



Full wwPDB EM Validation Report ⓘ

Oct 1, 2022 – 07:22 am BST

PDB ID : 8AT3
EMDB ID : EMD-15632
Title : Structure of the augmin holocomplex in open conformation
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2022-08-22
Resolution : 33.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

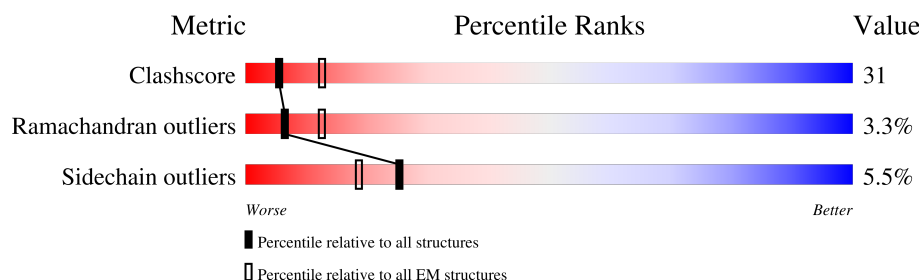
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 33.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	<div> <div>31%</div> <div>59%</div> <div>28%</div> <div>8%</div> <div>5%</div> </div>
2	B	597	<div> <div>27%</div> <div>57%</div> <div>27%</div> <div>9%</div> <div>7%</div> </div>
3	C	353	<div> <div>26%</div> <div>60%</div> <div>33%</div> <div>5%</div> <div>.</div> </div>
4	D	666	<div> <div>30%</div> <div>56%</div> <div>32%</div> <div>6%</div> <div>5%</div> </div>
5	E	222	<div> <div>19%</div> <div>48%</div> <div>37%</div> <div>9%</div> <div>.</div> </div>
6	F	978	<div> <div>5%</div> <div>22%</div> <div>13%</div> <div>.</div> <div>60%</div> </div>
7	G	348	<div> <div>17%</div> <div>47%</div> <div>36%</div> <div>9%</div> <div>5%</div> <div>.</div> </div>
8	H	367	<div> <div>33%</div> <div>18%</div> <div>.</div> <div>45%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24599 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 HAUS augmin-like complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	286	Total	C	N	O	S	0	0
			2282	1436	380	453	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ARG	GLN	variant	UNP Q3B8L5

- Molecule 2 is a protein called HAUS augmin-like complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	597	Total	C	N	O	S	0	0
			4771	2988	817	943	23		

- Molecule 3 is a protein called HAUS augmin like complex subunit 4 L homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	353	Total	C	N	O	S	0	0
			2885	1807	508	554	16		

- Molecule 4 is a protein called HAUS augmin-like complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	666	Total	C	N	O	S	0	0
			5415	3362	1000	1022	31		

- Molecule 5 is a protein called HAUS augmin like complex subunit 2 L homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	217	Total	C	N	O	S	0	0
			1717	1075	296	334	12		

- Molecule 6 is a protein called HAUS augmin like complex subunit 6 L homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	387	Total	C	N	O	S	0	0
			3171	2020	574	558	19		

- Molecule 7 is a protein called HAUS augmin like complex subunit 7 S homeolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	339	Total	C	N	O	S	0	0
			2687	1694	441	533	19		

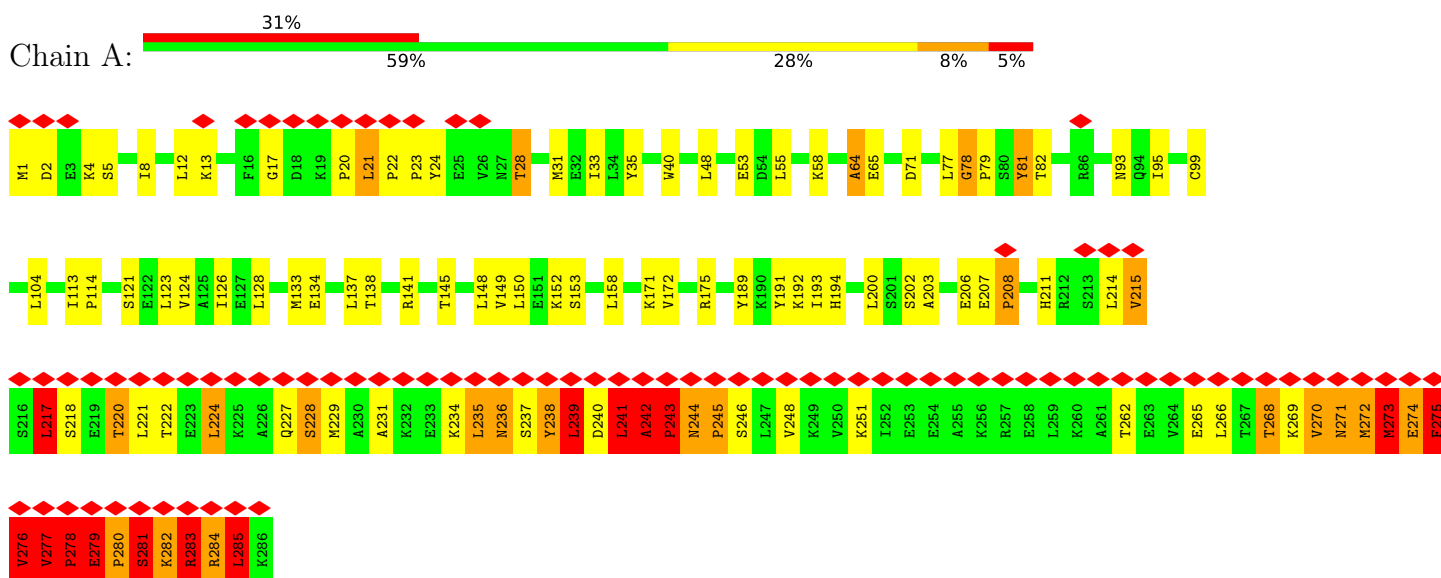
- Molecule 8 is a protein called HAUS augmin-like complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	203	Total	C	N	O	S	0	0
			1671	1048	285	331	7		

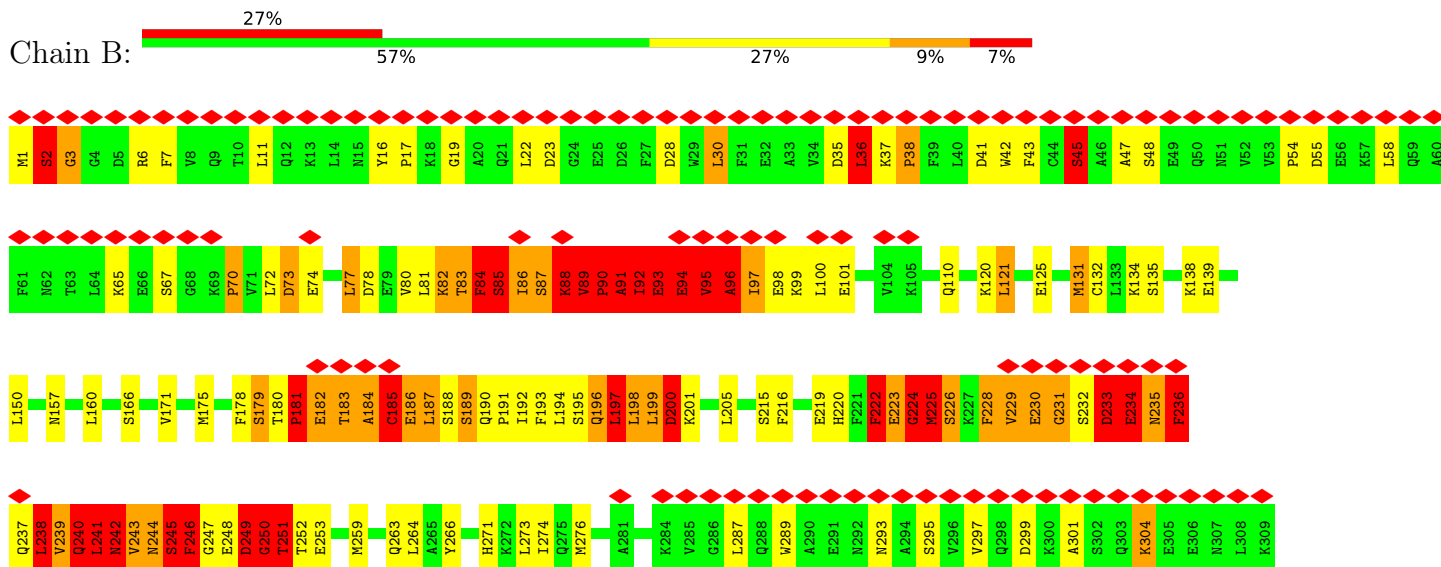
3 Residue-property plots

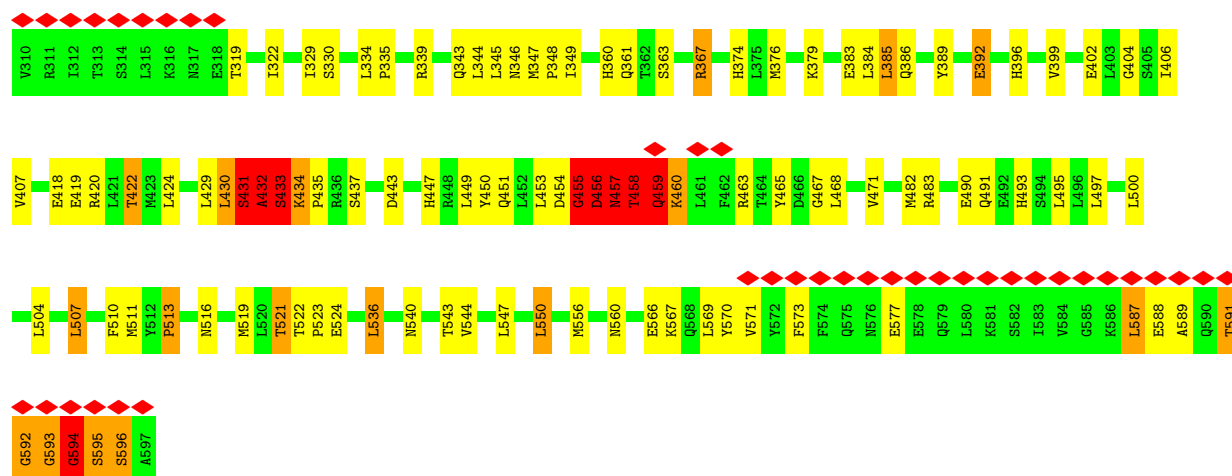
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: HAUS augmin-like complex subunit 1

