	122.09
1	H	96	VAL	N-CA-C	5.12	115.33	110.42
1	D	43	LYS	CA-C-O	5.12	125.85	119.97
1	E	43	LYS	CA-C-O	5.12	125.85	119.97
1	C	43	LYS	CA-C-O	5.11	125.85	119.97
1	E	178	PHE	O-C-N	5.11	125.92	121.17
1	A	191	ILE	CA-C-O	5.11	126.79	119.95
1	G	191	ILE	CA-C-O	5.11	126.79	119.95
1	D	191	ILE	CA-C-O	5.10	126.79	119.95
1	B	191	ILE	CA-C-O	5.09	126.77	119.95
1	F	191	ILE	CA-C-O	5.09	126.77	119.95
1	B	96	VAL	N-CA-C	5.09	115.30	110.42
1	F	207	PRO	O-C-N	5.08	127.46	121.46
1	A	207	PRO	O-C-N	5.08	127.46	121.46
1	E	191	ILE	CA-C-O	5.08	126.75	119.95
1	B	207	PRO	O-C-N	5.08	127.45	121.46
1	H	191	ILE	CA-C-O	5.08	126.75	119.95
1	C	191	ILE	CA-C-O	5.07	126.75	119.95
1	C	207	PRO	O-C-N	5.05	127.42	121.46
1	E	207	PRO	O-C-N	5.05	127.42	121.46
1	H	207	PRO	O-C-N	5.04	127.41	121.46
1	G	207	PRO	O-C-N	5.02	127.39	121.46
1	D	145	GLN	N-CA-C	5.02	117.01	110.53
1	D	207	PRO	O-C-N	5.02	127.38	121.46
1	F	145	GLN	N-CA-C	5.01	116.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	145	GLN	N-CA-C	5.01	116.99	110.53
1	C	145	GLN	N-CA-C	5.00	116.98	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1829	142	0
1	B	1777	0	1829	149	1
1	C	1777	0	1829	156	1
1	D	1777	0	1829	155	4
1	E	1777	0	1829	149	0
1	F	1777	0	1829	156	0
1	G	1777	0	1829	154	0
1	H	1777	0	1829	150	4
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
2	G	23	0	0	0	0
2	H	23	0	0	0	0
All	All	14400	0	14632	1124	5

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 39.

All (1124) 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:94:MET:HE2	1:B:66:VAL:H	1.05	1.20
1:C:94:MET:CE	1:D:66:VAL:H	1.55	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:HA	1:F:94:MET:HE1	1.26	1.12
1:C:94:MET:HE2	1:D:66:VAL:N	1.62	1.12
1:E:66:VAL:H	1:F:94:MET:CE	1.61	1.11
1:G:66:VAL:H	1:H:94:MET:HE2	0.97	1.11
1:G:65:LEU:HA	1:H:94:MET:HE1	1.31	1.10
1:E:94:MET:HE1	1:F:65:LEU:HA	1.33	1.09
1:C:66:VAL:H	1:D:94:MET:HE2	1.15	1.09
1:C:94:MET:CE	1:D:65:LEU:HA	1.83	1.08
1:C:94:MET:HE1	1:D:65:LEU:HA	1.09	1.08
1:E:94:MET:HE2	1:F:66:VAL:H	0.97	1.08
1:E:94:MET:CE	1:F:66:VAL:H	1.65	1.08
1:G:94:MET:HE2	1:H:66:VAL:H	1.06	1.07
1:A:66:VAL:H	1:B:94:MET:HE2	1.16	1.06
1:E:66:VAL:H	1:F:94:MET:HE2	0.90	1.05
1:G:66:VAL:H	1:H:94:MET:CE	1.71	1.03
1:A:94:MET:CE	1:B:66:VAL:H	1.71	1.03
1:E:66:VAL:N	1:F:94:MET:HE2	1.76	1.01
1:C:65:LEU:HA	1:D:94:MET:HE1	1.42	1.00
1:G:94:MET:CE	1:H:66:VAL:H	1.78	0.97
1:G:94:MET:HE1	1:H:65:LEU:HA	1.41	0.97
1:A:65:LEU:HA	1:B:94:MET:HE1	1.46	0.97
1:A:94:MET:HE1	1:B:65:LEU:HA	1.44	0.96
1:E:65:LEU:HA	1:F:94:MET:CE	1.96	0.96
1:G:65:LEU:HA	1:H:94:MET:CE	1.97	0.95
1:E:94:MET:HE2	1:F:66:VAL:N	1.82	0.94
1:C:94:MET:HE3	1:D:65:LEU:HB3	1.50	0.93
1:C:94:MET:HE2	1:D:66:VAL:H	0.76	0.93
1:G:66:VAL:N	1:H:94:MET:HE2	1.83	0.93
1:F:118:GLN:HG2	1:G:118:GLN:HG2	1.51	0.92
1:C:94:MET:HE1	1:D:65:LEU:CA	2.00	0.91
1:C:119:LYS:NZ	1:C:123:ASN:HB2	1.86	0.91
1:E:94:MET:CE	1:F:65:LEU:HA	2.02	0.90
1:E:119:LYS:NZ	1:E:123:ASN:HB2	1.86	0.90
1:G:119:LYS:NZ	1:G:123:ASN:HB2	1.86	0.90
1:F:119:LYS:NZ	1:F:123:ASN:HB2	1.86	0.89
1:A:119:LYS:NZ	1:A:123:ASN:HB2	1.86	0.89
1:C:65:LEU:HA	1:D:94:MET:CE	2.01	0.89
1:B:119:LYS:NZ	1:B:123:ASN:HB2	1.86	0.89
1:D:119:LYS:NZ	1:D:123:ASN:HB2	1.86	0.89
1:H:119:LYS:NZ	1:H:123:ASN:HB2	1.86	0.88
1:D:141:ARG:HG2	1:D:141:ARG:HH11	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.39	0.87
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.39	0.87
1:G:94:MET:CE	1:H:65:LEU:HA	2.04	0.87
1:E:141:ARG:HG2	1:E:141:ARG:HH11	1.39	0.87
1:H:141:ARG:HH11	1:H:141:ARG:HG2	1.39	0.87
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.39	0.86
1:F:141:ARG:HH11	1:F:141:ARG:HG2	1.39	0.86
1:G:141:ARG:HG2	1:G:141:ARG:HH11	1.39	0.86
1:F:118:GLN:CG	1:G:118:GLN:HG2	2.05	0.85
1:A:65:LEU:HA	1:B:94:MET:CE	2.08	0.84
1:A:66:VAL:H	1:B:94:MET:CE	1.91	0.83
1:C:94:MET:CE	1:D:65:LEU:CA	2.55	0.83
1:G:60:ILE:HD13	1:G:74:TYR:HE2	1.44	0.83
1:A:94:MET:HE2	1:B:66:VAL:N	1.91	0.82
1:C:60:ILE:HD13	1:C:74:TYR:HE2	1.44	0.82
1:F:60:ILE:HD13	1:F:74:TYR:HE2	1.44	0.81
1:G:119:LYS:HZ3	1:G:123:ASN:HB2	1.44	0.81
1:A:94:MET:CE	1:B:65:LEU:HA	2.10	0.81
1:D:60:ILE:HD13	1:D:74:TYR:HE2	1.44	0.81
1:G:94:MET:HE2	1:H:66:VAL:N	1.92	0.80
1:C:112:LEU:HA	1:C:113:LYS:HZ2	1.46	0.80
1:H:60:ILE:HD13	1:H:74:TYR:HE2	1.44	0.80
1:E:60:ILE:HD13	1:E:74:TYR:HE2	1.44	0.80
1:H:214:ARG:HG2	1:H:214:ARG:HH11	1.47	0.80
1:E:112:LEU:HA	1:E:113:LYS:HZ2	1.46	0.79
1:A:60:ILE:HD13	1:A:74:TYR:HE2	1.44	0.79
1:E:214:ARG:HG2	1:E:214:ARG:HH11	1.48	0.79
1:F:214:ARG:HG2	1:F:214:ARG:HH11	1.48	0.79
1:B:60:ILE:HD13	1:B:74:TYR:HE2	1.44	0.79
1:B:112:LEU:HA	1:B:113:LYS:HZ2	1.47	0.79
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.47	0.79
1:H:112:LEU:HB2	1:H:117:GLN:HG2	1.65	0.78
1:A:112:LEU:HB2	1:A:117:GLN:HG2	1.65	0.78
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.47	0.78
1:B:112:LEU:HB2	1:B:117:GLN:HG2	1.65	0.78
1:G:112:LEU:HB2	1:G:117:GLN:HG2	1.65	0.78
1:D:214:ARG:HH11	1:D:214:ARG:HG2	1.48	0.78
1:C:66:VAL:H	1:D:94:MET:CE	1.93	0.77
1:C:94:MET:CE	1:D:66:VAL:N	2.32	0.77
1:G:214:ARG:HG2	1:G:214:ARG:HH11	1.47	0.77
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HB2	1:D:117:GLN:HG2	1.65	0.77
1:E:112:LEU:HB2	1:E:117:GLN:HG2	1.65	0.77
1:H:112:LEU:HA	1:H:113:LYS:HZ2	1.50	0.77
1:A:112:LEU:HA	1:A:113:LYS:HZ2	1.48	0.77
1:E:66:VAL:N	1:F:94:MET:CE	2.41	0.77
1:F:118:GLN:NE2	1:G:118:GLN:HG2	2.00	0.77
1:C:37:THR:HB	1:C:40:GLN:HG3	1.67	0.76
1:D:37:THR:HB	1:D:40:GLN:HG3	1.67	0.76
1:F:112:LEU:HB2	1:F:117:GLN:HG2	1.65	0.76
1:B:37:THR:HB	1:B:40:GLN:HG3	1.67	0.76
1:E:94:MET:CE	1:F:66:VAL:N	2.46	0.76
1:F:118:GLN:CD	1:G:118:GLN:HG2	2.10	0.76
1:E:113:LYS:H	1:E:113:LYS:NZ	1.84	0.76
1:A:37:THR:HB	1:A:40:GLN:HG3	1.67	0.76
1:F:112:LEU:HA	1:F:113:LYS:HZ2	1.49	0.76
1:F:118:GLN:HG2	1:G:118:GLN:CG	2.16	0.76
1:G:112:LEU:HA	1:G:113:LYS:HZ2	1.50	0.76
1:G:37:THR:HB	1:G:40:GLN:HG3	1.67	0.75
1:C:112:LEU:HB2	1:C:117:GLN:HG2	1.65	0.75
1:B:119:LYS:HZ3	1:B:123:ASN:HB2	1.52	0.75
1:D:113:LYS:NZ	1:D:113:LYS:H	1.84	0.75
1:E:37:THR:HB	1:E:40:GLN:HG3	1.67	0.75
1:A:113:LYS:NZ	1:A:113:LYS:H	1.84	0.75
1:H:113:LYS:CE	1:H:113:LYS:H	2.00	0.75
1:H:113:LYS:H	1:H:113:LYS:NZ	1.84	0.75
1:B:113:LYS:NZ	1:B:113:LYS:H	1.84	0.75
1:C:119:LYS:HZ3	1:C:123:ASN:HB2	1.48	0.75
1:D:113:LYS:H	1:D:113:LYS:CE	2.00	0.75
1:F:37:THR:HB	1:F:40:GLN:HG3	1.67	0.75
1:F:113:LYS:NZ	1:F:113:LYS:H	1.84	0.74
1:F:119:LYS:HZ3	1:F:123:ASN:HB2	1.49	0.74
1:G:113:LYS:H	1:G:113:LYS:CE	2.00	0.74
1:E:65:LEU:HB3	1:F:94:MET:HE3	1.68	0.74
1:E:113:LYS:H	1:E:113:LYS:CE	2.00	0.74
1:H:37:THR:HB	1:H:40:GLN:HG3	1.67	0.74
1:H:119:LYS:HZ3	1:H:123:ASN:HB2	1.53	0.74
1:A:113:LYS:H	1:A:113:LYS:CE	2.00	0.74
1:C:193:THR:HA	1:C:196:ARG:NH1	2.03	0.74
1:H:193:THR:HA	1:H:196:ARG:NH1	2.03	0.74
1:D:193:THR:HA	1:D:196:ARG:NH1	2.03	0.74
1:G:113:LYS:H	1:G:113:LYS:NZ	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LYS:H	1:F:113:LYS:CE	2.00	0.74
1:C:113:LYS:H	1:C:113:LYS:NZ	1.84	0.74