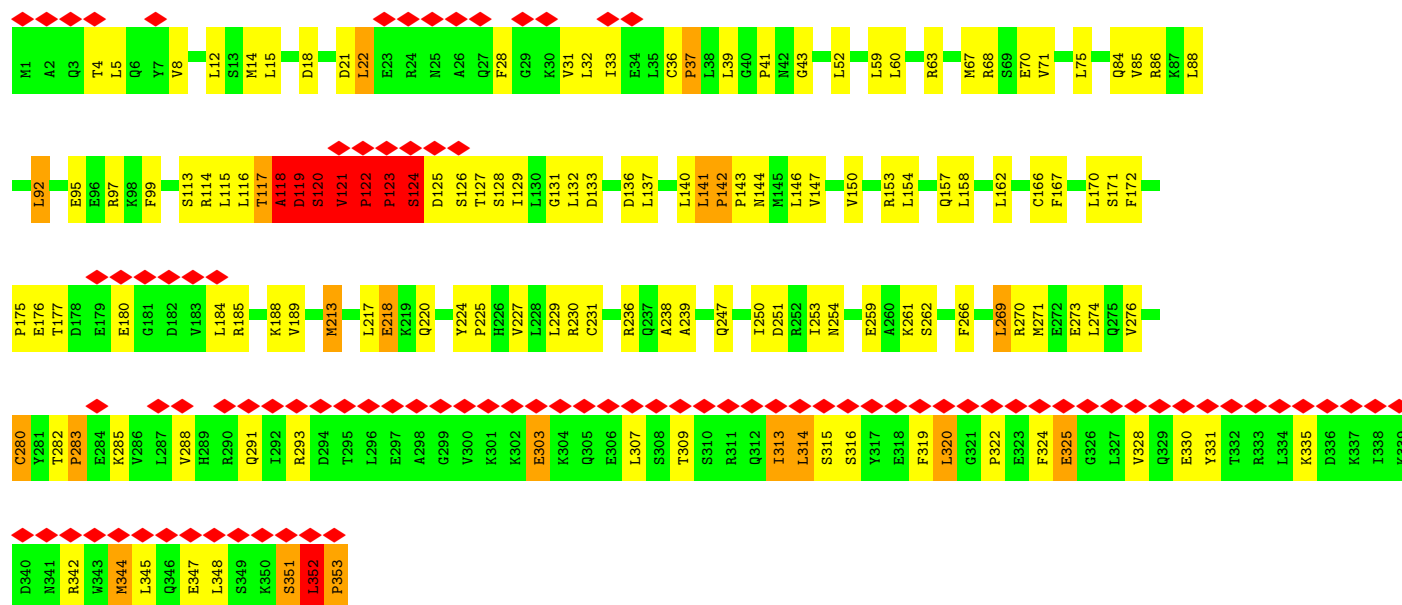


• Molecule 2: HAUS augmin-like complex subunit 3

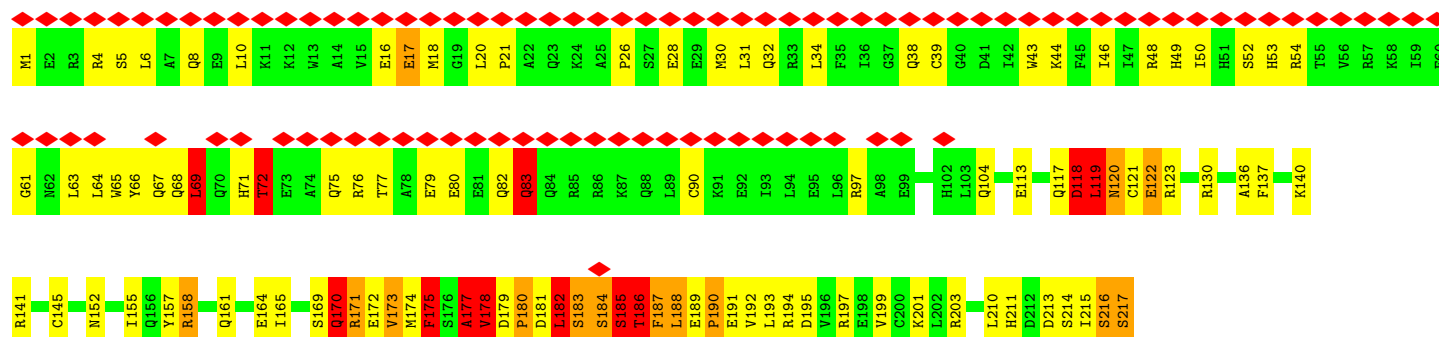


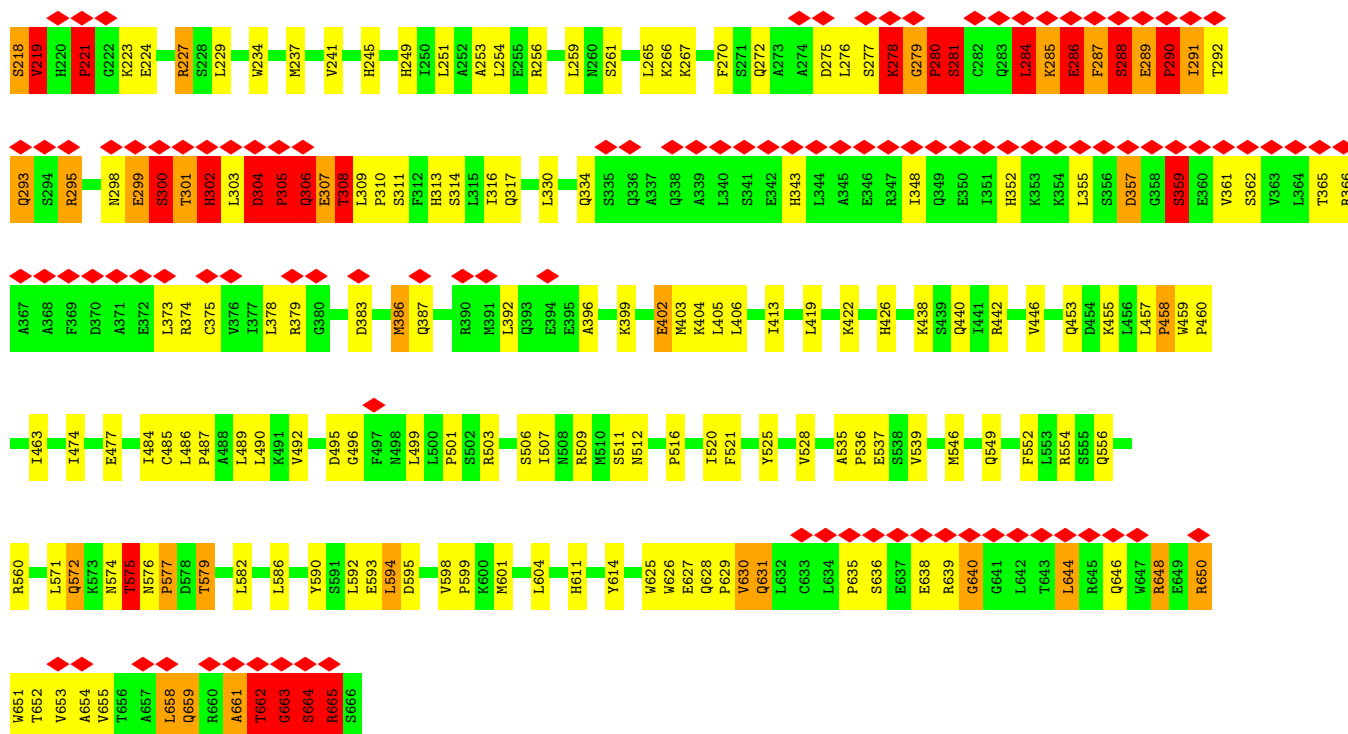


• Molecule 3: HAUS augmin like complex subunit 4 L homeolog

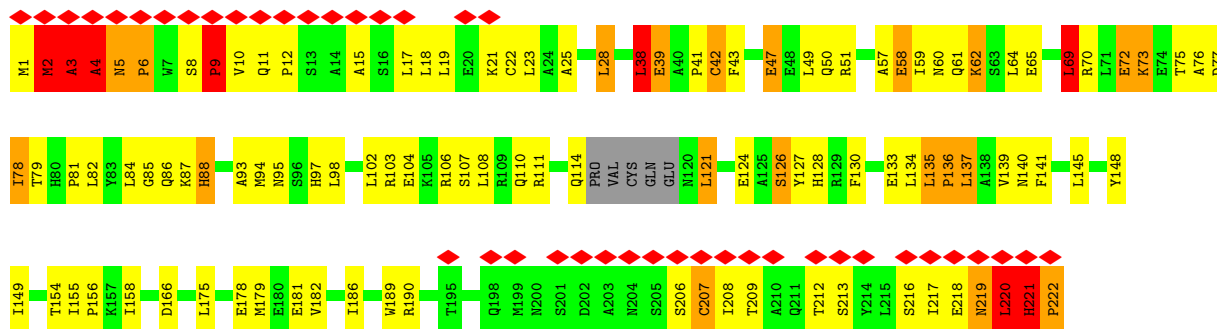


• Molecule 4: HAUS augmin-like complex subunit 5

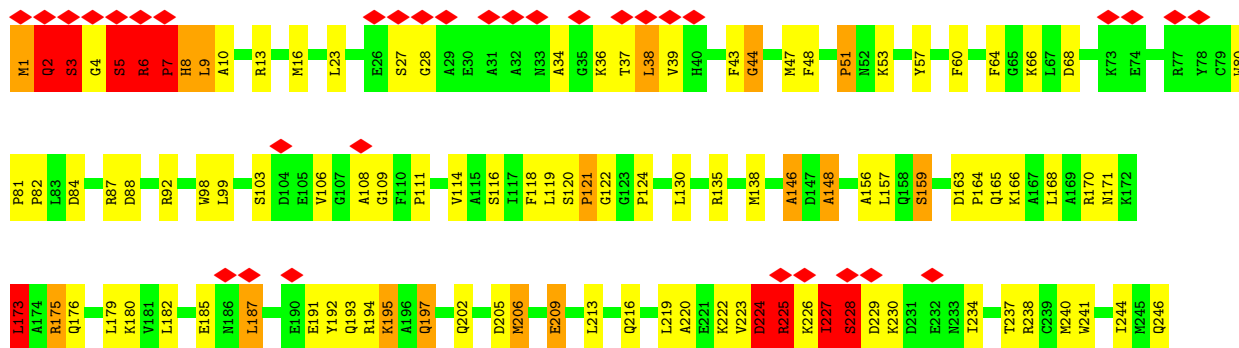


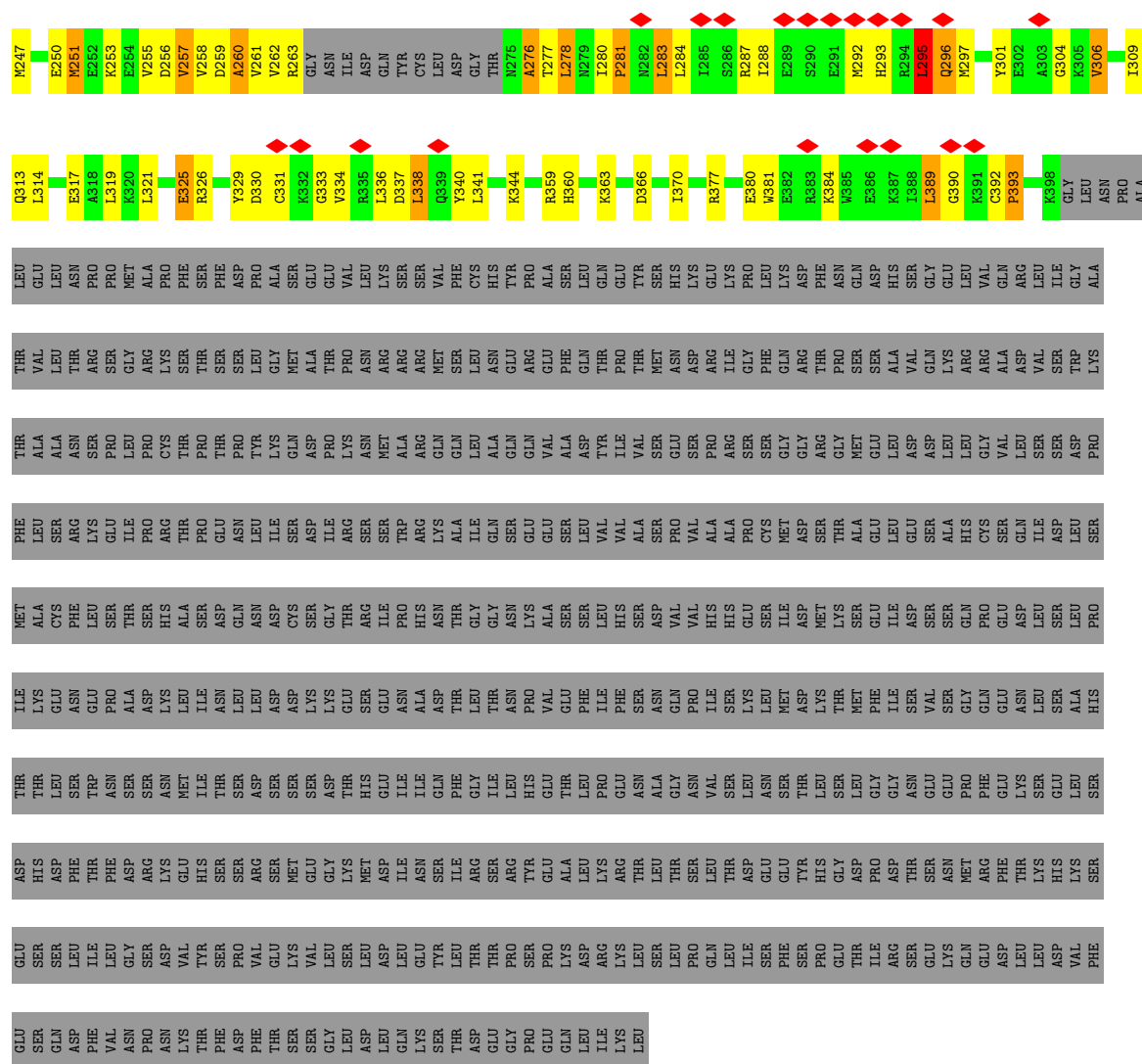


• Molecule 5: HAUS augmin like complex subunit 2 L homeolog

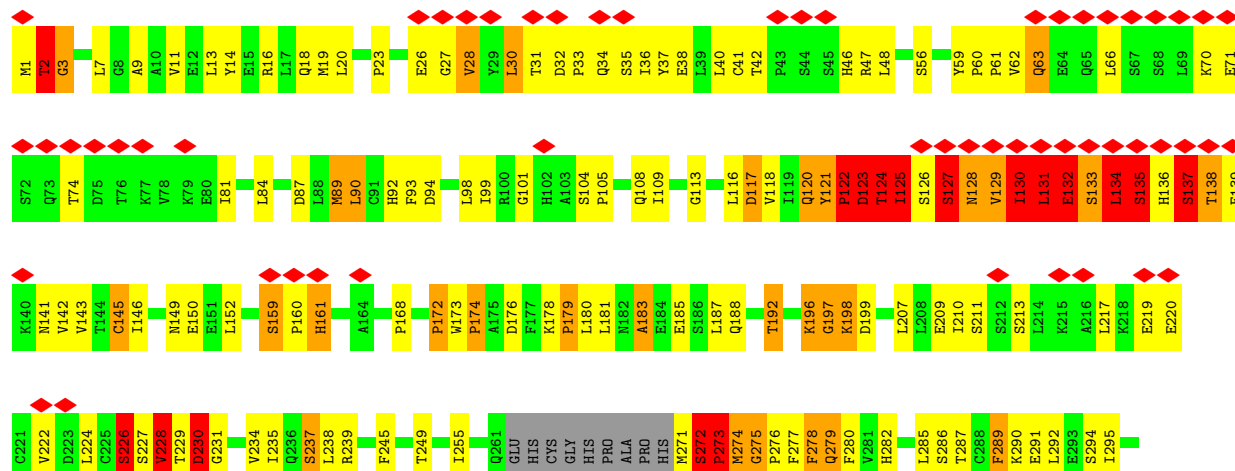


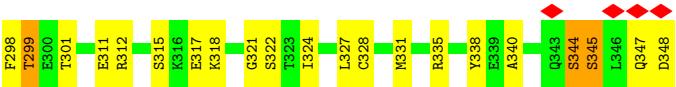
• Molecule 6: HAUS augmin like complex subunit 6 L homeolog



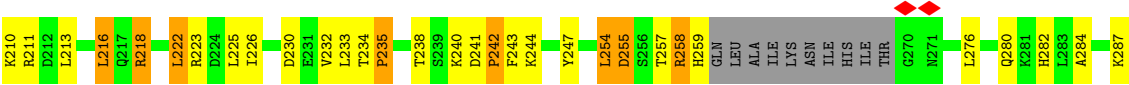
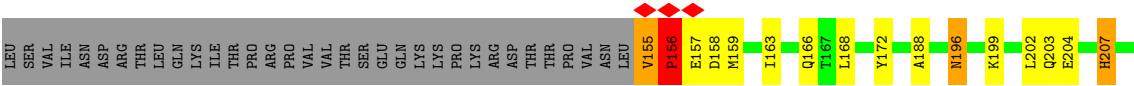
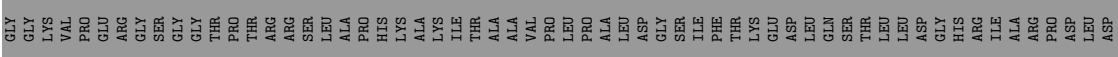
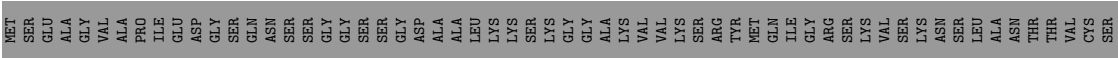
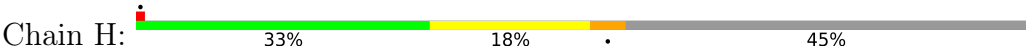


• Molecule 7: HAUS augmin like complex subunit 7 S homeolog





• Molecule 8: HAUS augmin-like complex subunit 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS L120C	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	101.8	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0245	Depositor
Map size (Å)	601.6, 601.6, 601.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.35, 2.35, 2.35	Depositor

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	1.47	38/2309 (1.6%)	1.41	48/3102 (1.5%)
2	B	1.19	41/4836 (0.8%)	1.36	76/6496 (1.2%)
3	C	0.99	23/2920 (0.8%)	1.18	29/3925 (0.7%)
4	D	1.10	55/5502 (1.0%)	1.24	61/7397 (0.8%)
5	E	1.34	40/1743 (2.3%)	1.08	17/2359 (0.7%)
6	F	1.22	55/3229 (1.7%)	1.12	34/4333 (0.8%)
7	G	1.19	48/2736 (1.8%)	1.31	37/3698 (1.0%)
8	H	1.12	19/1692 (1.1%)	0.95	6/2278 (0.3%)
All	All	1.19	319/24967 (1.3%)	1.24	308/33588 (0.9%)

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	14
2	B	0	68
3	C	0	11
4	D	0	39
5	E	0	11
6	F	0	19
7	G	0	27
8	H	0	1
All	All	0	190

All (319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	GLU	C-N	26.97	1.81	1.33
1	A	277	VAL	C-N	24.03	1.79	1.34
4	D	288	SER	C-N	19.16	1.78	1.34
2	B	591	THR	C-N	18.66	1.66	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	PRO	C-N	17.83	1.75	1.34
1	A	272	MET	C-N	-16.40	0.96	1.34
4	D	289	GLU	C-N	-16.28	1.03	1.34
1	A	283	ARG	C-N	15.78	1.70	1.34
1	A	284	ARG	C-N	15.54	1.69	1.34
6	F	34	ALA	C-N	14.96	1.59	1.33
3	C	319	PHE	C-N	13.89	1.66	1.34
1	A	276	VAL	C-N	13.54	1.65	1.34
2	B	392	GLU	C-N	-13.28	1.03	1.34
2	B	593	GLY	C-N	13.17	1.56	1.33
2	B	17	PRO	N-CD	-12.16	1.30	1.47
4	D	180	PRO	N-CD	-12.08	1.30	1.47
4	D	221	PRO	N-CD	-12.03	1.31	1.47
5	E	6	PRO	N-CD	-11.98	1.31	1.47
2	B	513	PRO	N-CD	-11.98	1.31	1.47
7	G	122	PRO	N-CD	-11.86	1.31	1.47
5	E	9	PRO	N-CD	-11.81	1.31	1.47
2	B	592	GLY	C-N	-11.80	1.11	1.33
8	H	367	PRO	N-CD	-11.80	1.31	1.47
4	D	21	PRO	N-CD	-11.79	1.31	1.47
1	A	245	PRO	N-CD	-11.78	1.31	1.47
4	D	576	ASN	C-N	11.75	1.56	1.34
1	A	22	PRO	N-CD	-11.66	1.31	1.47
4	D	26	PRO	N-CD	-11.63	1.31	1.47
2	B	54	PRO	N-CD	-11.54	1.31	1.47
2	B	90	PRO	N-CD	-11.48	1.31	1.47
5	E	222	PRO	N-CD	-11.46	1.31	1.47
1	A	208	PRO	N-CD	-11.42	1.31	1.47
4	D	280	PRO	N-CD	-11.26	1.32	1.47
3	C	283	PRO	N-CD	-11.18	1.32	1.47
6	F	7	PRO	N-CD	-11.07	1.32	1.47
1	A	282	LYS	C-N	11.07	1.59	1.34
3	C	353	PRO	N-CD	-11.06	1.32	1.47
4	D	495	ASP	C-N	11.06	1.52	1.33
5	E	41	PRO	N-CD	-11.01	1.32	1.47
4	D	290	PRO	N-CD	-10.99	1.32	1.47
3	C	322	PRO	N-CD	-10.94	1.32	1.47
3	C	122	PRO	N-CD	-10.93	1.32	1.47
2	B	191	PRO	N-CD	-10.83	1.32	1.47
2	B	181	PRO	N-CD	-10.81	1.32	1.47
1	A	274	GLU	C-N	10.45	1.58	1.34
4	D	305	PRO	N-CD	-10.39	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	82	PRO	N-CD	-10.33	1.33	1.47
7	G	23	PRO	N-CD	-10.17	1.33	1.47
1	A	273	MET	C-N	10.14	1.57	1.34
8	H	155	VAL	C-N	-10.11	1.15	1.34
6	F	106	VAL	C-N	10.11	1.51	1.33
2	B	560	ASN	C-N	10.04	1.57	1.34
4	D	635	PRO	N-CD	-9.94	1.33	1.47
6	F	121	PRO	N-CD	-9.93	1.33	1.47
3	C	123	PRO	N-CD	-9.90	1.33	1.47
2	B	70	PRO	N-CD	-9.78	1.34	1.47
8	H	156	PRO	N-CD	-9.75	1.34	1.47
6	F	1	MET	C-N	-9.69	1.11	1.34
7	G	196	LYS	C-N	9.66	1.50	1.33
6	F	148	ALA	C-N	9.65	1.50	1.33
1	A	278	PRO	N-CD	-9.49	1.34	1.47
8	H	295	PRO	N-CD	-9.33	1.34	1.47
6	F	393	PRO	N-CD	-9.28	1.34	1.47
1	A	269	LYS	C-N	-9.25	1.12	1.34
1	A	20	PRO	N-CD	-9.02	1.35	1.47
4	D	659	GLN	C-N	8.83	1.54	1.34
1	A	243	PRO	N-CD	-8.70	1.35	1.47
6	F	262	VAL	C-N	-8.55	1.14	1.34
6	F	121	PRO	C-N	-8.53	1.17	1.33
6	F	281	PRO	N-CD	-8.50	1.35	1.47
4	D	577	PRO	N-CD	-8.49	1.35	1.47
2	B	38	PRO	N-CD	-8.47	1.35	1.47
1	A	239	LEU	C-N	8.45	1.53	1.34
1	A	280	PRO	N-CD	-8.45	1.36	1.47
4	D	402	GLU	C-N	-8.45	1.14	1.34
2	B	587	LEU	C-N	8.35	1.53	1.34
6	F	146	ALA	C-N	-8.32	1.15	1.34
5	E	86	GLN	C-N	-8.31	1.15	1.34
5	E	133	GLU	C-N	-8.27	1.15	1.34
7	G	315	SER	C-N	8.25	1.53	1.34
7	G	275	GLY	C-N	-8.25	1.18	1.34
1	A	229	MET	C-N	-8.19	1.15	1.34
1	A	265	GLU	C-N	-8.11	1.15	1.34
5	E	25	ALA	C-N	8.07	1.47	1.33
2	B	455	GLY	C-N	8.07	1.52	1.34
4	D	72	THR	C-N	8.07	1.52	1.34
6	F	111	PRO	N-CD	-8.06	1.36	1.47
6	F	213	LEU	C-N	-7.98	1.15	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	160	PRO	N-CD	-7.96	1.36	1.47
1	A	206	GLU	C-N	-7.91	1.15	1.34
2	B	434	LYS	C-N	7.91	1.49	1.34
4	D	357	ASP	C-N	7.85	1.47	1.33
5	E	69	LEU	C-N	-7.84	1.16	1.34
7	G	27	GLY	C-N	7.84	1.52	1.34
5	E	12	PRO	N-CD	-7.79	1.36	1.47
1	A	268	THR	C-N	-7.78	1.16	1.34
3	C	41	PRO	N-CD	-7.77	1.36	1.47
6	F	81	PRO	N-CD	-7.76	1.36	1.47
7	G	226	SER	C-N	7.74	1.51	1.34
7	G	345	SER	C-N	7.73	1.51	1.34
6	F	80	TRP	C-N	-7.71	1.19	1.34
4	D	69	LEU	C-N	7.69	1.51	1.34
4	D	18	MET	C-N	7.68	1.46	1.33
7	G	174	PRO	N-CD	-7.67	1.37	1.47
1	A	242	ALA	C-N	-7.66	1.19	1.34
4	D	662	THR	C-N	7.61	1.46	1.33
7	G	289	PHE	C-N	-7.56	1.16	1.34
5	E	73	LYS	C-N	-7.55	1.16	1.34
2	B	435	PRO	N-CD	-7.53	1.37	1.47
4	D	177	ALA	C-N	-7.53	1.16	1.34
2	B	73	ASP	C-N	-7.51	1.16	1.34
6	F	258	VAL	C-N	-7.50	1.16	1.34
7	G	234	VAL	C-N	-7.50	1.16	1.34
4	D	227	ARG	C-N	-7.39	1.17	1.34
1	A	2	ASP	C-N	7.37	1.50	1.34
7	G	122	PRO	C-N	-7.33	1.17	1.34
4	D	180	PRO	C-N	7.29	1.50	1.34
6	F	27	SER	C-N	7.25	1.46	1.33
8	H	242	PRO	N-CD	-7.22	1.37	1.47
2	B	589	ALA	C-N	-7.19	1.17	1.34
5	E	11	GLN	C-N	-7.17	1.20	1.34
3	C	113	SER	C-N	-7.14	1.17	1.34
2	B	594	GLY	C-N	-7.14	1.17	1.34
5	E	82	LEU	C-N	-7.09	1.17	1.34
4	D	640	GLY	C-N	7.08	1.45	1.33
6	F	51	PRO	C-N	-7.08	1.17	1.34
4	D	221	PRO	C-N	-7.07	1.20	1.33
8	H	361	TYR	C-N	7.06	1.50	1.34
4	D	313	HIS	C-N	-7.03	1.17	1.34
6	F	209	GLU	C-N	-7.00	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	ARG	C-N	-6.99	1.18	1.34
1	A	17	GLY	C-N	6.96	1.50	1.34
6	F	253	LYS	C-N	-6.93	1.18	1.34
6	F	44	GLY	C-N	-6.93	1.18	1.34
2	B	215	SER	C-N	-6.93	1.18	1.34
3	C	314	LEU	C-N	-6.91	1.18	1.34
8	H	300	GLU	C-N	-6.88	1.18	1.34
6	F	108	ALA	C-N	-6.86	1.20	1.33
6	F	222	LYS	C-N	6.84	1.49	1.34
7	G	161	HIS	C-N	-6.82	1.18	1.34
5	E	93	ALA	C-N	-6.79	1.18	1.34
2	B	222	PHE	C-N	-6.79	1.18	1.34
8	H	196	ASN	C-N	-6.78	1.18	1.34
2	B	150	LEU	C-N	6.78	1.49	1.34
7	G	71	GLU	C-N	6.78	1.49	1.34
1	A	270	VAL	C-N	6.76	1.49	1.34
4	D	278	LYS	C-N	-6.75	1.20	1.33
7	G	130	ILE	C-N	6.68	1.49	1.34
3	C	37	PRO	N-CD	-6.67	1.38	1.47
5	E	78	ILE	C-N	-6.65	1.18	1.34
8	H	333	SER	C-N	-6.63	1.18	1.34
7	G	141	ASN	C-N	-6.62	1.18	1.34
6	F	260	ALA	C-N	-6.57	1.19	1.34
3	C	291	GLN	C-N	-6.54	1.19	1.34
5	E	58	GLU	C-N	-6.53	1.19	1.34
4	D	516	PRO	N-CD	-6.52	1.38	1.47
4	D	311	SER	C-N	-6.51	1.19	1.34
6	F	292	MET	C-N	6.50	1.49	1.34
5	E	61	GLN	C-N	-6.50	1.19	1.34
3	C	22	LEU	C-N	6.49	1.49	1.34
3	C	352	LEU	C-N	6.48	1.46	1.34
3	C	313	ILE	C-N	-6.47	1.19	1.34
1	A	81	TYR	C-N	6.45	1.48	1.34
2	B	516	ASN	C-N	-6.44	1.19	1.34
8	H	364	GLY	C-N	6.42	1.48	1.34
3	C	124	SER	C-N	6.41	1.48	1.34
6	F	202	GLN	C-N	-6.39	1.19	1.34
4	D	223	LYS	C-N	-6.38	1.19	1.34
1	A	222	THR	C-N	-6.38	1.19	1.34
8	H	218	ARG	C-N	-6.37	1.19	1.34
7	G	33	PRO	N-CD	-6.36	1.39	1.47
2	B	233	ASP	C-N	6.34	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	22	CYS	C-N	-6.34	1.19	1.34
2	B	523	PRO	N-CD	-6.33	1.39	1.47
4	D	652	THR	C-N	6.28	1.48	1.34
5	E	15	ALA	C-N	-6.28	1.19	1.34
1	A	23	PRO	N-CD	-6.28	1.39	1.47
6	F	380	GLU	C-N	-6.28	1.19	1.34
4	D	501	PRO	C-N	-6.27	1.19	1.34
4	D	496	GLY	C-N	6.24	1.48	1.34
4	D	310	PRO	N-CD	-6.23	1.39	1.47
5	E	88	HIS	C-N	-6.22	1.19	1.34
6	F	195	LYS	C-N	-6.19	1.19	1.34
2	B	363	SER	C-N	-6.17	1.19	1.34
3	C	142	PRO	N-CD	-6.16	1.39	1.47
7	G	120	GLN	C-N	-6.14	1.20	1.34
2	B	249	ASP	C-N	6.09	1.44	1.33
5	E	128	HIS	C-N	-6.08	1.20	1.34
5	E	8	SER	C-N	-6.08	1.22	1.34
2	B	23	ASP	C-N	-6.07	1.22	1.33
4	D	650	ARG	C-N	-6.07	1.20	1.34
8	H	297	HIS	C-N	-6.06	1.20	1.34
6	F	175	ARG	C-N	-6.06	1.20	1.34
5	E	95	ASN	C-N	-6.05	1.20	1.34
5	E	136	PRO	C-N	-6.05	1.20	1.34
2	B	367	ARG	C-N	-6.03	1.20	1.34
7	G	129	VAL	C-N	6.03	1.48	1.34
5	E	72	GLU	C-N	-6.03	1.20	1.34
7	G	287	THR	C-N	-6.02	1.20	1.34
4	D	661	ALA	C-N	-6.02	1.20	1.34
8	H	319	ASP	C-N	-6.00	1.20	1.34
7	G	26	GLU	C-N	-5.99	1.22	1.33
6	F	173	LEU	C-N	-5.98	1.20	1.34
7	G	299	THR	C-N	-5.97	1.20	1.34
4	D	638	GLU	C-N	-5.96	1.20	1.34
3	C	213	MET	C-N	-5.94	1.20	1.34
5	E	137	LEU	C-N	-5.93	1.20	1.34
5	E	51	ARG	C-N	-5.93	1.20	1.34
7	G	179	PRO	N-CD	-5.91	1.39	1.47
2	B	3	GLY	C-N	-5.89	1.22	1.33
4	D	511	SER	C-N	5.89	1.47	1.34
1	A	79	PRO	N-CD	-5.88	1.39	1.47
6	F	256	ASP	C-N	-5.87	1.20	1.34
6	F	329	TYR	C-N	5.87	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	347	GLN	C-N	5.85	1.47	1.34
4	D	83	GLN	C-N	5.84	1.47	1.34
4	D	224	GLU	C-N	5.84	1.47	1.34
7	G	290	LYS	C-N	-5.83	1.20	1.34
7	G	311	GLU	C-N	-5.81	1.20	1.34
4	D	653	VAL	C-N	-5.81	1.20	1.34
5	E	84	LEU	C-N	-5.79	1.22	1.33
7	G	159	SER	C-N	5.79	1.45	1.34
7	G	278	PHE	C-N	-5.76	1.20	1.34
6	F	205	ASP	C-N	-5.76	1.20	1.34
7	G	237	SER	C-N	-5.75	1.20	1.34
6	F	384	LYS	C-N	-5.73	1.20	1.34
4	D	190	PRO	N-CD	-5.73	1.39	1.47
3	C	143	PRO	N-CD	-5.72	1.39	1.47
7	G	89	MET	C-N	-5.72	1.20	1.34
5	E	9	PRO	C-N	-5.71	1.21	1.34
6	F	390	GLY	C-N	5.70	1.47	1.34
3	C	88	LEU	C-N	5.69	1.47	1.34
6	F	206	MET	C-N	-5.63	1.21	1.34
6	F	223	VAL	C-N	5.61	1.47	1.34
7	G	32	ASP	C-N	5.61	1.45	1.34
2	B	250	GLY	C-N	-5.60	1.21	1.34
6	F	306	VAL	C-N	-5.60	1.21	1.34
7	G	113	GLY	C-N	-5.60	1.21	1.34
5	E	81	PRO	C-N	-5.59	1.21	1.34
7	G	117	ASP	C-N	-5.58	1.21	1.34
8	H	222	LEU	C-N	-5.57	1.21	1.34
3	C	144	ASN	C-N	5.57	1.46	1.34
4	D	309	LEU	C-N	-5.55	1.23	1.34
6	F	120	SER	C-N	5.54	1.44	1.34
2	B	219	GLU	C-N	-5.52	1.21	1.34
3	C	325	GLU	C-N	5.51	1.43	1.33
6	F	251	MET	C-N	-5.51	1.21	1.34
4	D	572	GLN	C-N	5.50	1.46	1.34
4	D	53	HIS	C-N	-5.47	1.21	1.34
4	D	182	LEU	C-N	-5.46	1.21	1.34
1	A	82	THR	C-N	5.44	1.46	1.34
4	D	646	GLN	C-N	-5.38	1.21	1.34
4	D	396	ALA	C-N	5.38	1.46	1.34
6	F	43	PHE	C-N	5.37	1.42	1.33
7	G	213	SER	C-N	-5.37	1.21	1.34
2	B	422	THR	C-N	-5.37	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	CYS	C-N	5.36	1.46	1.34
2	B	360	HIS	C-N	-5.36	1.21	1.34
2	B	45	SER	C-N	-5.35	1.21	1.34
7	G	279	GLN	C-N	-5.35	1.21	1.34
6	F	246	GLN	C-N	-5.34	1.21	1.34
7	G	63	GLN	C-N	5.34	1.46	1.34
5	E	23	LEU	C-N	5.34	1.46	1.34
5	E	140	ASN	C-N	-5.33	1.21	1.34
7	G	90	LEU	C-N	5.32	1.46	1.34
6	F	237	THR	C-N	-5.29	1.21	1.34
4	D	16	GLU	C-N	-5.29	1.21	1.34
6	F	68	ASP	C-N	-5.28	1.21	1.34
6	F	276	ALA	C-N	5.28	1.46	1.34
7	G	286	SER	C-N	-5.28	1.22	1.34
6	F	194	ARG	C-N	-5.26	1.22	1.34
4	D	644	LEU	C-N	-5.26	1.22	1.34
5	E	62	LYS	C-N	-5.26	1.22	1.34
5	E	135	LEU	C-N	-5.26	1.24	1.34
6	F	191	GLU	C-N	-5.26	1.22	1.34
4	D	276	LEU	C-N	5.25	1.46	1.34
8	H	365	SER	C-N	5.25	1.46	1.34
4	D	158	ARG	C-N	-5.24	1.22	1.34
5	E	2	MET	C-N	-5.24	1.22	1.34
6	F	197	GLN	C-N	-5.24	1.22	1.34
3	C	331	TYR	C-N	-5.23	1.22	1.34
8	H	242	PRO	C-N	-5.23	1.22	1.34
7	G	181	LEU	C-N	5.23	1.46	1.34
6	F	363	LYS	C-N	5.21	1.46	1.34
1	A	241	LEU	C-N	5.21	1.46	1.34
6	F	103	SER	C-N	5.20	1.46	1.34
7	G	317	GLU	C-N	5.20	1.46	1.34
1	A	245	PRO	C-N	5.19	1.46	1.34
5	E	47	GLU	C-N	-5.18	1.22	1.34
7	G	282	HIS	C-N	-5.18	1.22	1.34
5	E	65	GLU	C-N	-5.16	1.22	1.34
6	F	81	PRO	C-N	5.16	1.44	1.34
3	C	118	ALA	C-N	5.16	1.46	1.34
1	A	78	GLY	C-N	-5.16	1.24	1.34
2	B	65	LYS	C-N	5.15	1.45	1.34
7	G	145	CYS	C-N	-5.13	1.22	1.34
6	F	109	GLY	C-N	-5.13	1.22	1.34
5	E	85	GLY	C-N	-5.13	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	235	PRO	N-CD	-5.13	1.40	1.47
7	G	30	LEU	C-N	-5.12	1.22	1.34
4	D	594	LEU	C-N	5.12	1.45	1.34
7	G	209	GLU	C-N	-5.11	1.22	1.34
7	G	124	THR	C-N	5.10	1.45	1.34
8	H	207	HIS	C-N	-5.10	1.22	1.34
8	H	344	SER	C-N	-5.09	1.22	1.34
1	A	64	ALA	C-N	-5.08	1.22	1.34
6	F	257	VAL	C-N	-5.08	1.22	1.34
5	E	98	LEU	C-N	-5.08	1.22	1.34
2	B	36	LEU	C-N	-5.06	1.22	1.34
4	D	665	ARG	C-N	-5.06	1.22	1.34
7	G	98	LEU	C-N	-5.06	1.22	1.34
6	F	224	ASP	C-N	-5.06	1.22	1.34
1	A	235	LEU	C-N	5.05	1.45	1.34
1	A	53	GLU	C-N	-5.05	1.22	1.34
5	E	126	SER	C-N	-5.04	1.22	1.34
2	B	224	GLY	C-N	-5.03	1.22	1.34
5	E	50	GLN	C-N	-5.02	1.22	1.34
7	G	104	SER	C-N	5.01	1.43	1.34
1	A	285	LEU	C-N	5.00	1.45	1.34