1:F:193:THR:HA	1:F:196:ARG:NH1	2.03	0.73
1:A:193:THR:HA	1:A:196:ARG:NH1	2.03	0.73
1:C:112:LEU:HD22	1:C:113:LYS:NZ	2.03	0.73
1:B:113:LYS:H	1:B:113:LYS:CE	2.00	0.73
1:E:112:LEU:HD22	1:E:113:LYS:NZ	2.03	0.73
1:G:193:THR:HA	1:G:196:ARG:NH1	2.03	0.73
1:C:113:LYS:H	1:C:113:LYS:CE	2.00	0.73
1:H:112:LEU:HD22	1:H:113:LYS:NZ	2.03	0.73
1:B:112:LEU:HD22	1:B:113:LYS:NZ	2.03	0.73
1:D:112:LEU:HA	1:D:113:LYS:HZ2	1.52	0.73
1:B:193:THR:HA	1:B:196:ARG:NH1	2.03	0.73
1:C:9:TYR:CG	1:C:10:PRO:HD2	2.24	0.73
1:G:9:TYR:CG	1:G:10:PRO:HD2	2.24	0.73
1:A:9:TYR:CG	1:A:10:PRO:HD2	2.24	0.73
1:A:112:LEU:HD22	1:A:113:LYS:NZ	2.03	0.73
1:F:9:TYR:CG	1:F:10:PRO:HD2	2.24	0.73
1:B:9:TYR:CG	1:B:10:PRO:HD2	2.24	0.72
1:D:112:LEU:HD22	1:D:113:LYS:NZ	2.03	0.72
1:E:193:THR:HA	1:E:196:ARG:NH1	2.03	0.72
1:D:9:TYR:CG	1:D:10:PRO:HD2	2.24	0.72
1:B:38:LYS:O	1:B:41:LEU:HB3	1.90	0.72
1:G:65:LEU:HB3	1:H:94:MET:HE3	1.71	0.72
1:F:112:LEU:HD22	1:F:113:LYS:NZ	2.03	0.72
1:E:38:LYS:O	1:E:41:LEU:HB3	1.90	0.72
1:H:9:TYR:CG	1:H:10:PRO:HD2	2.24	0.72
1:E:9:TYR:CG	1:E:10:PRO:HD2	2.24	0.71
1:C:65:LEU:HB3	1:D:94:MET:HE3	1.71	0.71
1:D:38:LYS:O	1:D:41:LEU:HB3	1.90	0.71
1:G:112:LEU:HD22	1:G:113:LYS:NZ	2.03	0.71
1:H:38:LYS:O	1:H:41:LEU:HB3	1.90	0.71
1:G:38:LYS:O	1:G:41:LEU:HB3	1.90	0.71
1:G:60:ILE:HD13	1:G:74:TYR:CE2	2.26	0.71
1:G:209:ASP:OD1	1:G:211:ILE:HB	1.91	0.71
1:C:209:ASP:OD1	1:C:211:ILE:HB	1.91	0.71
1:D:60:ILE:HD13	1:D:74:TYR:CE2	2.26	0.71
1:F:38:LYS:O	1:F:41:LEU:HB3	1.90	0.71
1:A:119:LYS:HZ3	1:A:123:ASN:HB2	1.55	0.70
1:A:209:ASP:OD1	1:A:211:ILE:HB	1.91	0.70
1:D:209:ASP:OD1	1:D:211:ILE:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ILE:HD13	1:F:74:TYR:CE2	2.26	0.70
1:E:60:ILE:HD13	1:E:74:TYR:CE2	2.26	0.70
1:A:104:GLU:O	1:A:108:MET:HG3	1.92	0.70
1:D:119:LYS:HZ3	1:D:123:ASN:HB2	1.53	0.70
1:G:104:GLU:O	1:G:108:MET:HG3	1.92	0.70
1:H:60:ILE:HD13	1:H:74:TYR:CE2	2.26	0.70
1:F:209:ASP:OD1	1:F:211:ILE:HB	1.91	0.70
1:A:38:LYS:O	1:A:41:LEU:HB3	1.90	0.70
1:C:60:ILE:HD13	1:C:74:TYR:CE2	2.26	0.70
1:B:209:ASP:OD1	1:B:211:ILE:HB	1.91	0.69
1:E:209:ASP:OD1	1:E:211:ILE:HB	1.91	0.69
1:H:104:GLU:O	1:H:108:MET:HG3	1.92	0.69
1:E:104:GLU:O	1:E:108:MET:HG3	1.92	0.69
1:F:104:GLU:O	1:F:108:MET:HG3	1.92	0.69
1:A:60:ILE:HD13	1:A:74:TYR:CE2	2.26	0.69
1:C:38:LYS:O	1:C:41:LEU:HB3	1.90	0.69
1:E:119:LYS:HZ2	1:E:123:ASN:HB2	1.57	0.69
1:B:60:ILE:HD13	1:B:74:TYR:CE2	2.26	0.69
1:A:94:MET:CE	1:B:66:VAL:N	2.53	0.69
1:D:104:GLU:O	1:D:108:MET:HG3	1.92	0.69
1:H:209:ASP:OD1	1:H:211:ILE:HB	1.91	0.69
1:C:104:GLU:O	1:C:108:MET:HG3	1.92	0.69
1:B:104:GLU:O	1:B:108:MET:HG3	1.92	0.68
1:E:94:MET:HE3	1:F:65:LEU:HB3	1.75	0.67
1:C:94:MET:HE3	1:D:65:LEU:CB	2.25	0.67
1:E:41:LEU:O	1:E:45:GLN:HG2	1.95	0.66
1:H:18:SER:CB	1:H:162:GLN:HE22	2.09	0.66
1:G:41:LEU:O	1:G:45:GLN:HG2	1.95	0.66
1:E:65:LEU:CA	1:F:94:MET:CE	2.71	0.66
1:C:41:LEU:O	1:C:45:GLN:HG2	1.95	0.66
1:D:41:LEU:O	1:D:45:GLN:HG2	1.96	0.66
1:D:18:SER:CB	1:D:162:GLN:HE22	2.09	0.66
1:E:18:SER:CB	1:E:162:GLN:HE22	2.09	0.66
1:A:41:LEU:O	1:A:45:GLN:HG2	1.96	0.65
1:G:18:SER:CB	1:G:162:GLN:HE22	2.09	0.65
1:B:41:LEU:O	1:B:45:GLN:HG2	1.96	0.65
1:H:41:LEU:O	1:H:45:GLN:HG2	1.96	0.65
1:A:18:SER:CB	1:A:162:GLN:HE22	2.09	0.65
1:C:18:SER:CB	1:C:162:GLN:HE22	2.09	0.65
1:B:18:SER:CB	1:B:162:GLN:HE22	2.09	0.65
1:A:113:LYS:O	1:A:116:ASP:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:HG3	1:B:69:ARG:HH11	1.62	0.65
1:D:69:ARG:HG3	1:D:69:ARG:HH11	1.62	0.65
1:F:18:SER:CB	1:F:162:GLN:HE22	2.09	0.65
1:F:41:LEU:O	1:F:45:GLN:HG2	1.96	0.65
1:E:119:LYS:HZ3	1:E:123:ASN:HB2	1.61	0.65
1:C:69:ARG:HG3	1:C:69:ARG:HH11	1.62	0.64
1:G:69:ARG:HG3	1:G:69:ARG:HH11	1.62	0.64
1:A:69:ARG:HG3	1:A:69:ARG:HH11	1.62	0.64
1:F:69:ARG:HG3	1:F:69:ARG:HH11	1.62	0.64
1:G:66:VAL:N	1:H:94:MET:CE	2.50	0.64
1:E:113:LYS:O	1:E:116:ASP:N	2.29	0.64
1:F:113:LYS:O	1:F:116:ASP:N	2.29	0.64
1:F:118:GLN:HG2	1:G:118:GLN:CD	2.22	0.64
1:A:65:LEU:HB3	1:B:94:MET:HE3	1.79	0.64
1:D:133:PHE:HB2	1:D:134:PRO:HD3	1.80	0.64
1:C:133:PHE:HB2	1:C:134:PRO:HD3	1.80	0.64
1:E:112:LEU:HA	1:E:113:LYS:NZ	2.13	0.64
1:C:113:LYS:O	1:C:116:ASP:N	2.29	0.63
1:H:113:LYS:O	1:H:116:ASP:N	2.29	0.63
1:B:112:LEU:HA	1:B:113:LYS:NZ	2.13	0.63
1:A:137:GLU:OE1	1:A:178:PHE:HB3	1.98	0.63
1:G:113:LYS:O	1:G:116:ASP:N	2.29	0.63
1:H:69:ARG:HG3	1:H:69:ARG:HH11	1.62	0.63
1:H:112:LEU:HA	1:H:113:LYS:NZ	2.13	0.63
1:A:112:LEU:HA	1:A:113:LYS:NZ	2.13	0.63
1:G:137:GLU:OE1	1:G:178:PHE:HB3	1.98	0.63
1:H:69:ARG:HH11	1:H:69:ARG:CG	2.12	0.63
1:B:137:GLU:OE1	1:B:178:PHE:HB3	1.98	0.63
1:D:137:GLU:OE1	1:D:178:PHE:HB3	1.98	0.63
1:E:69:ARG:HG3	1:E:69:ARG:HH11	1.62	0.63
1:F:39:GLU:O	1:F:43:LYS:HG3	1.99	0.63
1:B:69:ARG:HH11	1:B:69:ARG:CG	2.12	0.63
1:D:67:GLN:HB2	1:D:70:SER:HB2	1.81	0.63
1:E:69:ARG:HH11	1:E:69:ARG:CG	2.12	0.63
1:D:69:ARG:HH11	1:D:69:ARG:CG	2.12	0.63
1:F:69:ARG:HH11	1:F:69:ARG:CG	2.12	0.63
1:G:112:LEU:HA	1:G:113:LYS:NZ	2.13	0.63
1:G:215:THR:O	1:G:219:ILE:HG13	1.99	0.63
1:B:215:THR:O	1:B:219:ILE:HG13	1.99	0.63
1:C:112:LEU:HA	1:C:113:LYS:NZ	2.13	0.63
1:F:112:LEU:HA	1:F:113:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HA	1:D:113:LYS:NZ	2.13	0.62
1:E:67:GLN:HB2	1:E:70:SER:HB2	1.81	0.62
1:G:65:LEU:CA	1:H:94:MET:CE	2.74	0.62
1:G:39:GLU:O	1:G:43:LYS:HG3	1.99	0.62
1:E:215:THR:O	1:E:219:ILE:HG13	1.99	0.62
1:H:137:GLU:OE1	1:H:178:PHE:HB3	1.98	0.62
1:F:215:THR:O	1:F:219:ILE:HG13	1.99	0.62
1:G:94:MET:HE3	1:H:65:LEU:HB3	1.80	0.62
1:C:39:GLU:O	1:C:43:LYS:HG3	1.99	0.62
1:C:141:ARG:HG2	1:C:141:ARG:NH1	2.14	0.62
1:F:137:GLU:OE1	1:F:178:PHE:HB3	1.98	0.62
1:H:133:PHE:HB2	1:H:134:PRO:HD3	1.80	0.62
1:A:67:GLN:HB2	1:A:70:SER:HB2	1.81	0.62
1:A:215:THR:O	1:A:219:ILE:HG13	1.99	0.62
1:B:113:LYS:O	1:B:116:ASP:N	2.29	0.62
1:C:69:ARG:HH11	1:C:69:ARG:CG	2.12	0.62
1:F:133:PHE:HB2	1:F:134:PRO:HD3	1.80	0.62
1:G:133:PHE:HB2	1:G:134:PRO:HD3	1.80	0.62
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.12	0.62
1:C:215:THR:O	1:C:219:ILE:HG13	1.99	0.62
1:D:39:GLU:O	1:D:43:LYS:HG3	1.99	0.62
1:E:39:GLU:O	1:E:43:LYS:HG3	1.99	0.62
1:C:67:GLN:HB2	1:C:70:SER:HB2	1.81	0.62
1:C:137:GLU:OE1	1:C:178:PHE:HB3	1.98	0.62
1:D:215:THR:O	1:D:219:ILE:HG13	1.99	0.62
1:E:137:GLU:OE1	1:E:178:PHE:HB3	1.98	0.62
1:G:67:GLN:HB2	1:G:70:SER:HB2	1.81	0.62
1:A:133:PHE:HB2	1:A:134:PRO:HD3	1.80	0.62
1:B:133:PHE:HB2	1:B:134:PRO:HD3	1.80	0.62
1:E:133:PHE:HB2	1:E:134:PRO:HD3	1.80	0.62
1:A:119:LYS:HD3	1:A:119:LYS:C	2.25	0.62
1:D:119:LYS:HD3	1:D:119:LYS:C	2.25	0.62
1:G:69:ARG:HH11	1:G:69:ARG:CG	2.12	0.61
1:G:94:MET:CE	1:H:66:VAL:N	2.58	0.61
1:F:141:ARG:HG2	1:F:141:ARG:NH1	2.14	0.61
1:D:113:LYS:O	1:D:116:ASP:N	2.29	0.61
1:G:119:LYS:HD3	1:G:119:LYS:C	2.25	0.61
1:H:39:GLU:O	1:H:43:LYS:HG3	1.99	0.61
1:B:119:LYS:HD3	1:B:119:LYS:C	2.25	0.61
1:F:67:GLN:HB2	1:F:70:SER:HB2	1.81	0.61
1:F:137:GLU:CD	1:F:180:PHE:HB2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:O	1:A:43:LYS:HG3	1.99	0.61