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	130	ILE	O-C-N	-21.95	87.58	122.70
4	D	286	GLU	O-C-N	-21.61	88.13	122.70
3	C	117	THR	O-C-N	-21.59	88.16	122.70
2	B	392	GLU	O-C-N	-21.40	88.46	122.70
3	C	122	PRO	O-C-N	-21.14	80.94	121.10
1	A	283	ARG	O-C-N	-20.81	89.41	122.70
7	G	228	VAL	O-C-N	-20.31	90.20	122.70
4	D	301	THR	O-C-N	-20.13	90.49	122.70
4	D	306	GLN	O-C-N	-19.00	92.30	122.70
4	D	288	SER	O-C-N	-18.99	92.32	122.70
1	A	282	LYS	O-C-N	-18.60	92.94	122.70
6	F	1	MET	C-N-CA	18.57	168.13	121.70
7	G	127	SER	O-C-N	-18.49	93.11	122.70
7	G	137	SER	O-C-N	-18.14	93.68	122.70
4	D	284	LEU	O-C-N	-18.07	93.80	122.70
2	B	234	GLU	O-C-N	-17.50	94.69	122.70
2	B	591	THR	O-C-N	-17.45	93.54	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	304	ASP	O-C-N	-17.12	88.57	121.10
3	C	352	LEU	O-C-N	-16.76	89.25	121.10
1	A	275	PHE	O-C-N	-15.59	97.76	122.70
2	B	88	LYS	O-C-N	-15.58	97.78	122.70
2	B	392	GLU	CA-C-N	15.37	151.01	117.20
4	D	175	PHE	O-C-N	-15.13	98.48	122.70
3	C	119	ASP	O-C-N	-14.94	98.80	122.70
1	A	284	ARG	C-N-CA	14.57	158.13	121.70
2	B	594	GLY	O-C-N	-14.43	99.61	122.70
2	B	236	PHE	O-C-N	-13.94	100.40	122.70
4	D	186	THR	O-C-N	-13.92	100.43	122.70
2	B	596	SER	O-C-N	-13.79	100.64	122.70
2	B	392	GLU	C-N-CA	13.44	155.30	121.70
2	B	222	PHE	O-C-N	-13.38	101.29	122.70
2	B	231	GLY	O-C-N	-13.36	101.33	122.70
1	A	282	LYS	CA-C-N	13.23	146.30	117.20
4	D	662	THR	O-C-N	-12.98	101.14	123.20
1	A	278	PRO	O-C-N	-12.87	102.10	122.70
5	E	39	GLU	O-C-N	-12.72	102.34	122.70
2	B	238	LEU	O-C-N	-12.69	102.39	122.70
7	G	123	ASP	O-C-N	-12.54	102.64	122.70
4	D	216	SER	O-C-N	-12.51	102.68	122.70
2	B	249	ASP	O-C-N	-12.44	102.05	123.20
4	D	278	LYS	O-C-N	-12.37	102.18	123.20
2	B	245	SER	O-C-N	-12.30	103.02	122.70
1	A	277	VAL	O-C-N	-12.25	97.83	121.10
2	B	181	PRO	O-C-N	-12.14	103.27	122.70
2	B	246	PHE	O-C-N	-12.11	102.61	123.20
2	B	84	PHE	O-C-N	-12.08	103.37	122.70
5	E	220	LEU	O-C-N	-11.97	103.55	122.70
2	B	92	ILE	O-C-N	-11.71	103.96	122.70
6	F	295	LEU	O-C-N	-11.61	104.13	122.70
1	A	281	SER	O-C-N	11.47	141.06	122.70
7	G	196	LYS	C-N-CA	11.31	146.05	122.30
5	E	219	ASN	O-C-N	-11.24	104.72	122.70
5	E	221	HIS	O-C-N	-11.09	100.02	121.10
1	A	283	ARG	C-N-CA	11.06	149.35	121.70
2	B	225	MET	O-C-N	-11.01	105.08	122.70
2	B	95	VAL	O-C-N	-10.88	105.29	122.70
4	D	280	PRO	O-C-N	-10.86	105.33	122.70
7	G	133	SER	O-C-N	-10.84	105.35	122.70
3	C	320	LEU	O-C-N	-10.78	104.87	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PRO	C-N-CA	10.71	148.48	121.70
3	C	118	ALA	O-C-N	-10.67	105.63	122.70
2	B	592	GLY	O-C-N	-10.51	105.33	123.20
3	C	351	SER	O-C-N	-10.36	106.13	122.70
7	G	129	VAL	C-N-CA	10.31	147.47	121.70
3	C	123	PRO	O-C-N	-10.16	106.45	122.70
1	A	280	PRO	C-N-CA	9.97	146.62	121.70
4	D	177	ALA	O-C-N	-9.88	106.89	122.70
4	D	219	VAL	O-C-N	-9.68	107.21	122.70
2	B	223	GLU	C-N-CA	9.63	142.53	122.30
2	B	242	ASN	O-C-N	-9.61	107.32	122.70
4	D	218	SER	O-C-N	-9.54	107.43	122.70
2	B	593	GLY	O-C-N	-9.54	106.99	123.20
4	D	302	HIS	O-C-N	-9.54	107.44	122.70
6	F	224	ASP	O-C-N	-9.52	107.47	122.70
1	A	284	ARG	O-C-N	-9.42	107.62	122.70
2	B	93	GLU	O-C-N	-9.33	107.77	122.70
2	B	96	ALA	O-C-N	-9.26	107.89	122.70
8	H	156	PRO	O-C-N	-9.23	107.93	122.70
4	D	182	LEU	O-C-N	-9.23	107.94	122.70
7	G	230	ASP	O-C-N	-9.17	107.61	123.20
7	G	124	THR	C-N-CA	9.16	144.59	121.70
1	A	276	VAL	C-N-CA	9.06	144.35	121.70
1	A	283	ARG	CA-C-N	9.05	137.12	117.20
5	E	2	MET	O-C-N	-8.97	108.34	122.70
6	F	8	HIS	O-C-N	-8.96	108.37	122.70
1	A	282	LYS	C-N-CA	8.94	144.06	121.70
6	F	159	SER	O-C-N	-8.94	108.40	122.70
2	B	229	VAL	O-C-N	-8.86	108.53	122.70
4	D	184	SER	O-C-N	-8.85	108.54	122.70
1	A	281	SER	C-N-CA	-8.82	99.65	121.70
4	D	287	PHE	C-N-CA	8.80	143.71	121.70
1	A	281	SER	CA-C-N	-8.79	97.86	117.20
2	B	456	ASP	O-C-N	-8.76	108.68	122.70
6	F	227	ILE	O-C-N	-8.71	108.76	122.70
6	F	6	ARG	C-N-CD	-8.69	101.49	120.60
6	F	146	ALA	O-C-N	-8.64	108.87	122.70
2	B	592	GLY	CA-C-N	8.61	133.43	116.20
4	D	188	LEU	O-C-N	-8.59	108.96	122.70
7	G	128	ASN	O-C-N	-8.55	109.02	122.70
2	B	591	THR	C-N-CA	8.55	140.25	122.30
1	A	234	LYS	O-C-N	-8.49	109.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	178	VAL	O-C-N	-8.41	109.24	122.70
7	G	132	GLU	O-C-N	-8.41	109.24	122.70
2	B	2	SER	O-C-N	-8.41	108.91	123.20
6	F	228	SER	O-C-N	-8.35	109.35	122.70
1	A	236	ASN	O-C-N	-8.30	109.41	122.70
2	B	595	SER	O-C-N	-8.24	109.52	122.70
2	B	240	GLN	O-C-N	-8.22	109.55	122.70
7	G	137	SER	CA-C-N	8.20	135.24	117.20
6	F	108	ALA	O-C-N	-8.19	109.28	123.20
3	C	280	CYS	O-C-N	-8.19	109.60	122.70
2	B	237	GLN	C-N-CA	8.17	142.13	121.70
3	C	320	LEU	C-N-CA	8.16	139.44	122.30
6	F	6	ARG	O-C-N	-8.13	105.64	121.10
2	B	241	LEU	O-C-N	-8.10	109.74	122.70
7	G	199	ASP	O-C-N	-8.05	109.82	122.70
4	D	221	PRO	O-C-N	-8.04	109.53	123.20
2	B	230	GLU	O-C-N	-8.03	109.55	123.20
7	G	28	VAL	O-C-N	-8.01	109.88	122.70
3	C	344	MET	O-C-N	-7.99	109.91	122.70
2	B	432	ALA	C-N-CA	-7.92	101.91	121.70
2	B	242	ASN	C-N-CA	7.90	141.45	121.70
2	B	596	SER	CA-C-N	7.79	134.35	117.20
4	D	280	PRO	CA-C-N	7.79	134.33	117.20
4	D	576	ASN	C-N-CD	-7.75	103.55	120.60
6	F	3	SER	C-N-CA	7.72	138.51	122.30
4	D	280	PRO	C-N-CA	-7.71	102.42	121.70
6	F	225	ARG	O-C-N	-7.71	110.36	122.70
2	B	458	THR	O-C-N	-7.66	110.44	122.70
5	E	43	PHE	O-C-N	-7.66	110.45	122.70
5	E	219	ASN	CA-C-N	7.65	134.03	117.20
8	H	258	ARG	O-C-N	-7.65	110.47	122.70
3	C	320	LEU	CA-C-N	7.63	131.46	116.20
2	B	223	GLU	O-C-N	-7.55	110.37	123.20
6	F	3	SER	O-C-N	-7.54	110.38	123.20
7	G	137	SER	C-N-CA	7.54	140.54	121.70
7	G	197	GLY	O-C-N	-7.53	110.65	122.70
4	D	308	THR	O-C-N	-7.51	110.68	122.70
1	A	285	LEU	O-C-N	-7.50	110.69	122.70
2	B	459	GLN	O-C-N	-7.50	110.70	122.70
5	E	4	ALA	O-C-N	-7.49	110.71	122.70
5	E	221	HIS	CA-C-N	7.47	138.03	117.10
1	A	238	TYR	O-C-N	-7.44	110.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	348	LEU	O-C-N	-7.39	110.87	122.70
4	D	216	SER	C-N-CA	7.37	140.12	121.70
2	B	228	PHE	O-C-N	-7.36	110.92	122.70
4	D	458	PRO	O-C-N	-7.36	110.92	122.70
4	D	216	SER	CA-C-N	7.35	133.36	117.20
3	C	351	SER	CA-C-N	7.28	133.21	117.20
2	B	591	THR	CA-C-N	7.24	130.68	116.20
4	D	665	ARG	O-C-N	-7.23	111.13	122.70
3	C	119	ASP	C-N-CA	-7.22	103.66	121.70
4	D	663	GLY	C-N-CA	-7.21	103.66	121.70
3	C	347	GLU	O-C-N	-7.18	111.21	122.70
6	F	220	ALA	O-C-N	-7.17	111.22	122.70
2	B	88	LYS	C-N-CA	-7.16	103.79	121.70
6	F	223	VAL	O-C-N	-7.16	111.24	122.70
6	F	5	SER	O-C-N	-7.08	111.37	122.70
1	A	241	LEU	O-C-N	-7.04	111.43	122.70
8	H	255	ASP	O-C-N	-7.02	111.47	122.70
4	D	455	LYS	O-C-N	-6.98	111.53	122.70
2	B	225	MET	CA-C-N	6.96	132.52	117.20
5	E	42	CYS	O-C-N	-6.91	111.65	122.70
1	A	237	SER	O-C-N	-6.90	111.65	122.70
1	A	228	SER	O-C-N	-6.90	111.67	122.70
7	G	274	MET	O-C-N	-6.89	111.48	123.20
2	B	186	GLU	O-C-N	-6.89	111.67	122.70
5	E	3	ALA	O-C-N	-6.79	111.84	122.70
1	A	274	GLU	O-C-N	-6.76	111.88	122.70
2	B	16	TYR	O-C-N	-6.75	108.28	121.10
3	C	342	ARG	O-C-N	6.71	133.43	122.70
4	D	665	ARG	C-N-CA	-6.68	104.99	121.70
4	D	575	THR	O-C-N	-6.67	112.02	122.70
1	A	191	TYR	O-C-N	-6.65	112.07	122.70
4	D	303	LEU	C-N-CA	-6.64	105.11	121.70
2	B	91	ALA	O-C-N	-6.63	112.08	122.70
6	F	2	GLN	C-N-CA	6.54	138.06	121.70
1	A	279	GLU	O-C-N	-6.52	108.71	121.10
2	B	432	ALA	O-C-N	-6.49	112.32	122.70
2	B	556	MET	O-C-N	-6.49	112.32	122.70
1	A	202	SER	O-C-N	-6.47	112.35	122.70
6	F	226	LYS	O-C-N	-6.44	112.39	122.70
2	B	23	ASP	O-C-N	-6.43	112.27	123.20
7	G	196	LYS	O-C-N	-6.42	112.28	123.20
2	B	240	GLN	C-N-CA	6.42	137.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	MET	O-C-N	-6.41	112.45	122.70
2	B	182	GLU	O-C-N	-6.39	112.48	122.70
6	F	216	GLN	O-C-N	-6.32	112.58	122.70
4	D	281	SER	O-C-N	-6.32	112.59	122.70
7	G	183	ALA	C-N-CA	6.29	137.42	121.70
6	F	229	ASP	O-C-N	-6.28	112.65	122.70
2	B	23	ASP	C-N-CA	6.28	135.48	122.30
6	F	108	ALA	CA-C-N	6.26	128.72	116.20
1	A	221	LEU	O-C-N	-6.22	112.74	122.70
1	A	217	LEU	O-C-N	-6.21	112.77	122.70
4	D	288	SER	C-N-CA	6.20	137.20	121.70
2	B	185	CYS	C-N-CA	-6.19	106.22	121.70
1	A	243	PRO	O-C-N	-6.19	112.79	122.70
7	G	130	ILE	C-N-CA	6.18	137.15	121.70
2	B	82	LYS	O-C-N	6.18	132.59	122.70
7	G	273	PRO	O-C-N	-6.18	112.82	122.70
2	B	16	TYR	C-N-CD	-6.17	107.03	120.60
6	F	224	ASP	CA-C-N	6.17	130.77	117.20
3	C	316	SER	O-C-N	-6.16	112.85	122.70
1	A	224	LEU	O-C-N	-6.15	112.86	122.70
2	B	229	VAL	CA-C-N	6.14	130.71	117.20
2	B	304	LYS	O-C-N	-6.08	112.97	122.70
2	B	235	ASN	C-N-CA	6.07	136.89	121.70
4	D	289	GLU	O-C-N	6.07	132.64	121.10
6	F	8	HIS	CA-C-N	6.05	130.51	117.20
4	D	386	MET	O-C-N	6.04	132.36	122.70
4	D	279	GLY	C-N-CD	-6.03	107.34	120.60
2	B	47	ALA	O-C-N	-6.00	113.10	122.70
4	D	285	LYS	C-N-CA	6.00	136.69	121.70
4	D	359	SER	O-C-N	-5.99	113.12	122.70
4	D	17	GLU	O-C-N	-5.97	113.15	122.70
4	D	221	PRO	C-N-CA	5.96	134.81	122.30
2	B	223	GLU	CA-C-N	5.91	128.02	116.20
1	A	236	ASN	CA-C-N	5.87	130.11	117.20
7	G	274	MET	CA-C-N	5.85	127.91	116.20
5	E	217	ILE	O-C-N	-5.84	113.36	122.70
4	D	217	SER	O-C-N	-5.83	113.38	122.70
4	D	631	GLN	O-C-N	-5.82	113.38	122.70
3	C	120	SER	C-N-CA	5.78	136.14	121.70
2	B	299	ASP	O-C-N	-5.77	113.46	122.70
7	G	131	LEU	C-N-CA	-5.76	107.31	121.70
3	C	280	CYS	CA-C-N	5.75	129.85	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	404	LYS	O-C-N	5.74	131.89	122.70
1	A	231	ALA	O-C-N	-5.73	113.53	122.70
1	A	271	ASN	O-C-N	-5.73	113.53	122.70
2	B	250	GLY	O-C-N	-5.71	113.56	122.70
6	F	276	ALA	O-C-N	-5.71	113.57	122.70
7	G	20	LEU	O-C-N	-5.70	113.58	122.70
2	B	244	ASN	O-C-N	-5.68	113.61	122.70
7	G	172	PRO	O-C-N	-5.66	113.65	122.70
7	G	272	SER	O-C-N	-5.63	110.40	121.10
7	G	133	SER	C-N-CA	5.61	135.72	121.70
3	C	122	PRO	CA-C-N	5.60	132.78	117.10
7	G	126	SER	C-N-CA	-5.60	107.69	121.70
3	C	344	MET	CA-C-N	5.59	129.50	117.20
5	E	42	CYS	C-N-CA	5.57	135.63	121.70
7	G	127	SER	C-N-CA	-5.57	107.78	121.70
1	A	242	ALA	O-C-N	-5.55	110.55	121.10
2	B	433	SER	O-C-N	-5.55	113.82	122.70
1	A	203	ALA	O-C-N	-5.53	113.80	123.20
2	B	90	PRO	O-C-N	-5.53	113.85	122.70
2	B	593	GLY	C-N-CA	5.52	133.90	122.30
5	E	41	PRO	O-C-N	5.52	131.53	122.70
3	C	121	VAL	C-N-CD	-5.48	108.55	120.60
7	G	135	SER	O-C-N	-5.48	113.93	122.70
4	D	288	SER	CA-C-N	5.47	129.24	117.20
1	A	194	HIS	O-C-N	5.43	131.38	122.70
4	D	185	SER	O-C-N	-5.42	114.03	122.70
5	E	43	PHE	C-N-CA	5.42	135.24	121.70
1	A	284	ARG	CA-C-N	5.41	129.10	117.20
1	A	234	LYS	CA-C-N	5.39	129.07	117.20
4	D	38	GLN	O-C-N	-5.38	114.09	122.70
4	D	278	LYS	C-N-CA	-5.38	111.01	122.30
7	G	226	SER	C-N-CA	5.37	135.12	121.70
7	G	122	PRO	O-C-N	-5.37	114.11	122.70
7	G	70	LYS	O-C-N	-5.36	114.13	122.70
2	B	23	ASP	CA-C-N	5.35	126.91	116.20
4	D	48	ARG	O-C-N	-5.34	114.16	122.70
3	C	293	ARG	O-C-N	5.33	131.23	122.70
4	D	5	SER	O-C-N	-5.32	114.18	122.70
4	D	300	SER	O-C-N	-5.32	114.18	122.70
8	H	305	PHE	O-C-N	-5.32	114.19	122.70
2	B	295	SER	O-C-N	-5.29	114.23	122.70
4	D	277	SER	O-C-N	-5.29	114.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	122	PRO	C-N-CD	5.29	139.50	128.40
1	A	215	VAL	O-C-N	5.28	131.15	122.70
6	F	227	ILE	CA-C-N	5.27	128.79	117.20
2	B	431	SER	C-N-CA	5.27	134.87	121.70
4	D	275	ASP	O-C-N	-5.26	114.28	122.70
1	A	236	ASN	C-N-CA	5.26	134.84	121.70
1	A	234	LYS	C-N-CA	5.25	134.84	121.70
8	H	258	ARG	CA-C-N	5.24	128.73	117.20
2	B	521	THR	O-C-N	5.23	131.07	122.70
3	C	348	LEU	CA-C-N	5.20	128.65	117.20
6	F	106	VAL	O-C-N	-5.18	114.40	123.20
1	A	238	TYR	CA-C-N	5.17	128.58	117.20
3	C	319	PHE	O-C-N	-5.17	114.44	122.70
7	G	129	VAL	O-C-N	-5.16	114.44	122.70
4	D	458	PRO	CA-C-N	5.16	128.55	117.20
1	A	270	VAL	O-C-N	-5.15	114.46	122.70
4	D	630	VAL	O-C-N	-5.15	114.46	122.70
6	F	304	GLY	O-C-N	-5.14	114.47	122.70
2	B	85	SER	O-C-N	-5.14	114.48	122.70
4	D	664	SER	O-C-N	-5.13	114.48	122.70
8	H	238	THR	O-C-N	-5.13	114.49	122.70
4	D	627	GLU	O-C-N	-5.12	114.51	122.70
7	G	3	GLY	O-C-N	-5.12	114.50	123.20
6	F	389	LEU	O-C-N	-5.11	114.51	123.20
7	G	198	LYS	O-C-N	-5.10	114.54	122.70
6	F	209	GLU	O-C-N	-5.09	114.56	122.70
6	F	296	GLN	O-C-N	-5.09	114.56	122.70
1	A	280	PRO	O-C-N	5.08	130.82	122.70
5	E	216	SER	O-C-N	-5.07	114.58	122.70
3	C	342	ARG	CA-C-N	-5.07	106.05	117.20
2	B	594	GLY	CA-C-N	5.07	128.35	117.20
1	A	285	LEU	CA-C-N	5.07	128.34	117.20
1	A	244	ASN	C-N-CD	-5.05	109.49	120.60
2	B	457	ASN	C-N-CA	-5.04	109.09	121.70
6	F	366	ASP	O-C-N	-5.04	114.64	122.70
6	F	220	ALA	CA-C-N	5.03	128.28	117.20
4	D	188	LEU	C-N-CA	5.03	134.28	121.70
5	E	43	PHE	CA-C-N	5.02	128.25	117.20
3	C	344	MET	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (190) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	LEU	Mainchain
1	A	242	ALA	Mainchain
1	A	243	PRO	Mainchain
1	A	273	MET	Peptide
1	A	274	GLU	Mainchain,Peptide
1	A	275	PHE	Mainchain,Peptide
1	A	276	VAL	Peptide
1	A	278	PRO	Mainchain,Peptide
1	A	279	GLU	Mainchain
1	A	281	SER	Peptide
1	A	285	LEU	Peptide
2	B	1	MET	Mainchain
2	B	179	SER	Mainchain
2	B	181	PRO	Mainchain
2	B	182	GLU	Mainchain
2	B	183	THR	Mainchain
2	B	184	ALA	Mainchain
2	B	185	CYS	Mainchain
2	B	186	GLU	Mainchain
2	B	187	LEU	Mainchain
2	B	189	SER	Mainchain
2	B	2	SER	Mainchain
2	B	222	PHE	Mainchain
2	B	224	GLY	Mainchain
2	B	225	MET	Mainchain
2	B	230	GLU	Mainchain,Peptide
2	B	231	GLY	Mainchain,Peptide
2	B	232	SER	Mainchain
2	B	233	ASP	Mainchain,Peptide
2	B	234	GLU	Mainchain
2	B	235	ASN	Mainchain
2	B	236	PHE	Mainchain
2	B	238	LEU	Mainchain
2	B	239	VAL	Mainchain
2	B	240	GLN	Mainchain
2	B	241	LEU	Mainchain
2	B	242	ASN	Mainchain
2	B	244	ASN	Mainchain
2	B	245	SER	Mainchain
2	B	246	PHE	Mainchain,Peptide
2	B	247	GLY	Mainchain
2	B	249	ASP	Mainchain
2	B	250	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	B	251	THR	Mainchain
2	B	304	LYS	Mainchain
2	B	430	LEU	Mainchain
2	B	432	ALA	Mainchain
2	B	433	SER	Mainchain
2	B	434	LYS	Mainchain
2	B	455	GLY	Mainchain
2	B	456	ASP	Mainchain
2	B	457	ASN	Mainchain
2	B	458	THR	Mainchain
2	B	459	GLN	Mainchain
2	B	460	LYS	Mainchain
2	B	593	GLY	Mainchain
2	B	594	GLY	Mainchain
2	B	595	SER	Mainchain,Peptide
2	B	596	SER	Mainchain,Peptide
2	B	67	SER	Mainchain
2	B	84	PHE	Mainchain
2	B	85	SER	Mainchain
2	B	86	ILE	Mainchain
2	B	87	SER	Mainchain
2	B	88	LYS	Mainchain
2	B	89	VAL	Mainchain
2	B	90	PRO	Mainchain
2	B	91	ALA	Mainchain
2	B	92	ILE	Mainchain
2	B	93	GLU	Mainchain
2	B	94	GLU	Mainchain
2	B	95	VAL	Mainchain
2	B	96	ALA	Mainchain
3	C	117	THR	Mainchain
3	C	118	ALA	Mainchain
3	C	119	ASP	Mainchain
3	C	121	VAL	Mainchain
3	C	122	PRO	Mainchain
3	C	123	PRO	Mainchain
3	C	124	SER	Mainchain
3	C	126	SER	Mainchain
3	C	320	LEU	Mainchain
3	C	352	LEU	Mainchain,Peptide
4	D	118	ASP	Mainchain
4	D	119	LEU	Mainchain