1:B:67:GLN:HB2	1:B:70:SER:HB2	1.81	0.61
1:B:137:GLU:CD	1:B:180:PHE:HB2	2.26	0.61
1:C:137:GLU:CD	1:C:180:PHE:HB2	2.26	0.61
1:H:215:THR:O	1:H:219:ILE:HG13	1.99	0.61
1:C:119:LYS:C	1:C:119:LYS:HD3	2.25	0.61
1:G:137:GLU:CD	1:G:180:PHE:HB2	2.26	0.61
1:H:119:LYS:HD3	1:H:119:LYS:C	2.25	0.61
1:A:119:LYS:HZ2	1:A:123:ASN:HB2	1.63	0.61
1:A:137:GLU:CD	1:A:180:PHE:HB2	2.26	0.61
1:B:39:GLU:O	1:B:43:LYS:HG3	1.99	0.61
1:F:37:THR:HG22	1:F:39:GLU:H	1.66	0.61
1:G:37:THR:HG22	1:G:39:GLU:H	1.66	0.61
1:E:119:LYS:C	1:E:119:LYS:HD3	2.25	0.61
1:F:119:LYS:HD3	1:F:119:LYS:C	2.25	0.61
1:A:37:THR:HG22	1:A:39:GLU:H	1.66	0.60
1:H:37:THR:HG22	1:H:39:GLU:H	1.66	0.60
1:D:137:GLU:CD	1:D:180:PHE:HB2	2.26	0.60
1:H:67:GLN:HB2	1:H:70:SER:HB2	1.81	0.60
1:C:37:THR:HG22	1:C:39:GLU:H	1.66	0.60
1:H:137:GLU:CD	1:H:180:PHE:HB2	2.26	0.60
1:D:119:LYS:HZ2	1:D:123:ASN:HB2	1.65	0.60
1:E:37:THR:HG22	1:E:39:GLU:H	1.66	0.60
1:E:137:GLU:CD	1:E:180:PHE:HB2	2.26	0.60
1:G:141:ARG:HG2	1:G:141:ARG:NH1	2.14	0.60
1:E:94:MET:CE	1:F:65:LEU:CA	2.78	0.60
1:C:94:MET:CE	1:D:65:LEU:CB	2.80	0.60
1:B:37:THR:HG22	1:B:39:GLU:H	1.66	0.59
1:E:141:ARG:HG2	1:E:141:ARG:NH1	2.14	0.59
1:D:37:THR:HG22	1:D:39:GLU:H	1.66	0.59
1:D:112:LEU:HD22	1:D:113:LYS:HZ1	1.69	0.58
1:C:109:HIS:HB3	1:C:110:PRO:HD3	1.86	0.58
1:H:109:HIS:HB3	1:H:110:PRO:HD3	1.86	0.57
1:A:94:MET:HE3	1:B:65:LEU:HB3	1.86	0.57
1:B:197:PHE:CZ	1:B:204:LYS:HB2	2.40	0.57
1:D:197:PHE:CZ	1:D:204:LYS:HB2	2.40	0.57
1:F:80:ASN:HD21	1:F:84:LYS:HE2	1.70	0.57
1:G:80:ASN:HD21	1:G:84:LYS:HE2	1.70	0.57
1:F:197:PHE:CZ	1:F:204:LYS:HB2	2.40	0.57
1:A:197:PHE:CZ	1:A:204:LYS:HB2	2.40	0.57
1:F:109:HIS:HB3	1:F:110:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:PHE:CZ	1:H:204:LYS:HB2	2.40	0.57
1:B:109:HIS:HB3	1:B:110:PRO:HD3	1.86	0.57
1:D:109:HIS:HB3	1:D:110:PRO:HD3	1.86	0.56
1:E:197:PHE:CZ	1:E:204:LYS:HB2	2.40	0.56
1:B:80:ASN:HD21	1:B:84:LYS:HE2	1.70	0.56
1:D:80:ASN:HD21	1:D:84:LYS:HE2	1.70	0.56
1:A:109:HIS:HB3	1:A:110:PRO:HD3	1.86	0.56
1:D:141:ARG:HG2	1:D:141:ARG:NH1	2.14	0.56
1:G:112:LEU:HD22	1:G:113:LYS:HZ1	1.70	0.56
1:G:197:PHE:CZ	1:G:204:LYS:HB2	2.40	0.56
1:C:80:ASN:HD21	1:C:84:LYS:HE2	1.70	0.56
1:E:80:ASN:HD21	1:E:84:LYS:HE2	1.70	0.56
1:F:112:LEU:HD22	1:F:113:LYS:HZ1	1.70	0.56
1:H:211:ILE:HD12	1:H:211:ILE:N	2.21	0.56
1:A:164:ILE:O	1:A:168:GLU:HG3	2.06	0.56
1:F:211:ILE:HD12	1:F:211:ILE:N	2.21	0.56
1:C:197:PHE:CZ	1:C:204:LYS:HB2	2.40	0.56
1:E:109:HIS:HB3	1:E:110:PRO:HD3	1.86	0.56
1:E:112:LEU:HD22	1:E:113:LYS:HZ1	1.71	0.56
1:B:164:ILE:O	1:B:168:GLU:HG3	2.06	0.56
1:B:211:ILE:N	1:B:211:ILE:HD12	2.21	0.56
1:G:211:ILE:N	1:G:211:ILE:HD12	2.21	0.56
1:A:211:ILE:HD12	1:A:211:ILE:N	2.21	0.56
1:E:211:ILE:HD12	1:E:211:ILE:N	2.21	0.56
1:G:94:MET:CE	1:H:65:LEU:CA	2.83	0.56
1:H:112:LEU:HD22	1:H:113:LYS:HZ1	1.70	0.56
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.14	0.55
1:B:141:ARG:HG2	1:B:141:ARG:NH1	2.14	0.55
1:G:109:HIS:HB3	1:G:110:PRO:HD3	1.86	0.55
1:F:118:GLN:NE2	1:G:118:GLN:CG	2.69	0.55
1:C:65:LEU:CA	1:D:94:MET:CE	2.80	0.55
1:E:164:ILE:O	1:E:168:GLU:HG3	2.06	0.55
1:H:80:ASN:HD21	1:H:84:LYS:HE2	1.70	0.55
1:A:80:ASN:HD21	1:A:84:LYS:HE2	1.70	0.55
1:B:119:LYS:HZ2	1:B:123:ASN:HB2	1.68	0.55
1:C:164:ILE:O	1:C:168:GLU:HG3	2.06	0.55
1:H:164:ILE:O	1:H:168:GLU:HG3	2.06	0.55
1:C:66:VAL:N	1:D:94:MET:HE2	2.01	0.55
1:C:112:LEU:HD22	1:C:113:LYS:HZ1	1.71	0.55
1:C:211:ILE:HD12	1:C:211:ILE:N	2.21	0.55
1:D:211:ILE:N	1:D:211:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:ILE:O	1:G:168:GLU:HG3	2.06	0.55
1:G:178:PHE:O	1:G:182:GLN:HG3	2.07	0.55
1:H:178:PHE:O	1:H:182:GLN:HG3	2.07	0.55
1:C:178:PHE:O	1:C:182:GLN:HG3	2.07	0.55
1:D:178:PHE:O	1:D:182:GLN:HG3	2.07	0.55
1:A:178:PHE:O	1:A:182:GLN:HG3	2.07	0.54
1:C:94:MET:CE	1:D:65:LEU:HB3	2.29	0.54
1:A:51:LEU:HB3	1:A:66:VAL:HG21	1.90	0.54
1:D:164:ILE:O	1:D:168:GLU:HG3	2.06	0.54
1:E:92:ILE:HD13	1:E:154:SER:HB2	1.90	0.54
1:H:92:ILE:HD13	1:H:154:SER:HB2	1.89	0.54
1:E:178:PHE:O	1:E:182:GLN:HG3	2.07	0.54
1:F:164:ILE:O	1:F:168:GLU:HG3	2.06	0.54
1:H:119:LYS:HZ2	1:H:123:ASN:HB2	1.66	0.54
1:B:51:LEU:HB3	1:B:66:VAL:HG21	1.90	0.54
1:D:51:LEU:HB3	1:D:66:VAL:HG21	1.90	0.54
1:B:112:LEU:HD22	1:B:113:LYS:HZ1	1.70	0.54
1:F:51:LEU:HB3	1:F:66:VAL:HG21	1.90	0.54
1:B:178:PHE:O	1:B:182:GLN:HG3	2.07	0.54
1:D:175:LEU:O	1:D:178:PHE:N	2.38	0.54
1:B:92:ILE:HD13	1:B:154:SER:HB2	1.90	0.53
1:C:113:LYS:O	1:C:115:ASP:N	2.41	0.53
1:F:178:PHE:O	1:F:182:GLN:HG3	2.07	0.53
1:G:113:LYS:O	1:G:115:ASP:N	2.41	0.53
1:F:145:GLN:HB3	1:F:151:ASN:OD1	2.09	0.53
1:A:92:ILE:O	1:A:96:VAL:HG23	2.09	0.53
1:B:145:GLN:HB3	1:B:151:ASN:OD1	2.09	0.53
1:F:92:ILE:O	1:F:96:VAL:HG23	2.09	0.53
1:G:51:LEU:HB3	1:G:66:VAL:HG21	1.90	0.53
1:A:145:GLN:HB3	1:A:151:ASN:OD1	2.09	0.53
1:D:92:ILE:HD13	1:D:154:SER:HB2	1.89	0.53
1:F:92:ILE:HD13	1:F:154:SER:HB2	1.90	0.53
1:A:92:ILE:HD13	1:A:154:SER:HB2	1.89	0.53
1:B:113:LYS:O	1:B:115:ASP:N	2.41	0.53
1:E:113:LYS:O	1:E:115:ASP:N	2.41	0.53
1:G:145:GLN:HB3	1:G:151:ASN:OD1	2.09	0.53
1:H:37:THR:CB	1:H:40:GLN:HG3	2.39	0.53
1:H:145:GLN:HB3	1:H:151:ASN:OD1	2.09	0.53
1:A:112:LEU:HD22	1:A:113:LYS:HZ1	1.70	0.53
1:D:113:LYS:O	1:D:115:ASP:N	2.41	0.53
1:F:113:LYS:O	1:F:115:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:LYS:O	1:H:115:ASP:N	2.41	0.53
1:E:51:LEU:HB3	1:E:66:VAL:HG21	1.90	0.53
1:A:113:LYS:O	1:A:115:ASP:N	2.41	0.53
1:C:92:ILE:O	1:C:96:VAL:HG23	2.09	0.53
1:E:92:ILE:O	1:E:96:VAL:HG23	2.09	0.53
1:E:175:LEU:O	1:E:178:PHE:N	2.38	0.53
1:G:92:ILE:HD13	1:G:154:SER:HB2	1.90	0.53
1:E:145:GLN:HB3	1:E:151:ASN:OD1	2.09	0.52
1:C:51:LEU:HB3	1:C:66:VAL:HG21	1.90	0.52
1:G:175:LEU:O	1:G:178:PHE:N	2.38	0.52
1:H:92:ILE:O	1:H:96:VAL:HG23	2.09	0.52
1:C:92:ILE:HD13	1:C:154:SER:HB2	1.89	0.52
1:D:92:ILE:O	1:D:96:VAL:HG23	2.09	0.52
1:G:184:TYR:CZ	1:G:188:LEU:HD11	2.45	0.52
1:A:184:TYR:CZ	1:A:188:LEU:HD11	2.45	0.52
1:D:184:TYR:CZ	1:D:188:LEU:HD11	2.45	0.52
1:F:184:TYR:CZ	1:F:188:LEU:HD11	2.45	0.52
1:H:214:ARG:HH11	1:H:214:ARG:CG	2.21	0.52
1:C:37:THR:CB	1:C:40:GLN:HG3	2.39	0.52
1:E:143:HIS:ND1	1:E:145:GLN:N	2.53	0.52
1:B:92:ILE:O	1:B:96:VAL:HG23	2.09	0.52
1:G:92:ILE:O	1:G:96:VAL:HG23	2.09	0.52
1:F:179:PRO:HB3	1:H:42:TYR:CZ	2.45	0.52
1:B:184:TYR:CZ	1:B:188:LEU:HD11	2.45	0.52
1:D:143:HIS:ND1	1:D:145:GLN:N	2.53	0.52
1:E:37:THR:CB	1:E:40:GLN:HG3	2.39	0.52
1:H:51:LEU:HB3	1:H:66:VAL:HG21	1.90	0.52
1:C:145:GLN:HB3	1:C:151:ASN:OD1	2.09	0.52
1:F:214:ARG:HG2	1:F:214:ARG:NH1	2.23	0.52
1:H:184:TYR:CZ	1:H:188:LEU:HD11	2.45	0.52
1:A:214:ARG:HH11	1:A:214:ARG:CG	2.21	0.51
1:D:145:GLN:HB3	1:D:151:ASN:OD1	2.09	0.51
1:D:214:ARG:HG2	1:D:214:ARG:NH1	2.23	0.51
1:C:143:HIS:ND1	1:C:145:GLN:N	2.53	0.51
1:C:184:TYR:CZ	1:C:188:LEU:HD11	2.45	0.51
1:F:119:LYS:HZ2	1:F:123:ASN:HB2	1.70	0.51
1:D:59:GLU:HA	1:D:63:MET:O	2.11	0.51
1:D:113:LYS:H	1:D:113:LYS:HZ3	1.57	0.51
1:B:59:GLU:HA	1:B:63:MET:O	2.10	0.51
1:C:85:ASN:O	1:C:89:ARG:HB2	2.11	0.51
1:E:184:TYR:CZ	1:E:188:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ASN:O	1:F:89:ARG:HB2	2.11	0.51
1:G:211:ILE:HD12	1:G:211:ILE:H	1.76	0.51
1:A:59:GLU:HA	1:A:63:MET:O	2.11	0.51
1:D:85:ASN:O	1:D:89:ARG:HB2	2.11	0.51
1:B:175:LEU:O	1:B:178:PHE:N	2.38	0.51
1:B:143:HIS:ND1	1:B:145:GLN:N	2.53	0.51
1:C:59:GLU:HA	1:C:63:MET:O	2.11	0.51
1:D:214:ARG:HH11	1:D:214:ARG:CG	2.21	0.51
1:E:214:ARG:HH11	1:E:214:ARG:CG	2.21	0.51
1:F:37:THR:CB	1:F:40:GLN:HG3	2.39	0.51
1:F:214:ARG:HH11	1:F:214:ARG:CG	2.21	0.51
1:G:59:GLU:HA	1:G:63:MET:O	2.10	0.51
1:H:175:LEU:O	1:H:178:PHE:N	2.38	0.51
1:A:85:ASN:O	1:A:89:ARG:HB2	2.11	0.51
1:E:59:GLU:HA	1:E:63:MET:O	2.11	0.51
1:G:214:ARG:HH11	1:G:214:ARG:CG	2.21	0.51
1:A:211:ILE:HD12	1:A:211:ILE:H	1.76	0.50
1:F:59:GLU:HA	1:F:63:MET:O	2.11	0.50
1:H:112:LEU:CB	1:H:117:GLN:HG2	2.40	0.50
1:B:214:ARG:HH11	1:B:214:ARG:CG	2.21	0.50
1:C:192:PRO:O	1:C:196:ARG:HG3	2.12	0.50
1:E:211:ILE:HD12	1:E:211:ILE:H	1.76	0.50
1:F:118:GLN:HE21	1:G:118:GLN:CG	2.25	0.50
1:G:85:ASN:O	1:G:89:ARG:HB2	2.11	0.50
1:C:94:MET:HG2	1:D:66:VAL:O	2.11	0.50
1:C:211:ILE:HD12	1:C:211:ILE:H	1.76	0.50
1:D:60:ILE:CD1	1:D:74:TYR:HE2	2.21	0.50
1:B:85:ASN:O	1:B:89:ARG:HB2	2.11	0.50
1:C:175:LEU:O	1:C:178:PHE:N	2.38	0.50
1:D:211:ILE:HD12	1:D:211:ILE:H	1.76	0.50
1:F:175:LEU:O	1:F:178:PHE:N	2.38	0.50
1:A:65:LEU:CA	1:B:94:MET:CE	2.86	0.50
1:B:192:PRO:O	1:B:196:ARG:HG3	2.12	0.50
1:H:59:GLU:HA	1:H:63:MET:O	2.10	0.50
1:E:85:ASN:O	1:E:89:ARG:HB2	2.11	0.50
1:G:60:ILE:CD1	1:G:74:TYR:HE2	2.21	0.50
1:A:192:PRO:O	1:A:196:ARG:HG3	2.12	0.50
1:D:192:PRO:O	1:D:196:ARG:HG3	2.12	0.50
1:F:192:PRO:O	1:F:196:ARG:HG3	2.12	0.50
1:G:192:PRO:O	1:G:196:ARG:HG3	2.12	0.50
1:H:211:ILE:HD12	1:H:211:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:CD1	1:B:74:TYR:HE2	2.21	0.49
1:C:9:TYR:CE1	1:C:56:PRO:HD3	2.47	0.49
1:G:9:TYR:CE1	1:G:56:PRO:HD3	2.47	0.49
1:H:9:TYR:CE1	1:H:56:PRO:HD3	2.47	0.49
1:H:192:PRO:O	1:H:196:ARG:HG3	2.12	0.49
1:B:18:SER:HB3	1:B:162:GLN:HE22	1.78	0.49
1:C:119:LYS:HZ2	1:C:123:ASN:HB2	1.71	0.49
1:D:9:TYR:CE1	1:D:56:PRO:HD3	2.47	0.49
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.21	0.49
1:F:179:PRO:HB3	1:H:42:TYR:CE2	2.47	0.49
1:G:143:HIS:ND1	1:G:145:GLN:N	2.53	0.49
1:B:211:ILE:HD12	1:B:211:ILE:H	1.76	0.49
1:C:18:SER:HB3	1:C:162:GLN:HE22	1.78	0.49
1:F:47:GLY:O	1:F:48:ASN:HB2	2.13	0.49
1:A:9:TYR:CE1	1:A:56:PRO:HD3	2.47	0.49
1:H:18:SER:HB3	1:H:162:GLN:HE22	1.78	0.49
1:A:47:GLY:O	1:A:48:ASN:HB2	2.12	0.49
1:A:143:HIS:ND1	1:A:145:GLN:N	2.53	0.49
1:B:47:GLY:O	1:B:48:ASN:HB2	2.13	0.49
1:D:7:LEU:HD12	1:D:7:LEU:N	2.27	0.49
1:G:37:THR:CB	1:G:40:GLN:HG3	2.39	0.49
1:H:85:ASN:O	1:H:89:ARG:HB2	2.11	0.49
1:B:9:TYR:CE1	1:B:56:PRO:HD3	2.47	0.49
1:D:37:THR:CB	1:D:40:GLN:HG3	2.39	0.49
1:E:192:PRO:O	1:E:196:ARG:HG3	2.12	0.49
1:F:211:ILE:HD12	1:F:211:ILE:H	1.76	0.49
1:H:47:GLY:O	1:H:48:ASN:HB2	2.13	0.49
1:F:9:TYR:CE1	1:F:56:PRO:HD3	2.47	0.49
1:E:9:TYR:CE1	1:E:56:PRO:HD3	2.47	0.49
1:H:7:LEU:HD12	1:H:7:LEU:N	2.28	0.49
1:B:37:THR:CB	1:B:40:GLN:HG3	2.39	0.49
1:F:18:SER:HB3	1:F:162:GLN:HE22	1.78	0.49
1:A:112:LEU:CB	1:A:117:GLN:HG2	2.40	0.48
1:C:47:GLY:O	1:C:48:ASN:HB2	2.13	0.48
1:H:141:ARG:HG2	1:H:141:ARG:NH1	2.14	0.48
1:A:7:LEU:HD12	1:A:7:LEU:N	2.27	0.48
1:A:94:MET:CE	1:B:65:LEU:CA	2.88	0.48
1:C:7:LEU:N	1:C:7:LEU:HD12	2.27	0.48
1:H:60:ILE:CD1	1:H:74:TYR:HE2	2.21	0.48
1:C:65:LEU:CB	1:D:94:MET:HE3	2.42	0.48
1:B:112:LEU:CB	1:B:117:GLN:HG2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:CD1	1:C:74:TYR:HE2	2.21	0.48
1:D:78:LYS:HD2	1:D:78:LYS:HA	1.43	0.48
1:G:58:VAL:O	1:G:65:LEU:N	2.44	0.48
1:D:58:VAL:O	1:D:65:LEU:N	2.44	0.48
1:E:58:VAL:O	1:E:65:LEU:N	2.44	0.48
1:C:141:ARG:HD2	1:C:180:PHE:CE2	2.49	0.48
1:F:133:PHE:N	1:F:134:PRO:CD	2.77	0.48
1:E:112:LEU:CB	1:E:117:GLN:HG2	2.41	0.48
1:G:7:LEU:N	1:G:7:LEU:HD12	2.27	0.48
1:H:141:ARG:HD2	1:H:180:PHE:CE2	2.49	0.48
1:B:7:LEU:N	1:B:7:LEU:HD12	2.28	0.48
1:D:47:GLY:O	1:D:48:ASN:HB2	2.13	0.48
1:E:207:PRO:HA	1:E:208:PRO:HD3	1.52	0.48
1:H:113:LYS:H	1:H:113:LYS:HZ3	1.61	0.48
1:E:87:LYS:HA	1:E:87:LYS:HD3	1.61	0.48
1:G:18:SER:HB3	1:G:162:GLN:HE22	1.78	0.48
1:A:109:HIS:N	1:A:110:PRO:HD2	2.29	0.47
1:D:18:SER:HB3	1:D:162:GLN:HE22	1.78	0.47
1:E:7:LEU:N	1:E:7:LEU:HD12	2.28	0.47
1:E:18:SER:HB3	1:E:162:GLN:HE22	1.78	0.47
1:E:141:ARG:HD2	1:E:180:PHE:CE2	2.49	0.47
1:G:47:GLY:O	1:G:48:ASN:HB2	2.12	0.47
1:H:143:HIS:ND1	1:H:145:GLN:N	2.53	0.47
1:A:37:THR:CB	1:A:40:GLN:HG3	2.39	0.47
1:D:109:HIS:N	1:D:110:PRO:HD2	2.29	0.47
1:D:141:ARG:HD2	1:D:180:PHE:CE2	2.49	0.47
1:E:109:HIS:N	1:E:110:PRO:HD2	2.29	0.47
1:F:112:LEU:CB	1:F:117:GLN:HG2	2.41	0.47
1:A:175:LEU:O	1:A:178:PHE:N	2.38	0.47
1:B:214:ARG:HG2	1:B:214:ARG:NH1	2.23	0.47
1:H:214:ARG:HG2	1:H:214:ARG:NH1	2.23	0.47
1:A:18:SER:HB3	1:A:162:GLN:HE22	1.78	0.47
1:B:109:HIS:N	1:B:110:PRO:HD2	2.29	0.47
1:G:214:ARG:CG	1:G:214:ARG:NH1	2.78	0.47
1:B:133:PHE:N	1:B:134:PRO:CD	2.77	0.47
1:B:214:ARG:CG	1:B:214:ARG:NH1	2.78	0.47
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.78	0.47
1:D:133:PHE:N	1:D:134:PRO:CD	2.77	0.47
1:F:7:LEU:HD12	1:F:7:LEU:N	2.27	0.47
1:F:109:HIS:N	1:F:110:PRO:HD2	2.29	0.47
1:G:109:HIS:N	1:G:110:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:ARG:HD2	1:G:180:PHE:CE2	2.49	0.47
1:B:141:ARG:HD2	1:B:180:PHE:CE2	2.49	0.47
1:B:170:LYS:C	1:B:171:ILE:HG13	2.40	0.47
1:C:109:HIS:N	1:C:110:PRO:HD2	2.30	0.47
1:C:112:LEU:CB	1:C:117:GLN:HG2	2.41	0.47
1:E:65:LEU:CB	1:F:94:MET:HE3	2.41	0.47
1:F:60:ILE:CD1	1:F:74:TYR:HE2	2.21	0.47
1:F:193:THR:HA	1:F:196:ARG:HH12	1.79	0.47
1:G:129:ILE:HD12	1:G:129:ILE:HG23	1.66	0.47
1:A:133:PHE:N	1:A:134:PRO:CD	2.77	0.47
1:A:141:ARG:HD2	1:A:180:PHE:CE2	2.49	0.47
1:A:170:LYS:C	1:A:171:ILE:HG13	2.40	0.47
1:C:84:LYS:O	1:C:85:ASN:HB3	2.15	0.47
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.64	0.47
1:C:170:LYS:C	1:C:171:ILE:HG13	2.40	0.47
1:D:23:LEU:HD23	1:D:23:LEU:HA	1.72	0.47
1:E:47:GLY:O	1:E:48:ASN:HB2	2.13	0.47
1:E:133:PHE:N	1:E:134:PRO:CD	2.77	0.47
1:F:44:LEU:HD12	1:F:44:LEU:HA	1.68	0.47
1:F:170:LYS:C	1:F:171:ILE:HG13	2.40	0.47
1:G:65:LEU:CB	1:H:94:MET:HE3	2.43	0.47
1:G:133:PHE:N	1:G:134:PRO:CD	2.77	0.47
1:A:66:VAL:N	1:B:94:MET:CE	2.71	0.47
1:F:141:ARG:HD2	1:F:180:PHE:CE2	2.49	0.47
1:F:207:PRO:HA	1:F:208:PRO:HD3	1.52	0.47
1:H:129:ILE:HG23	1:H:129:ILE:HD12	1.66	0.47
1:H:133:PHE:N	1:H:134:PRO:CD	2.77	0.47
1:H:214:ARG:HA	1:H:214:ARG:HD2	1.60	0.47
1:D:84:LYS:O	1:D:85:ASN:HB3	2.15	0.47
1:D:113:LYS:N	1:D:113:LYS:CD	2.78	0.47
1:D:211:ILE:H	1:D:211:ILE:CD1	2.28	0.47
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.64	0.47
1:G:119:LYS:HZ2	1:G:123:ASN:HB2	1.76	0.47
1:C:66:VAL:N	1:D:94:MET:CE	2.72	0.47
1:C:133:PHE:N	1:C:134:PRO:CD	2.77	0.47
1:G:113:LYS:N	1:G:113:LYS:CD	2.78	0.47
1:G:181:LEU:HD23	1:G:181:LEU:HA	1.73	0.47
1:H:58:VAL:O	1:H:65:LEU:N	2.44	0.47
1:H:109:HIS:N	1:H:110:PRO:HD2	2.29	0.47