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Mol	Chain	Res	Type	Group
4	D	120	ASN	Mainchain
4	D	175	PHE	Mainchain
4	D	177	ALA	Mainchain
4	D	178	VAL	Mainchain
4	D	181	ASP	Mainchain
4	D	182	LEU	Mainchain
4	D	183	SER	Mainchain,Peptide
4	D	184	SER	Mainchain
4	D	185	SER	Mainchain
4	D	186	THR	Mainchain
4	D	187	PHE	Mainchain
4	D	188	LEU	Mainchain
4	D	216	SER	Mainchain
4	D	218	SER	Mainchain
4	D	219	VAL	Mainchain
4	D	221	PRO	Mainchain
4	D	278	LYS	Mainchain
4	D	279	GLY	Peptide
4	D	281	SER	Mainchain
4	D	284	LEU	Mainchain
4	D	286	GLU	Mainchain
4	D	300	SER	Peptide
4	D	301	THR	Mainchain
4	D	302	HIS	Mainchain,Peptide
4	D	304	ASP	Mainchain
4	D	305	PRO	Mainchain
4	D	306	GLN	Mainchain
4	D	307	GLU	Mainchain
4	D	308	THR	Mainchain
4	D	357	ASP	Mainchain
4	D	359	SER	Mainchain
4	D	662	THR	Mainchain
4	D	663	GLY	Mainchain
4	D	664	SER	Mainchain
4	D	665	ARG	Mainchain
5	E	1	MET	Mainchain
5	E	2	MET	Mainchain
5	E	220	LEU	Mainchain,Peptide
5	E	221	HIS	Mainchain,Peptide
5	E	3	ALA	Mainchain
5	E	38	LEU	Mainchain
5	E	39	GLU	Mainchain