1:H:211:ILE:H	1:H:211:ILE:CD1	2.28	0.47
1:A:214:ARG:HD2	1:A:214:ARG:HA	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:LEU:HA	1:E:100:LEU:HD23	1.64	0.46
1:G:193:THR:HA	1:G:196:ARG:HH12	1.79	0.46
1:G:211:ILE:H	1:G:211:ILE:CD1	2.28	0.46
1:C:52:PHE:O	1:C:54:GLN:HG3	2.16	0.46
1:F:9:TYR:CD1	1:F:10:PRO:HD2	2.51	0.46
1:G:214:ARG:HG2	1:G:214:ARG:NH1	2.23	0.46
1:H:193:THR:HA	1:H:196:ARG:HH12	1.79	0.46
1:B:214:ARG:HD2	1:B:214:ARG:HA	1.60	0.46
1:C:178:PHE:HA	1:C:179:PRO:HD2	1.38	0.46
1:E:113:LYS:N	1:E:113:LYS:CD	2.78	0.46
1:G:178:PHE:HA	1:G:179:PRO:HD2	1.38	0.46
1:H:170:LYS:C	1:H:171:ILE:HG13	2.40	0.46
1:A:52:PHE:O	1:A:54:GLN:HG3	2.16	0.46
1:A:58:VAL:O	1:A:65:LEU:N	2.44	0.46
1:A:207:PRO:HA	1:A:208:PRO:HD3	1.52	0.46
1:A:211:ILE:H	1:A:211:ILE:CD1	2.28	0.46
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.74	0.46
1:D:9:TYR:CD1	1:D:10:PRO:HD2	2.51	0.46
1:H:113:LYS:CD	1:H:113:LYS:N	2.78	0.46
1:H:191:ILE:CG2	1:H:192:PRO:HD2	2.46	0.46
1:A:78:LYS:HD2	1:A:78:LYS:HA	1.43	0.46
1:B:52:PHE:O	1:B:54:GLN:HG3	2.16	0.46
1:B:117:GLN:O	1:B:121:VAL:HG23	2.16	0.46
1:C:9:TYR:CD1	1:C:10:PRO:HD2	2.51	0.46
1:C:193:THR:HA	1:C:196:ARG:HH12	1.79	0.46
1:E:60:ILE:CD1	1:E:74:TYR:HE2	2.21	0.46
1:E:113:LYS:HA	1:E:114:PRO:HD3	1.50	0.46
1:E:170:LYS:C	1:E:171:ILE:HG13	2.40	0.46
1:G:9:TYR:CD1	1:G:10:PRO:HD2	2.51	0.46
1:G:191:ILE:CG2	1:G:192:PRO:HD2	2.46	0.46
1:H:52:PHE:O	1:H:54:GLN:HG3	2.16	0.46
1:H:113:LYS:HA	1:H:114:PRO:HD3	1.50	0.46
1:C:113:LYS:CD	1:C:113:LYS:N	2.79	0.46
1:D:170:LYS:C	1:D:171:ILE:HG13	2.40	0.46
1:E:117:GLN:O	1:E:121:VAL:HG23	2.16	0.46
1:E:193:THR:HA	1:E:196:ARG:HH12	1.79	0.46
1:G:84:LYS:O	1:G:85:ASN:HB3	2.15	0.46
1:A:113:LYS:CD	1:A:113:LYS:N	2.78	0.46
1:D:191:ILE:HA	1:D:192:PRO:HD3	1.49	0.46
1:E:9:TYR:CD1	1:E:10:PRO:HD2	2.51	0.46
1:F:84:LYS:O	1:F:85:ASN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:LYS:H	1:G:113:LYS:HZ3	1.61	0.46
1:C:59:GLU:OE1	1:G:211:ILE:HD11	2.16	0.46
1:C:181:LEU:HD23	1:C:181:LEU:HA	1.74	0.46
1:E:191:ILE:CG2	1:E:192:PRO:HD2	2.46	0.46
1:F:113:LYS:CD	1:F:113:LYS:N	2.78	0.46
1:F:191:ILE:CG2	1:F:192:PRO:HD2	2.46	0.46
1:F:214:ARG:NH1	1:F:214:ARG:CG	2.78	0.46
1:H:44:LEU:HD12	1:H:44:LEU:HA	1.68	0.46
1:H:214:ARG:CG	1:H:214:ARG:NH1	2.78	0.46
1:B:193:THR:HA	1:B:196:ARG:HH12	1.79	0.46
1:C:214:ARG:HA	1:C:214:ARG:HD2	1.60	0.46
1:D:44:LEU:HD12	1:D:44:LEU:HA	1.68	0.46
1:D:52:PHE:O	1:D:54:GLN:HG3	2.16	0.46
1:F:214:ARG:HD2	1:F:214:ARG:HA	1.60	0.46
1:H:9:TYR:CD1	1:H:10:PRO:HD2	2.51	0.46
1:H:207:PRO:HA	1:H:208:PRO:HD3	1.52	0.46
1:B:113:LYS:N	1:B:113:LYS:CD	2.78	0.46
1:B:191:ILE:CG2	1:B:192:PRO:HD2	2.46	0.46
1:B:211:ILE:H	1:B:211:ILE:CD1	2.28	0.46
1:C:211:ILE:H	1:C:211:ILE:CD1	2.28	0.46
1:F:148:LEU:HD23	1:F:148:LEU:HA	1.79	0.46
1:G:207:PRO:HA	1:G:208:PRO:HD3	1.52	0.46
1:H:84:LYS:O	1:H:85:ASN:HB3	2.15	0.46
1:H:117:GLN:O	1:H:121:VAL:HG23	2.16	0.46
1:A:84:LYS:O	1:A:85:ASN:HB3	2.15	0.45
1:B:84:LYS:O	1:B:85:ASN:HB3	2.15	0.45
1:E:52:PHE:O	1:E:54:GLN:HG3	2.16	0.45
1:G:129:ILE:O	1:G:129:ILE:HG22	2.16	0.45
1:C:65:LEU:HD23	1:D:94:MET:HE1	1.98	0.45
1:E:211:ILE:H	1:E:211:ILE:CD1	2.28	0.45
1:F:78:LYS:HA	1:F:78:LYS:HD2	1.43	0.45
1:G:170:LYS:C	1:G:171:ILE:HG13	2.40	0.45
1:A:9:TYR:CD1	1:A:10:PRO:HD2	2.50	0.45
1:A:191:ILE:CG2	1:A:192:PRO:HD2	2.46	0.45
1:B:78:LYS:HD2	1:B:78:LYS:HA	1.43	0.45
1:B:213:VAL:CG1	1:B:217:TYR:CE2	3.00	0.45
1:C:106:LEU:HD11	1:C:167:LEU:HG	1.98	0.45
1:C:191:ILE:CG2	1:C:192:PRO:HD2	2.46	0.45
1:D:191:ILE:CG2	1:D:192:PRO:HD2	2.46	0.45
1:F:117:GLN:O	1:F:121:VAL:HG23	2.16	0.45
1:G:117:GLN:O	1:G:121:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:VAL:CG1	1:G:217:TYR:CE2	3.00	0.45
1:D:117:GLN:O	1:D:121:VAL:HG23	2.16	0.45
1:E:84:LYS:O	1:E:85:ASN:HB3	2.15	0.45
1:B:9:TYR:CD1	1:B:10:PRO:HD2	2.51	0.45
1:D:213:VAL:CG1	1:D:217:TYR:CE2	3.00	0.45
1:D:214:ARG:NH1	1:D:214:ARG:CG	2.78	0.45
1:G:103:LEU:O	1:G:106:LEU:HB2	2.17	0.45
1:G:106:LEU:HD11	1:G:167:LEU:HG	1.99	0.45
1:B:23:LEU:HA	1:B:23:LEU:HD23	1.72	0.45
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.79	0.45
1:F:7:LEU:N	1:F:7:LEU:CD1	2.80	0.45
1:F:211:ILE:H	1:F:211:ILE:CD1	2.28	0.45
1:G:109:HIS:ND1	1:G:170:LYS:NZ	2.65	0.45
1:A:7:LEU:N	1:A:7:LEU:CD1	2.80	0.45
1:A:129:ILE:HD12	1:A:129:ILE:HG23	1.66	0.45
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.74	0.45
1:D:9:TYR:HE1	1:D:56:PRO:HD3	1.82	0.45
1:D:193:THR:HA	1:D:196:ARG:HH12	1.79	0.45
1:E:219:ILE:HG22	1:E:219:ILE:O	2.17	0.45
1:F:52:PHE:O	1:F:54:GLN:HG3	2.16	0.45
1:F:58:VAL:O	1:F:65:LEU:N	2.44	0.45
1:F:103:LEU:O	1:F:106:LEU:HB2	2.17	0.45
1:F:106:LEU:HD11	1:F:167:LEU:HG	1.98	0.45
1:G:113:LYS:HA	1:G:114:PRO:HD3	1.50	0.45
1:H:106:LEU:HD11	1:H:167:LEU:HG	1.99	0.45
1:H:175:LEU:HA	1:H:175:LEU:HD23	1.74	0.45
1:A:117:GLN:O	1:A:121:VAL:HG23	2.16	0.45
1:B:58:VAL:O	1:B:65:LEU:N	2.44	0.45
1:B:114:PRO:HA	1:B:117:GLN:HG3	1.99	0.45
1:C:67:GLN:O	1:C:70:SER:HB2	2.17	0.45
1:C:103:LEU:O	1:C:106:LEU:HB2	2.17	0.45
1:E:103:LEU:O	1:E:106:LEU:HB2	2.17	0.45
1:E:214:ARG:CG	1:E:214:ARG:NH1	2.78	0.45
1:A:106:LEU:HD11	1:A:167:LEU:HG	1.99	0.45
1:C:9:TYR:HE1	1:C:56:PRO:HD3	1.82	0.45
1:C:117:GLN:O	1:C:121:VAL:HG23	2.16	0.45
1:D:43:LYS:HG3	1:D:43:LYS:H	1.41	0.45
1:E:129:ILE:O	1:E:129:ILE:HG22	2.16	0.45
1:E:191:ILE:HA	1:E:192:PRO:HD3	1.49	0.45
1:A:109:HIS:ND1	1:A:170:LYS:NZ	2.65	0.45
1:A:213:VAL:CG1	1:A:217:TYR:CE2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:VAL:CG1	1:C:217:TYR:CE2	3.00	0.45
1:H:67:GLN:O	1:H:70:SER:HB2	2.17	0.45
1:H:213:VAL:CG1	1:H:217:TYR:CE2	3.00	0.45
1:A:43:LYS:HG3	1:A:43:LYS:H	1.41	0.44
1:A:113:LYS:H	1:A:113:LYS:HZ3	1.65	0.44
1:A:214:ARG:CG	1:A:214:ARG:NH1	2.78	0.44
1:B:67:GLN:O	1:B:70:SER:HB2	2.17	0.44
1:B:109:HIS:ND1	1:B:170:LYS:NZ	2.65	0.44
1:B:213:VAL:HG12	1:B:217:TYR:CD2	2.52	0.44
1:B:219:ILE:O	1:B:219:ILE:HG22	2.17	0.44
1:D:67:GLN:O	1:D:70:SER:HB2	2.17	0.44
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.74	0.44
1:D:181:LEU:HD23	1:D:181:LEU:HA	1.74	0.44
1:D:213:VAL:HG12	1:D:217:TYR:CD2	2.53	0.44
1:E:213:VAL:CG1	1:E:217:TYR:CE2	3.00	0.44
1:G:9:TYR:HE1	1:G:56:PRO:HD3	1.82	0.44
1:H:7:LEU:N	1:H:7:LEU:CD1	2.80	0.44
1:A:60:ILE:CD1	1:A:74:TYR:HE2	2.21	0.44
1:A:114:PRO:HA	1:A:117:GLN:HG3	2.00	0.44
1:C:78:LYS:HD2	1:C:78:LYS:HA	1.43	0.44
1:C:86:LEU:HD12	1:C:86:LEU:HA	1.83	0.44
1:C:219:ILE:O	1:C:219:ILE:HG22	2.17	0.44
1:D:106:LEU:HD11	1:D:167:LEU:HG	1.99	0.44
1:H:103:LEU:O	1:H:106:LEU:HB2	2.17	0.44
1:H:114:PRO:HA	1:H:117:GLN:HG3	2.00	0.44
1:C:8:HIS:O	1:C:9:TYR:HB2	2.18	0.44
1:D:7:LEU:N	1:D:7:LEU:CD1	2.80	0.44
1:D:103:LEU:O	1:D:106:LEU:HB2	2.17	0.44
1:D:129:ILE:O	1:D:129:ILE:HG22	2.16	0.44
1:E:173:ASN:OD1	1:E:173:ASN:N	2.49	0.44
1:E:213:VAL:HG12	1:E:217:TYR:CD2	2.52	0.44
1:F:6:LYS:C	1:F:7:LEU:HD12	2.43	0.44
1:F:109:HIS:ND1	1:F:170:LYS:NZ	2.65	0.44
1:A:173:ASN:OD1	1:A:173:ASN:N	2.49	0.44
1:E:6:LYS:C	1:E:7:LEU:HD12	2.43	0.44
1:E:67:GLN:O	1:E:70:SER:HB2	2.17	0.44
1:E:106:LEU:HD11	1:E:167:LEU:HG	1.99	0.44
1:E:178:PHE:HA	1:E:179:PRO:HD2	1.38	0.44
1:F:67:GLN:O	1:F:70:SER:HB2	2.17	0.44
1:F:113:LYS:H	1:F:113:LYS:HZ3	1.62	0.44
1:F:213:VAL:CG1	1:F:217:TYR:CE2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:O	1:A:9:TYR:HB2	2.18	0.44
1:A:193:THR:HA	1:A:196:ARG:HH12	1.79	0.44
1:B:6:LYS:C	1:B:7:LEU:HD12	2.43	0.44
1:C:214:ARG:HG2	1:C:214:ARG:NH1	2.23	0.44
1:E:181:LEU:HD23	1:E:181:LEU:HA	1.73	0.44
1:E:214:ARG:HG2	1:E:214:ARG:NH1	2.23	0.44
1:F:191:ILE:O	1:F:194:ILE:HB	2.18	0.44
1:F:213:VAL:HG12	1:F:217:TYR:CD2	2.52	0.44
1:F:219:ILE:O	1:F:219:ILE:HG22	2.17	0.44
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.64	0.44
1:G:213:VAL:HG12	1:G:217:TYR:CD2	2.52	0.44
1:H:6:LYS:C	1:H:7:LEU:HD12	2.43	0.44
1:A:9:TYR:HE1	1:A:56:PRO:HD3	1.82	0.44
1:B:9:TYR:HE1	1:B:56:PRO:HD3	1.82	0.44
1:C:109:HIS:ND1	1:C:170:LYS:NZ	2.65	0.44
1:D:191:ILE:O	1:D:194:ILE:HB	2.18	0.44
1:E:7:LEU:N	1:E:7:LEU:CD1	2.80	0.44
1:G:191:ILE:O	1:G:194:ILE:HB	2.18	0.44
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.72	0.44
1:A:213:VAL:HG12	1:A:217:TYR:CD2	2.53	0.44
1:C:7:LEU:N	1:C:7:LEU:CD1	2.80	0.44
1:C:213:VAL:HG12	1:C:217:TYR:CD2	2.53	0.44
1:D:207:PRO:HA	1:D:208:PRO:HD3	1.52	0.44
1:E:44:LEU:HD12	1:E:44:LEU:HA	1.68	0.44
1:G:6:LYS:C	1:G:7:LEU:HD12	2.43	0.44
1:G:52:PHE:O	1:G:54:GLN:HG3	2.16	0.44
1:H:178:PHE:N	1:H:179:PRO:CD	2.78	0.44
1:A:67:GLN:O	1:A:70:SER:HB2	2.17	0.44
1:A:103:LEU:O	1:A:106:LEU:HB2	2.17	0.44
1:B:7:LEU:N	1:B:7:LEU:CD1	2.80	0.44
1:B:191:ILE:O	1:B:194:ILE:HB	2.18	0.44
1:D:6:LYS:C	1:D:7:LEU:HD12	2.43	0.44
1:D:109:HIS:ND1	1:D:170:LYS:NZ	2.65	0.44
1:E:175:LEU:HD23	1:E:175:LEU:HA	1.74	0.44
1:E:191:ILE:O	1:E:194:ILE:HB	2.18	0.44
1:F:143:HIS:ND1	1:F:145:GLN:N	2.53	0.44
1:H:181:LEU:HD23	1:H:181:LEU:HA	1.74	0.44
1:H:213:VAL:HG12	1:H:217:TYR:CD2	2.52	0.44
1:A:191:ILE:O	1:A:194:ILE:HB	2.18	0.44
1:C:6:LYS:C	1:C:7:LEU:HD12	2.43	0.44
1:C:188:LEU:O	1:C:191:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:LEU:O	1:D:191:ILE:HG13	2.18	0.44
1:G:114:PRO:HA	1:G:117:GLN:HG3	2.00	0.44
1:H:188:LEU:O	1:H:191:ILE:HG13	2.18	0.44
1:B:8:HIS:O	1:B:9:TYR:HB2	2.18	0.43
1:B:103:LEU:O	1:B:106:LEU:HB2	2.17	0.43
1:C:191:ILE:HA	1:C:192:PRO:HD3	1.49	0.43
1:D:178:PHE:HA	1:D:179:PRO:HD2	1.38	0.43
1:D:219:ILE:O	1:D:219:ILE:HG22	2.17	0.43
1:E:9:TYR:HE1	1:E:56:PRO:HD3	1.82	0.43
1:F:109:HIS:N	1:F:110:PRO:CD	2.81	0.43
1:F:173:ASN:OD1	1:F:173:ASN:N	2.49	0.43
1:G:67:GLN:O	1:G:70:SER:HB2	2.17	0.43
1:H:113:LYS:NZ	1:H:113:LYS:N	2.62	0.43
1:H:191:ILE:O	1:H:194:ILE:HB	2.18	0.43
1:B:43:LYS:HG3	1:B:43:LYS:H	1.41	0.43
1:B:191:ILE:HA	1:B:192:PRO:HD3	1.49	0.43
1:C:55:VAL:HA	1:C:56:PRO:C	2.43	0.43
1:C:58:VAL:O	1:C:65:LEU:N	2.44	0.43
1:D:106:LEU:HD23	1:D:106:LEU:HA	1.83	0.43
1:F:55:VAL:HA	1:F:56:PRO:C	2.43	0.43
1:G:219:ILE:O	1:G:219:ILE:HG22	2.17	0.43
1:D:112:LEU:CB	1:D:117:GLN:HG2	2.41	0.43
1:D:129:ILE:HD12	1:D:129:ILE:HG23	1.66	0.43
1:E:109:HIS:ND1	1:E:170:LYS:NZ	2.65	0.43
1:F:9:TYR:HE1	1:F:56:PRO:HD3	1.82	0.43
1:F:23:LEU:HD23	1:F:23:LEU:HA	1.72	0.43
1:F:87:LYS:HA	1:F:87:LYS:HD3	1.61	0.43
1:G:7:LEU:N	1:G:7:LEU:CD1	2.80	0.43
1:G:18:SER:HB3	1:G:162:GLN:NE2	2.34	0.43
1:G:188:LEU:O	1:G:191:ILE:HG13	2.18	0.43
1:H:9:TYR:HE1	1:H:56:PRO:HD3	1.82	0.43
1:B:18:SER:HB3	1:B:162:GLN:NE2	2.34	0.43
1:B:42:TYR:HA	1:B:45:GLN:HG3	2.01	0.43
1:D:8:HIS:O	1:D:9:TYR:HB2	2.18	0.43
1:E:55:VAL:HA	1:E:56:PRO:C	2.43	0.43
1:E:94:MET:HE3	1:F:65:LEU:CB	2.47	0.43
1:F:18:SER:HB3	1:F:162:GLN:NE2	2.34	0.43
1:G:55:VAL:HA	1:G:56:PRO:C	2.43	0.43
1:G:175:LEU:HD23	1:G:175:LEU:HA	1.74	0.43
1:H:191:ILE:HA	1:H:192:PRO:HD3	1.49	0.43
1:H:219:ILE:O	1:H:219:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:HB3	1:A:162:GLN:NE2	2.33	0.43
1:A:148:LEU:HA	1:A:148:LEU:HD23	1.79	0.43
1:A:219:ILE:O	1:A:219:ILE:HG22	2.17	0.43
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.64	0.43
1:B:106:LEU:HD11	1:B:167:LEU:HG	1.98	0.43
1:B:178:PHE:N	1:B:179:PRO:CD	2.78	0.43
1:B:207:PRO:HA	1:B:208:PRO:HD3	1.52	0.43
1:C:109:HIS:N	1:C:110:PRO:CD	2.81	0.43
1:E:148:LEU:HD23	1:E:148:LEU:HA	1.79	0.43
1:G:178:PHE:N	1:G:179:PRO:CD	2.78	0.43
1:A:109:HIS:N	1:A:110:PRO:CD	2.81	0.43
1:B:55:VAL:HA	1:B:56:PRO:C	2.43	0.43
1:C:114:PRO:HA	1:C:117:GLN:HG3	2.00	0.43
1:F:188:LEU:O	1:F:191:ILE:HG13	2.18	0.43
1:A:6:LYS:C	1:A:7:LEU:HD12	2.43	0.43
1:C:37:THR:HG22	1:C:38:LYS:N	2.34	0.43
1:C:87:LYS:HD3	1:C:87:LYS:HA	1.61	0.43
1:C:97:GLU:HB3	1:D:67:GLN:OE1	2.19	0.43
1:C:129:ILE:HG23	1:C:129:ILE:HD12	1.66	0.43
1:D:92:ILE:HD13	1:D:154:SER:CB	2.49	0.43
1:E:8:HIS:O	1:E:9:TYR:HB2	2.18	0.43
1:E:37:THR:HG22	1:E:38:LYS:N	2.34	0.43
1:E:42:TYR:HA	1:E:45:GLN:HG3	2.01	0.43
1:E:113:LYS:NZ	1:E:113:LYS:N	2.62	0.43
1:F:8:HIS:O	1:F:9:TYR:HB2	2.18	0.43
1:F:9:TYR:O	1:F:34:PHE:HA	2.19	0.43
1:G:9:TYR:O	1:G:34:PHE:HA	2.19	0.43
1:G:37:THR:HG22	1:G:38:LYS:N	2.34	0.43
1:H:109:HIS:ND1	1:H:170:LYS:NZ	2.65	0.43
1:H:178:PHE:HA	1:H:179:PRO:HD2	1.38	0.43
1:A:92:ILE:HD13	1:A:154:SER:CB	2.49	0.43
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.73	0.43
1:C:94:MET:CE	1:D:65:LEU:C	2.91	0.43
1:D:9:TYR:O	1:D:34:PHE:HA	2.19	0.43
1:D:114:PRO:HA	1:D:117:GLN:HG3	1.99	0.43
1:E:106:LEU:HD23	1:E:106:LEU:HA	1.82	0.43
1:F:113:LYS:HA	1:F:114:PRO:HD3	1.50	0.43
1:H:9:TYR:O	1:H:34:PHE:HA	2.19	0.43
1:H:42:TYR:HA	1:H:45:GLN:HG3	2.01	0.43
1:H:55:VAL:HA	1:H:56:PRO:C	2.43	0.43
1:H:198:LEU:HA	1:H:198:LEU:HD23	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:O	1:A:34:PHE:HA	2.19	0.43
1:B:9:TYR:O	1:B:34:PHE:HA	2.19	0.43
1:C:18:SER:HB3	1:C:162:GLN:NE2	2.34	0.43
1:C:44:LEU:HD12	1:C:44:LEU:HA	1.68	0.43
1:D:100:LEU:HD23	1:D:100:LEU:HA	1.64	0.43
1:E:114:PRO:HA	1:E:117:GLN:HG3	2.00	0.43
1:E:198:LEU:HA	1:E:198:LEU:HD23	1.85	0.43
1:F:159:ILE:HD12	1:F:159:ILE:HG23	1.81	0.43
1:G:8:HIS:O	1:G:9:TYR:HB2	2.18	0.43
1:G:173:ASN:OD1	1:G:173:ASN:N	2.49	0.43
1:H:18:SER:HB3	1:H:162:GLN:NE2	2.34	0.43
1:B:92:ILE:HD13	1:B:154:SER:CB	2.49	0.42
1:B:129:ILE:HD12	1:B:129:ILE:HG23	1.66	0.42
1:F:129:ILE:O	1:F:129:ILE:HG22	2.16	0.42
1:H:100:LEU:HD23	1:H:100:LEU:HA	1.64	0.42
1:C:191:ILE:O	1:C:194:ILE:HB	2.18	0.42
1:D:109:HIS:N	1:D:110:PRO:CD	2.81	0.42
1:D:143:HIS:ND1	1:D:145:GLN:HG3	2.34	0.42
1:E:214:ARG:HA	1:E:214:ARG:HD2	1.60	0.42
1:F:114:PRO:HA	1:F:117:GLN:HG3	2.00	0.42
1:A:37:THR:HG22	1:A:38:LYS:N	2.34	0.42
1:A:42:TYR:HA	1:A:45:GLN:HG3	2.01	0.42
1:A:92:ILE:CD1	1:A:154:SER:HB2	2.50	0.42
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.64	0.42
1:A:188:LEU:O	1:A:191:ILE:HG13	2.18	0.42
1:C:9:TYR:O	1:C:34:PHE:HA	2.19	0.42
1:C:143:HIS:ND1	1:C:145:GLN:HG3	2.34	0.42
1:E:78:LYS:HD2	1:E:78:LYS:HA	1.43	0.42
1:E:188:LEU:O	1:E:191:ILE:HG13	2.18	0.42
1:G:109:HIS:N	1:G:110:PRO:CD	2.81	0.42
1:G:191:ILE:HA	1:G:192:PRO:HD3	1.49	0.42
1:H:109:HIS:N	1:H:110:PRO:CD	2.81	0.42
1:H:129:ILE:O	1:H:129:ILE:HG22	2.16	0.42
1:A:55:VAL:HA	1:A:56:PRO:C	2.43	0.42
1:B:92:ILE:CD1	1:B:154:SER:HB2	2.50	0.42