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Mol	Chain	Res	Type	Group
5	E	4	ALA	Mainchain
5	E	5	ASN	Mainchain
6	F	1	MET	Mainchain,Peptide
6	F	122	GLY	Mainchain
6	F	146	ALA	Mainchain
6	F	159	SER	Mainchain
6	F	2	GLN	Mainchain,Peptide
6	F	225	ARG	Mainchain
6	F	227	ILE	Mainchain
6	F	228	SER	Mainchain
6	F	276	ALA	Mainchain
6	F	295	LEU	Mainchain
6	F	3	SER	Mainchain
6	F	336	LEU	Mainchain
6	F	36	LYS	Mainchain
6	F	39	VAL	Mainchain
6	F	4	GLY	Mainchain
6	F	5	SER	Mainchain
6	F	6	ARG	Mainchain
7	G	1	MET	Mainchain
7	G	121	TYR	Mainchain
7	G	122	PRO	Mainchain
7	G	123	ASP	Mainchain
7	G	124	THR	Mainchain
7	G	125	ILE	Mainchain
7	G	127	SER	Mainchain
7	G	128	ASN	Mainchain
7	G	130	ILE	Mainchain
7	G	131	LEU	Mainchain,Peptide
7	G	132	GLU	Mainchain
7	G	133	SER	Mainchain,Peptide
7	G	134	LEU	Mainchain
7	G	135	SER	Mainchain
7	G	137	SER	Mainchain
7	G	196	LYS	Mainchain
7	G	198	LYS	Mainchain
7	G	2	THR	Mainchain
7	G	226	SER	Mainchain
7	G	227	SER	Mainchain
7	G	228	VAL	Mainchain
7	G	230	ASP	Mainchain
7	G	272	SER	Mainchain