1:B:143:HIS:ND1	1:B:145:GLN:HG3	2.34	0.42
1:B:178:PHE:HA	1:B:179:PRO:HD2	1.38	0.42
1:B:188:LEU:O	1:B:191:ILE:HG13	2.18	0.42
1:D:214:ARG:HA	1:D:214:ARG:HD2	1.60	0.42
1:A:113:LYS:HB2	1:A:113:LYS:HE2	1.91	0.42
1:A:143:HIS:ND1	1:A:145:GLN:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HG22	1:B:38:LYS:N	2.34	0.42
1:D:42:TYR:HA	1:D:45:GLN:HG3	2.01	0.42
1:E:43:LYS:HG3	1:E:43:LYS:H	1.41	0.42
1:F:42:TYR:HA	1:F:45:GLN:HG3	2.01	0.42
1:G:198:LEU:HA	1:G:198:LEU:HD23	1.85	0.42
1:B:109:HIS:N	1:B:110:PRO:CD	2.81	0.42
1:D:37:THR:HG22	1:D:38:LYS:N	2.34	0.42
1:D:55:VAL:HA	1:D:56:PRO:C	2.43	0.42
1:G:143:HIS:ND1	1:G:145:GLN:HG3	2.34	0.42
1:D:18:SER:HB3	1:D:162:GLN:NE2	2.34	0.42
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.79	0.42
1:E:143:HIS:ND1	1:E:145:GLN:HG3	2.34	0.42
1:F:86:LEU:HA	1:F:86:LEU:HD12	1.83	0.42
1:F:113:LYS:HB2	1:F:113:LYS:HE2	1.91	0.42
1:F:146:SER:HB3	1:F:187:LYS:NZ	2.35	0.42
1:H:8:HIS:O	1:H:9:TYR:HB2	2.18	0.42
1:H:37:THR:HG22	1:H:38:LYS:N	2.34	0.42
1:C:92:ILE:CD1	1:C:154:SER:HB2	2.50	0.42
1:C:170:LYS:C	1:C:172:PRO:HD3	2.45	0.42
1:E:18:SER:HB3	1:E:162:GLN:NE2	2.34	0.42
1:F:95:TYR:N	1:F:95:TYR:CD1	2.87	0.42
1:G:148:LEU:HD23	1:G:148:LEU:HA	1.79	0.42
1:H:106:LEU:HD23	1:H:106:LEU:HA	1.83	0.42
1:A:25:ALA:C	1:A:27:GLY:H	2.28	0.42
1:B:25:ALA:C	1:B:27:GLY:H	2.28	0.42
1:B:159:ILE:HD12	1:B:159:ILE:HG23	1.81	0.42
1:C:12:GLY:HA3	1:C:212:TYR:CE1	2.55	0.42
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.61	0.42
1:B:146:SER:HB3	1:B:187:LYS:NZ	2.35	0.42
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.83	0.42
1:C:207:PRO:HA	1:C:208:PRO:HD3	1.52	0.42
1:D:81:LEU:HA	1:D:81:LEU:HD23	1.83	0.42
1:D:173:ASN:OD1	1:D:173:ASN:N	2.49	0.42
1:G:92:ILE:CD1	1:G:154:SER:HB2	2.50	0.42
1:G:146:SER:HB3	1:G:187:LYS:NZ	2.35	0.42
1:G:214:ARG:HD2	1:G:214:ARG:HA	1.60	0.42
1:H:92:ILE:HD13	1:H:154:SER:CB	2.49	0.42
1:H:146:SER:HB3	1:H:187:LYS:NZ	2.35	0.42
1:H:173:ASN:OD1	1:H:173:ASN:N	2.49	0.42
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.83	0.41
1:C:42:TYR:HA	1:C:45:GLN:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:HIS:N	1:E:110:PRO:CD	2.81	0.41
1:F:37:THR:HG22	1:F:38:LYS:N	2.34	0.41
1:F:129:ILE:HG23	1:F:129:ILE:HD12	1.66	0.41
1:F:143:HIS:ND1	1:F:145:GLN:HG3	2.34	0.41
1:H:95:TYR:N	1:H:95:TYR:CD1	2.87	0.41
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.83	0.41
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.83	0.41
1:C:43:LYS:HG3	1:C:43:LYS:H	1.41	0.41
1:D:12:GLY:HA3	1:D:212:TYR:CE1	2.55	0.41
1:D:66:VAL:O	1:D:67:GLN:HB2	2.20	0.41
1:E:9:TYR:O	1:E:34:PHE:HA	2.19	0.41
1:E:12:GLY:HA3	1:E:212:TYR:CE1	2.55	0.41
1:E:60:ILE:CD1	1:E:74:TYR:CE2	3.00	0.41
1:E:146:SER:HB3	1:E:187:LYS:NZ	2.35	0.41
1:G:95:TYR:N	1:G:95:TYR:CD1	2.87	0.41
1:H:66:VAL:O	1:H:67:GLN:HB2	2.20	0.41
1:A:146:SER:HB3	1:A:187:LYS:NZ	2.35	0.41
1:C:25:ALA:C	1:C:27:GLY:H	2.28	0.41
1:E:113:LYS:C	1:E:115:ASP:N	2.78	0.41
1:F:92:ILE:HD13	1:F:154:SER:CB	2.49	0.41
1:A:170:LYS:C	1:A:172:PRO:HD3	2.45	0.41
1:A:218:ASN:HD22	1:A:218:ASN:HA	1.65	0.41
1:C:129:ILE:O	1:C:129:ILE:HG22	2.16	0.41
1:C:133:PHE:N	1:C:133:PHE:CD1	2.88	0.41
1:C:146:SER:HB3	1:C:187:LYS:NZ	2.35	0.41
1:D:211:ILE:N	1:D:211:ILE:CD1	2.84	0.41
1:D:218:ASN:HD22	1:D:218:ASN:HA	1.65	0.41
1:E:92:ILE:HD13	1:E:154:SER:CB	2.49	0.41
1:E:170:LYS:C	1:E:172:PRO:HD3	2.45	0.41
1:F:66:VAL:O	1:F:67:GLN:HB2	2.20	0.41
1:F:113:LYS:C	1:F:115:ASP:N	2.78	0.41
1:G:112:LEU:CB	1:G:117:GLN:HG2	2.41	0.41
1:B:113:LYS:NZ	1:B:113:LYS:N	2.62	0.41
1:C:92:ILE:HD13	1:C:154:SER:CB	2.49	0.41
1:D:146:SER:HB3	1:D:187:LYS:NZ	2.35	0.41
1:G:42:TYR:HA	1:G:45:GLN:HG3	2.01	0.41
1:G:66:VAL:O	1:G:67:GLN:HB2	2.20	0.41
1:H:25:ALA:C	1:H:27:GLY:H	2.28	0.41
1:H:87:LYS:HD3	1:H:87:LYS:HA	1.61	0.41
1:A:159:ILE:HG23	1:A:159:ILE:HD12	1.81	0.41
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HB2	1:B:113:LYS:HE2	1.91	0.41
1:B:161:LEU:O	1:B:165:LEU:HG	2.21	0.41
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.72	0.41
1:C:106:LEU:HD23	1:C:106:LEU:HA	1.83	0.41
1:C:113:LYS:C	1:C:115:ASP:N	2.78	0.41
1:E:206:PRO:CB	1:E:207:PRO:CD	2.99	0.41
1:F:12:GLY:HA3	1:F:212:TYR:CE1	2.55	0.41
1:F:92:ILE:CD1	1:F:154:SER:HB2	2.50	0.41
1:G:87:LYS:HD3	1:G:87:LYS:HA	1.61	0.41
1:G:113:LYS:HB2	1:G:113:LYS:HE2	1.91	0.41
1:H:12:GLY:HA3	1:H:212:TYR:CE1	2.55	0.41
1:B:66:VAL:O	1:B:67:GLN:HB2	2.20	0.41
1:B:113:LYS:C	1:B:115:ASP:N	2.78	0.41
1:D:198:LEU:HD23	1:D:198:LEU:HA	1.85	0.41
1:E:211:ILE:N	1:E:211:ILE:CD1	2.84	0.41
1:G:81:LEU:HD23	1:G:81:LEU:HA	1.83	0.41
1:H:92:ILE:CD1	1:H:154:SER:HB2	2.50	0.41
1:H:143:HIS:ND1	1:H:145:GLN:HG3	2.34	0.41
1:H:170:LYS:C	1:H:172:PRO:HD3	2.45	0.41
1:B:113:LYS:HA	1:B:114:PRO:HD3	1.50	0.41
1:C:66:VAL:O	1:C:67:GLN:HB2	2.21	0.41
1:D:25:ALA:C	1:D:27:GLY:H	2.28	0.41
1:F:45:GLN:HE21	1:F:45:GLN:HB3	1.64	0.41
1:F:170:LYS:C	1:F:172:PRO:HD3	2.45	0.41
1:G:92:ILE:HD13	1:G:154:SER:CB	2.49	0.41
1:G:211:ILE:N	1:G:211:ILE:CD1	2.84	0.41
1:H:206:PRO:CB	1:H:207:PRO:CD	2.99	0.41
1:H:211:ILE:N	1:H:211:ILE:CD1	2.84	0.41
1:A:45:GLN:HE21	1:A:45:GLN:HB3	1.64	0.41
1:A:211:ILE:N	1:A:211:ILE:CD1	2.84	0.41
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.85	0.41
1:C:161:LEU:O	1:C:165:LEU:HG	2.21	0.41
1:D:60:ILE:CD1	1:D:74:TYR:CE2	2.99	0.41
1:D:86:LEU:HD12	1:D:86:LEU:HA	1.83	0.41
1:D:170:LYS:C	1:D:172:PRO:HD3	2.45	0.41
1:D:188:LEU:C	1:D:190:ASN:N	2.79	0.41
1:E:66:VAL:O	1:E:67:GLN:HB2	2.20	0.41
1:F:25:ALA:C	1:F:27:GLY:H	2.28	0.41
1:G:113:LYS:H	1:G:113:LYS:CD	2.34	0.41
1:G:161:LEU:O	1:G:165:LEU:HG	2.21	0.41
1:G:170:LYS:C	1:G:172:PRO:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:PHE:N	1:H:133:PHE:CD1	2.88	0.41
1:A:66:VAL:O	1:A:67:GLN:HB2	2.20	0.41
1:A:113:LYS:NZ	1:A:113:LYS:N	2.62	0.41
1:A:113:LYS:H	1:A:113:LYS:CD	2.34	0.41
1:A:113:LYS:C	1:A:115:ASP:N	2.79	0.41
1:A:178:PHE:HA	1:A:179:PRO:HD2	1.38	0.41
1:A:206:PRO:CB	1:A:207:PRO:CD	2.99	0.41
1:B:170:LYS:C	1:B:172:PRO:HD3	2.45	0.41
1:C:112:LEU:CA	1:C:113:LYS:HZ2	2.26	0.41
1:C:173:ASN:OD1	1:C:173:ASN:N	2.49	0.41
1:E:57:MET:HA	1:E:65:LEU:O	2.21	0.41
1:G:12:GLY:HA3	1:G:212:TYR:CE1	2.55	0.41
1:G:55:VAL:HB	1:G:56:PRO:HA	2.03	0.41
1:H:81:LEU:HD23	1:H:81:LEU:HA	1.83	0.41
1:H:161:LEU:O	1:H:165:LEU:HG	2.21	0.41
1:A:12:GLY:HA3	1:A:212:TYR:CE1	2.55	0.40
1:B:129:ILE:HA	1:B:129:ILE:HD13	1.84	0.40
1:F:57:MET:HA	1:F:65:LEU:O	2.21	0.40
1:F:161:LEU:O	1:F:165:LEU:HG	2.21	0.40
1:A:129:ILE:O	1:A:129:ILE:HG22	2.16	0.40
1:B:12:GLY:HA3	1:B:212:TYR:CE1	2.55	0.40
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.79	0.40
1:C:65:LEU:CB	1:D:94:MET:CE	3.00	0.40
1:E:95:TYR:N	1:E:95:TYR:CD1	2.87	0.40
1:F:45:GLN:HG2	1:F:45:GLN:H	1.60	0.40
1:F:171:ILE:N	1:F:172:PRO:HD3	2.35	0.40
1:H:23:LEU:HD23	1:H:23:LEU:HA	1.72	0.40
1:H:57:MET:HA	1:H:65:LEU:O	2.21	0.40
1:B:55:VAL:HB	1:B:56:PRO:HA	2.03	0.40
1:B:60:ILE:CD1	1:B:74:TYR:CE2	2.99	0.40
1:B:206:PRO:CB	1:B:207:PRO:CD	2.99	0.40
1:C:113:LYS:HA	1:C:114:PRO:HD3	1.50	0.40
1:C:129:ILE:HD13	1:C:129:ILE:HA	1.84	0.40
1:D:87:LYS:HA	1:D:87:LYS:HD3	1.61	0.40
1:D:92:ILE:CD1	1:D:154:SER:HB2	2.50	0.40
1:E:25:ALA:C	1:E:27:GLY:H	2.28	0.40
1:E:92:ILE:CD1	1:E:154:SER:HB2	2.50	0.40
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.74	0.40
1:G:60:ILE:CD1	1:G:74:TYR:CE2	2.99	0.40
1:H:43:LYS:HG3	1:H:43:LYS:H	1.41	0.40
1:B:113:LYS:H	1:B:113:LYS:CD	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:CA	1:C:113:LYS:NZ	2.84	0.40
1:D:113:LYS:C	1:D:115:ASP:N	2.79	0.40
1:E:81:LEU:HD23	1:E:81:LEU:HA	1.83	0.40
1:E:113:LYS:HB2	1:E:113:LYS:HE2	1.91	0.40
1:E:161:LEU:O	1:E:165:LEU:HG	2.21	0.40
1:G:25:ALA:C	1:G:27:GLY:H	2.28	0.40
1:G:113:LYS:C	1:G:115:ASP:N	2.78	0.40
1:H:133:PHE:CB	1:H:134:PRO:HD3	2.51	0.40
1:A:52:PHE:O	1:A:53:GLN:HB2	2.22	0.40
1:B:52:PHE:O	1:B:53:GLN:HB2	2.22	0.40
1:B:57:MET:HA	1:B:65:LEU:O	2.21	0.40
1:B:133:PHE:CB	1:B:134:PRO:HD3	2.51	0.40
1:B:188:LEU:C	1:B:190:ASN:N	2.79	0.40
1:E:55:VAL:HB	1:E:56:PRO:HA	2.03	0.40
1:F:178:PHE:HA	1:F:179:PRO:HD2	1.38	0.40

All (5) 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:196:ARG:NH2	1:H:200:PRO:CG[4_455]	1.34	0.86
1:D:196:ARG:NH2	1:H:200:PRO:CB[4_455]	1.74	0.46
1:D:196:ARG:CZ	1:H:200:PRO:CB[4_455]	2.12	0.08
1:B:118:GLN:CG	1:C:118:GLN:CG[1_554]	2.16	0.04
1:D:196:ARG:CZ	1:H:200:PRO:CG[4_455]	2.18	0.02

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	215/222 (97%)	200 (93%)	13 (6%)	2 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	215/222 (97%)	201 (94%)	12 (6%)	2 (1%)	14	48
1	C	215/222 (97%)	200 (93%)	13 (6%)	2 (1%)	14	48
1	D	215/222 (97%)	201 (94%)	12 (6%)	2 (1%)	14	48
1	E	215/222 (97%)	200 (93%)	13 (6%)	2 (1%)	14	48
1	F	215/222 (97%)	201 (94%)	12 (6%)	2 (1%)	14	48
1	G	215/222 (97%)	200 (93%)	13 (6%)	2 (1%)	14	48
1	H	215/222 (97%)	201 (94%)	12 (6%)	2 (1%)	14	48
All	All	1720/1776 (97%)	1604 (93%)	100 (6%)	16 (1%)	14	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	B	114	PRO
1	C	114	PRO
1	D	114	PRO
1	E	114	PRO
1	F	114	PRO
1	G	114	PRO
1	H	114	PRO
1	A	176	SER
1	B	176	SER
1	C	176	SER
1	D	176	SER
1	E	176	SER
1	F	176	SER
1	G	176	SER
1	H	176	SER

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	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	B	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	C	197/200 (98%)	171 (87%)	26 (13%)	4	18
1	D	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	E	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	F	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	G	197/200 (98%)	170 (86%)	27 (14%)	3	17
1	H	197/200 (98%)	170 (86%)	27 (14%)	3	17
All	All	1576/1600 (98%)	1361 (86%)	215 (14%)	3	17

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	33	GLU
1	A	36	GLU
1	A	39	GLU
1	A	40	GLN
1	A	45	GLN
1	A	54	GLN
1	A	60	ILE
1	A	68	THR
1	A	69	ARG
1	A	82	PHE
1	A	92	ILE
1	A	107	ILE
1	A	112	LEU
1	A	113	LYS
1	A	115	ASP
1	A	119	LYS
1	A	127	LYS
1	A	141	ARG
1	A	145	GLN
1	A	146	SER
1	A	152	GLN
1	A	174	ILE
1	A	187	LYS
1	A	189	SER
1	A	214	ARG
1	A	219	ILE

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Mol	Chain	Res	Type
1	B	18	SER
1	B	33	GLU
1	B	36	GLU
1	B	39	GLU
1	B	40	GLN
1	B	45	GLN
1	B	54	GLN
1	B	60	ILE
1	B	68	THR
1	B	69	ARG
1	B	82	PHE
1	B	92	ILE
1	B	107	ILE
1	B	112	LEU
1	B	113	LYS
1	B	115	ASP
1	B	119	LYS
1	B	127	LYS
1	B	141	ARG
1	B	145	GLN
1	B	146	SER
1	B	152	GLN
1	B	174	ILE
1	B	187	LYS
1	B	189	SER
1	B	214	ARG
1	B	219	ILE
1	C	18	SER
1	C	33	GLU
1	C	36	GLU
1	C	39	GLU
1	C	40	GLN
1	C	45	GLN
1	C	54	GLN
1	C	60	ILE
1	C	68	THR
1	C	69	ARG
1	C	92	ILE
1	C	107	ILE
1	C	112	LEU
1	C	113	LYS
1	C	115	ASP

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Mol	Chain	Res	Type
1	C	119	LYS
1	C	127	LYS
1	C	141	ARG
1	C	145	GLN
1	C	146	SER
1	C	152	GLN
1	C	174	ILE
1	C	187	LYS
1	C	189	SER
1	C	214	ARG
1	C	219	ILE
1	D	18	SER
1	D	33	GLU
1	D	36	GLU
1	D	39	GLU
1	D	40	GLN
1	D	45	GLN
1	D	54	GLN
1	D	60	ILE
1	D	68	THR
1	D	69	ARG
1	D	82	PHE
1	D	92	ILE
1	D	107	ILE
1	D	112	LEU
1	D	113	LYS
1	D	115	ASP
1	D	119	LYS
1	D	127	LYS
1	D	141	ARG
1	D	145	GLN
1	D	146	SER
1	D	152	GLN
1	D	174	ILE
1	D	187	LYS
1	D	189	SER
1	D	214	ARG
1	D	219	ILE
1	E	18	SER
1	E	33	GLU
1	E	36	GLU
1	E	39	GLU

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Mol	Chain	Res	Type
1	E	40	GLN
1	E	45	GLN
1	E	54	GLN
1	E	60	ILE
1	E	68	THR
1	E	69	ARG
1	E	82	PHE
1	E	92	ILE
1	E	107	ILE
1	E	112	LEU
1	E	113	LYS
1	E	115	ASP
1	E	119	LYS
1	E	127	LYS
1	E	141	ARG
1	E	145	GLN
1	E	146	SER
1	E	152	GLN
1	E	174	ILE
1	E	187	LYS
1	E	189	SER
1	E	214	ARG
1	E	219	ILE
1	F	18	SER
1	F	33	GLU
1	F	36	GLU
1	F	39	GLU
1	F	40	GLN
1	F	45	GLN
1	F	54	GLN
1	F	60	ILE
1	F	68	THR
1	F	69	ARG
1	F	82	PHE
1	F	92	ILE
1	F	107	ILE
1	F	112	LEU
1	F	113	LYS
1	F	115	ASP
1	F	119	LYS
1	F	127	LYS
1	F	141	ARG

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Mol	Chain	Res	Type
1	F	145	GLN
1	F	146	SER
1	F	152	GLN
1	F	174	ILE
1	F	187	LYS
1	F	189	SER
1	F	214	ARG
1	F	219	ILE
1	G	18	SER
1	G	33	GLU
1	G	36	GLU
1	G	39	GLU
1	G	40	GLN
1	G	45	GLN
1	G	54	GLN
1	G	60	ILE
1	G	68	THR
1	G	69	ARG
1	G	82	PHE
1	G	92	ILE
1	G	107	ILE
1	G	112	LEU
1	G	113	LYS
1	G	115	ASP
1	G	119	LYS
1	G	127	LYS
1	G	141	ARG
1	G	145	GLN
1	G	146	SER
1	G	152	GLN
1	G	174	ILE
1	G	187	LYS
1	G	189	SER
1	G	214	ARG
1	G	219	ILE
1	H	18	SER
1	H	33	GLU
1	H	36	GLU
1	H	39	GLU
1	H	40	GLN
1	H	45	GLN
1	H	54	GLN

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Mol	Chain	Res	Type
1	H	60	ILE
1	H	68	THR
1	H	69	ARG
1	H	82	PHE
1	H	92	ILE
1	H	107	ILE
1	H	112	LEU
1	H	113	LYS
1	H	115	ASP
1	H	119	LYS
1	H	127	LYS
1	H	141	ARG
1	H	145	GLN
1	H	146	SER
1	H	152	GLN
1	H	174	ILE
1	H	187	LYS
1	H	189	SER
1	H	214	ARG
1	H	219	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	54	GLN
1	A	80	ASN
1	A	126	GLN
1	A	162	GLN
1	A	182	GLN
1	A	218	ASN
1	B	54	GLN
1	B	80	ASN
1	B	126	GLN
1	B	162	GLN
1	B	182	GLN
1	B	218	ASN
1	C	45	GLN
1	C	54	GLN
1	C	80	ASN
1	C	162	GLN
1	C	182	GLN

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Mol	Chain	Res	Type
1	C	218	ASN
1	D	45	GLN
1	D	54	GLN
1	D	80	ASN
1	D	126	GLN
1	D	162	GLN
1	D	182	GLN
1	D	218	ASN
1	E	54	GLN
1	E	80	ASN
1	E	126	GLN
1	E	162	GLN
1	E	218	ASN
1	F	45	GLN
1	F	54	GLN
1	F	80	ASN
1	F	118	GLN
1	F	162	GLN
1	F	218	ASN
1	G	54	GLN
1	G	80	ASN
1	G	162	GLN
1	G	218	ASN
1	H	45	GLN
1	H	54	GLN
1	H	80	ASN
1	H	162	GLN
1	H	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/222 (97%)	-1.43	0 100 100	1, 14, 74, 131	0
1	B	217/222 (97%)	-1.45	0 100 100	1, 14, 74, 131	0
1	C	217/222 (97%)	-1.36	0 100 100	1, 14, 74, 131	0
1	D	217/222 (97%)	-1.35	0 100 100	1, 14, 74, 131	0
1	E	217/222 (97%)	-1.45	0 100 100	1, 14, 74, 131	0
1	F	217/222 (97%)	-1.43	0 100 100	1, 14, 74, 131	0
1	G	217/222 (97%)	-1.43	0 100 100	1, 14, 74, 131	0
1	H	217/222 (97%)	-1.41	0 100 100	1, 14, 74, 131	0
All	All	1736/1776 (97%)	-1.41	0 100 100	1, 14, 74, 131	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.