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Mol	Chain	Res	Type	Group
7	G	28	VAL	Mainchain
7	G	3	GLY	Mainchain
8	H	156	PRO	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	2282	0	2354	224	0
2	B	4771	0	4777	438	0
3	C	2885	0	2950	242	0
4	D	5415	0	5436	545	0
5	E	1717	0	1709	197	0
6	F	3171	0	3232	260	0
7	G	2687	0	2641	264	0
8	H	1671	0	1673	218	0
All	All	24599	0	24772	1532	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:ILE:CG2	6:F:334:VAL:HG21	1.33	1.58
1:A:278:PRO:HB2	1:A:279:GLU:CB	1.32	1.57
2:B:490:GLU:CA	4:D:560:ARG:NH2	1.71	1.51
1:A:281:SER:CB	1:A:283:ARG:HD2	1.41	1.48
1:A:284:ARG:C	1:A:285:LEU:N	1.69	1.45
6:F:247:MET:HB2	8:H:240:LYS:NZ	1.23	1.44
5:E:114:GLN:CD	7:G:277:PHE:CZ	1.86	1.41
1:A:283:ARG:C	1:A:284:ARG:N	1.70	1.41
1:A:71:ASP:HB3	3:C:114:ARG:NH2	1.18	1.40
1:A:280:PRO:C	1:A:281:SER:N	1.75	1.40
2:B:402:GLU:OE2	4:D:158:ARG:CZ	1.64	1.40
1:A:278:PRO:CG	1:A:279:GLU:HB2	1.51	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:326:ARG:NH1	8:H:295:PRO:HD3	1.30	1.39
5:E:155:ILE:CG2	6:F:334:VAL:CG2	2.00	1.38
2:B:138:LYS:CD	3:C:84:GLN:NE2	1.86	1.38
4:D:288:SER:C	4:D:289:GLU:N	1.78	1.37
2:B:131:MET:CE	3:C:85:VAL:HG21	1.51	1.37
5:E:189:TRP:CZ3	8:H:340:ILE:HD12	1.58	1.37
2:B:138:LYS:CE	3:C:84:GLN:HE22	1.37	1.36
5:E:155:ILE:HG23	6:F:334:VAL:CG2	1.55	1.36
5:E:114:GLN:OE1	7:G:277:PHE:CE2	1.75	1.36
5:E:104:GLU:OE2	5:E:127:TYR:CE2	1.78	1.36
1:A:138:THR:OG1	2:B:92:ILE:CD1	1.75	1.34
5:E:189:TRP:CZ3	8:H:340:ILE:CD1	2.09	1.34
2:B:223:GLU:C	2:B:224:GLY:N	1.81	1.34
2:B:404:GLY:HA2	4:D:459:TRP:CH2	1.63	1.34
5:E:189:TRP:CH2	8:H:340:ILE:CD1	2.10	1.34
1:A:277:VAL:C	1:A:278:PRO:N	1.79	1.33
6:F:326:ARG:HH12	8:H:295:PRO:CD	1.41	1.33
1:A:58:LYS:NZ	4:D:506:SER:OG	1.62	1.31
1:A:278:PRO:CB	1:A:279:GLU:CB	2.07	1.31
1:A:145:THR:HG21	4:D:69:LEU:CD1	1.61	1.30
3:C:63:ARG:NH2	4:D:535:ALA:HB2	1.43	1.29
4:D:307:GLU:CD	7:G:324:ILE:HD11	1.50	1.29
6:F:377:ARG:HH12	8:H:343:GLN:CB	1.45	1.29
2:B:222:PHE:CD1	2:B:241:LEU:HD13	1.68	1.28
5:E:107:SER:HB2	7:G:276:PRO:CD	1.62	1.28
5:E:189:TRP:CH2	8:H:340:ILE:HD12	1.64	1.28
2:B:132:CYS:SG	4:D:119:LEU:HG	1.73	1.27
1:A:278:PRO:CB	1:A:279:GLU:HB2	1.62	1.27
6:F:247:MET:SD	8:H:240:LYS:HG3	1.73	1.27
2:B:80:VAL:CG1	4:D:65:TRP:CZ3	2.16	1.27
5:E:114:GLN:OE1	7:G:277:PHE:CE1	1.88	1.27
1:A:278:PRO:HB2	1:A:279:GLU:CG	1.64	1.26
2:B:125:GLU:OE1	4:D:113:GLU:OE2	1.53	1.26
2:B:138:LYS:CE	3:C:84:GLN:NE2	1.99	1.26
1:A:152:LYS:NZ	2:B:73:ASP:OD2	1.66	1.26
2:B:138:LYS:HD2	3:C:84:GLN:CD	1.56	1.26
5:E:106:ARG:HH11	7:G:271:MET:CA	1.49	1.26
1:A:277:VAL:O	1:A:278:PRO:C	1.74	1.25
3:C:118:ALA:C	3:C:120:SER:H	1.40	1.25
8:H:259:HIS:C	8:H:291:GLU:HG2	1.54	1.25
2:B:120:LYS:NZ	3:C:171:SER:O	1.70	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LYS:NZ	3:C:84:GLN:OE1	1.69	1.25
8:H:359:GLN:HG2	8:H:363:ASP:OD2	1.07	1.24
5:E:104:GLU:OE2	5:E:127:TYR:HE2	0.99	1.24
3:C:63:ARG:HH22	4:D:535:ALA:CB	1.51	1.24
4:D:662:THR:C	4:D:664:SER:H	1.32	1.24
5:E:60:ASN:HB3	8:H:207:HIS:CE1	1.72	1.24
1:A:278:PRO:CB	1:A:279:GLU:HG3	1.67	1.23
4:D:298:ASN:ND2	4:D:300:SER:HB3	1.53	1.23
6:F:53:LYS:HE2	6:F:57:TYR:OH	1.37	1.23
4:D:185:SER:OG	4:D:187:PHE:HD2	1.21	1.22
4:D:307:GLU:CD	7:G:324:ILE:CD1	2.08	1.22
6:F:263:ARG:C	7:G:279:GLN:NE2	1.93	1.22
4:D:307:GLU:OE2	7:G:324:ILE:HD12	1.39	1.21
2:B:138:LYS:HE3	3:C:84:GLN:NE2	1.52	1.21
2:B:97:ILE:HD12	4:D:82:GLN:CD	1.61	1.21
1:A:278:PRO:CB	1:A:279:GLU:CG	2.17	1.20
7:G:274:MET:CE	8:H:280:GLN:HB2	1.72	1.20
1:A:281:SER:OG	1:A:283:ARG:NE	1.73	1.20
1:A:281:SER:OG	1:A:283:ARG:CD	1.89	1.20
2:B:138:LYS:CD	3:C:84:GLN:HE22	1.48	1.19
7:G:274:MET:HE2	8:H:280:GLN:HB2	1.20	1.19
1:A:148:LEU:HD13	2:B:80:VAL:CG2	1.72	1.19
6:F:260:ALA:CB	8:H:258:ARG:HH12	1.55	1.19
6:F:260:ALA:HB1	8:H:258:ARG:NH1	1.55	1.19
2:B:132:CYS:CA	4:D:119:LEU:HD21	1.72	1.17
6:F:260:ALA:CB	8:H:258:ARG:NH1	2.06	1.17
6:F:359:ARG:HG3	8:H:328:GLN:OE1	1.43	1.17
1:A:189:TYR:HD1	3:C:271:MET:HE1	1.04	1.17
3:C:118:ALA:O	3:C:120:SER:N	1.77	1.17
5:E:130:PHE:CE2	6:F:263:ARG:O	1.96	1.17
4:D:352:HIS:HB3	4:D:366:ARG:NH2	1.59	1.17
7:G:59:TYR:CD1	7:G:62:VAL:HG23	1.80	1.17
8:H:294:MET:CE	8:H:298:ALA:HB3	1.73	1.17
6:F:250:GLU:OE2	8:H:244:LYS:NZ	1.77	1.16
4:D:307:GLU:OE2	7:G:324:ILE:CD1	1.92	1.16
5:E:107:SER:HB2	7:G:276:PRO:HD3	1.27	1.16
6:F:53:LYS:CE	6:F:57:TYR:OH	1.93	1.16
4:D:177:ALA:HA	4:D:256:ARG:HH21	1.11	1.16
4:D:352:HIS:CB	4:D:366:ARG:HH21	1.56	1.16
1:A:71:ASP:CB	3:C:114:ARG:NH2	2.09	1.15
1:A:148:LEU:CD1	2:B:80:VAL:CG2	2.23	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASP:OD1	4:D:49:HIS:CE1	1.99	1.15
2:B:132:CYS:SG	4:D:119:LEU:CG	2.33	1.15
7:G:59:TYR:HD1	7:G:62:VAL:HG23	1.00	1.15
4:D:185:SER:OG	4:D:187:PHE:CD2	1.91	1.15
8:H:294:MET:HE1	8:H:298:ALA:CB	1.77	1.15
1:A:278:PRO:HB3	1:A:279:GLU:HG3	1.29	1.15
8:H:259:HIS:C	8:H:291:GLU:CG	2.15	1.15
6:F:377:ARG:HH12	8:H:343:GLN:CA	1.60	1.14
6:F:377:ARG:NH1	8:H:343:GLN:HA	1.62	1.14
2:B:132:CYS:HA	4:D:119:LEU:CD2	1.77	1.13
4:D:175:PHE:CE1	4:D:193:LEU:HD21	1.83	1.13
4:D:662:THR:C	4:D:664:SER:N	1.95	1.13
2:B:490:GLU:HA	4:D:560:ARG:NH2	0.81	1.13
4:D:298:ASN:HD21	4:D:300:SER:HB3	0.99	1.13
7:G:143:VAL:HG22	8:H:159:MET:HE3	1.16	1.13
2:B:80:VAL:CG1	4:D:65:TRP:CH2	2.32	1.13
6:F:325:GLU:OE2	6:F:325:GLU:HA	1.39	1.13
6:F:377:ARG:NH1	8:H:343:GLN:CA	2.10	1.13
4:D:199:VAL:HG21	4:D:241:VAL:HG21	1.18	1.12
4:D:352:HIS:HB3	4:D:366:ARG:HH21	0.95	1.11
6:F:10:ALA:O	6:F:13:ARG:HG2	1.49	1.11
5:E:106:ARG:HH11	7:G:271:MET:N	1.47	1.10
7:G:280:PHE:HE2	8:H:258:ARG:O	1.32	1.10
5:E:106:ARG:HH11	7:G:271:MET:C	1.45	1.10
2:B:80:VAL:HG12	4:D:65:TRP:CZ3	1.85	1.10
2:B:77:LEU:HD21	4:D:61:GLY:HA3	1.20	1.10
1:A:148:LEU:CD1	2:B:80:VAL:HG22	1.78	1.10
2:B:97:ILE:HD11	4:D:82:GLN:HB3	1.10	1.10
8:H:359:GLN:CG	8:H:363:ASP:OD2	2.00	1.10
1:A:189:TYR:CD1	3:C:271:MET:CE	2.34	1.09
2:B:138:LYS:CG	3:C:84:GLN:NE2	2.15	1.09
1:A:145:THR:HG21	4:D:69:LEU:HD11	1.24	1.09
3:C:131:GLY:O	4:D:140:LYS:NZ	1.86	1.09
2:B:55:ASP:CG	4:D:49:HIS:HE1	1.56	1.09
7:G:280:PHE:CE2	8:H:258:ARG:O	2.06	1.09
1:A:281:SER:CB	1:A:283:ARG:CD	2.31	1.08
7:G:143:VAL:HG22	8:H:159:MET:CE	1.81	1.08
7:G:312:ARG:HH12	8:H:323:ALA:HB2	1.07	1.08
6:F:206:MET:CE	8:H:199:LYS:HG3	1.84	1.08
2:B:175:MET:HG3	4:D:460:PRO:HG3	1.27	1.08
1:A:189:TYR:CD1	3:C:271:MET:HE1	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:ASN:HB3	8:H:207:HIS:NE2	1.68	1.08
8:H:294:MET:CE	8:H:298:ALA:CB	2.29	1.07
2:B:97:ILE:HD11	4:D:82:GLN:CB	1.84	1.07
6:F:377:ARG:NH1	8:H:343:GLN:CB	2.18	1.07
2:B:443:ASP:OD1	4:D:509:ARG:NH2	1.88	1.06
3:C:63:ARG:NH2	4:D:535:ALA:CB	2.13	1.06
1:A:152:LYS:NZ	2:B:73:ASP:CG	2.09	1.06
5:E:104:GLU:OE2	5:E:124:GLU:OE2	1.71	1.06
6:F:173:LEU:HD12	7:G:118:VAL:HG21	1.19	1.06
1:A:58:LYS:NZ	4:D:506:SER:CB	2.19	1.06
4:D:8:GLN:HG3	4:D:28:GLU:OE1	1.53	1.06
5:E:106:ARG:NH1	7:G:271:MET:C	1.95	1.06
2:B:490:GLU:HA	4:D:560:ARG:CZ	1.85	1.06
5:E:104:GLU:OE1	5:E:126:SER:OG	1.73	1.06
5:E:114:GLN:OE1	7:G:277:PHE:CZ	0.71	1.06
2:B:135:SER:OG	4:D:121:CYS:SG	2.10	1.05
1:A:149:VAL:HG13	2:B:70:PRO:HG2	1.35	1.05
5:E:189:TRP:CH2	8:H:340:ILE:HD13	1.88	1.05
7:G:130:ILE:HG22	7:G:131:LEU:N	1.72	1.05
2:B:80:VAL:HG11	4:D:65:TRP:CH2	1.89	1.05
2:B:567:LYS:NZ	4:D:626:TRP:O	1.87	1.05
6:F:173:LEU:CD1	7:G:118:VAL:HG21	1.86	1.05
3:C:63:ARG:HH22	4:D:535:ALA:HB2	0.99	1.04
6:F:173:LEU:HD12	7:G:118:VAL:CG2	1.86	1.04
2:B:138:LYS:CD	3:C:84:GLN:CD	2.20	1.04
7:G:280:PHE:CE1	8:H:287:LYS:HG3	1.90	1.04
2:B:77:LEU:HD21	4:D:61:GLY:CA	1.87	1.04
4:D:4:ARG:HG3	4:D:32:GLN:NE2	1.73	1.04
7:G:124:THR:HG22	7:G:125:ILE:HG13	1.39	1.04
2:B:131:MET:HE3	3:C:85:VAL:HG21	1.40	1.03
6:F:247:MET:CB	8:H:240:LYS:NZ	2.18	1.03
2:B:483:ARG:HH21	4:D:549:GLN:NE2	1.57	1.03
1:A:145:THR:HG21	4:D:69:LEU:HD13	1.40	1.03
5:E:155:ILE:HG21	6:F:334:VAL:CG2	1.86	1.03
2:B:77:LEU:CD2	4:D:61:GLY:HA3	1.89	1.02
1:A:128:LEU:HD22	4:D:97:ARG:NH2	1.74	1.02
2:B:138:LYS:HG3	3:C:84:GLN:NE2	1.73	1.02
1:A:278:PRO:HG2	1:A:279:GLU:HB2	1.07	1.02
5:E:102:LEU:CD2	7:G:255:ILE:HD12	1.88	1.02
6:F:377:ARG:HH12	8:H:343:GLN:CG	1.72	1.02
2:B:407:VAL:HG21	4:D:459:TRP:CZ3	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:305:PRO:O	4:D:307:GLU:N	1.93	1.01
2:B:94:GLU:O	2:B:96:ALA:N	1.93	1.01
1:A:278:PRO:HB2	1:A:279:GLU:CA	1.78	1.01
2:B:132:CYS:HA	4:D:119:LEU:HD21	1.04	1.01
1:A:113:ILE:HG23	3:C:172:PHE:CZ	1.96	1.01
6:F:227:ILE:HA	8:H:223:ARG:HH22	1.26	1.01
1:A:266:LEU:HD12	3:C:345:LEU:HG	1.42	1.00
3:C:273:GLU:OE2	4:D:614:TYR:OH	1.79	1.00
2:B:138:LYS:CE	3:C:84:GLN:OE1	2.09	1.00
5:E:102:LEU:HD22	7:G:255:ILE:HD12	1.43	1.00
4:D:189:GLU:OE2	4:D:197:ARG:NH2	1.95	1.00
6:F:227:ILE:HA	8:H:223:ARG:NH2	1.75	1.00
2:B:138:LYS:HE3	3:C:84:GLN:HE22	1.04	0.99
3:C:118:ALA:C	3:C:120:SER:N	2.07	0.99
3:C:236:ARG:HH12	4:D:575:THR:HA	1.22	0.99
1:A:138:THR:OG1	2:B:92:ILE:HD12	1.62	0.99
1:A:279:GLU:CB	1:A:280:PRO:HD3	1.92	0.99
6:F:192:TYR:HH	7:G:173:TRP:HE1	1.04	0.98
3:C:63:ARG:NH1	4:D:537:GLU:OE2	1.94	0.98
2:B:379:LYS:NZ	2:B:383:GLU:OE1	1.96	0.98
1:A:281:SER:HB3	1:A:283:ARG:HD2	1.00	0.98
2:B:424:LEU:HD22	4:D:484:ILE:CD1	1.94	0.98
6:F:359:ARG:CG	8:H:328:GLN:OE1	2.11	0.98
2:B:55:ASP:CG	4:D:49:HIS:CE1	2.36	0.98
4:D:175:PHE:CD1	4:D:193:LEU:HD21	1.98	0.98
6:F:206:MET:HE3	8:H:199:LYS:HG3	1.45	0.98
5:E:104:GLU:CD	5:E:124:GLU:CD	2.23	0.97
5:E:49:LEU:HD23	8:H:196:ASN:HD22	1.24	0.97
4:D:509:ARG:HD3	4:D:521:PHE:CE2	1.98	0.97
1:A:281:SER:OG	1:A:283:ARG:HD2	1.56	0.97
2:B:138:LYS:CE	3:C:84:GLN:CD	2.31	0.97
3:C:229:LEU:HD21	4:D:571:LEU:HD12	1.43	0.97
4:D:509:ARG:NH1	4:D:521:PHE:HZ	1.61	0.97
7:G:62:VAL:HG12	7:G:66:LEU:HD12	1.47	0.97
4:D:177:ALA:HA	4:D:256:ARG:NH2	1.80	0.96
1:A:278:PRO:CG	1:A:279:GLU:CB	2.39	0.96
2:B:131:MET:CE	3:C:85:VAL:CG2	2.43	0.96
2:B:297:VAL:HG11	4:D:355:LEU:HD11	1.47	0.96
4:D:175:PHE:HD1	4:D:193:LEU:HD11	1.27	0.96
1:A:279:GLU:HB3	1:A:280:PRO:HD3	1.44	0.96
8:H:294:MET:HE1	8:H:298:ALA:HB3	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:PHE:CE2	4:D:141:ARG:NH1	2.33	0.96
5:E:130:PHE:CZ	6:F:263:ARG:O	2.19	0.96
6:F:260:ALA:HB1	8:H:258:ARG:HH12	0.82	0.96
2:B:138:LYS:CG	3:C:84:GLN:HE22	1.75	0.95
1:A:138:THR:OG1	2:B:92:ILE:HD13	1.64	0.95
2:B:407:VAL:CG2	4:D:459:TRP:HZ3	1.77	0.95
1:A:12:LEU:HB3	1:A:21:LEU:HD21	1.49	0.95
1:A:278:PRO:HG2	1:A:279:GLU:CB	1.95	0.95
4:D:374:ARG:NH1	5:E:218:GLU:OE1	1.99	0.95
7:G:62:VAL:HG12	7:G:66:LEU:CD1	1.96	0.95
6:F:57:TYR:OH	6:F:88:ASP:OD1	1.84	0.95
5:E:97:HIS:NE2	8:H:247:TYR:OH	1.92	0.95
5:E:106:ARG:NH1	7:G:271:MET:N	2.14	0.95
7:G:59:TYR:HD1	7:G:62:VAL:CG2	1.79	0.94
2:B:490:GLU:HG2	4:D:560:ARG:CZ	1.97	0.94
2:B:404:GLY:HA2	4:D:459:TRP:HH2	1.25	0.94
2:B:522:THR:HG23	4:D:590:TYR:CE2	2.03	0.94
7:G:47:ARG:NH1	7:G:108:GLN:OE1	2.00	0.94
2:B:483:ARG:HH21	4:D:549:GLN:HE22	1.04	0.94
4:D:197:ARG:CG	4:D:201:LYS:HE3	1.97	0.94
2:B:84:PHE:HE2	4:D:65:TRP:CE3	1.86	0.94
5:E:107:SER:HA	7:G:273:PRO:HA	1.48	0.94
2:B:91:ALA:O	2:B:93:GLU:N	2.01	0.94
6:F:326:ARG:NH1	8:H:295:PRO:CD	2.12	0.94
4:D:658:LEU:O	4:D:662:THR:OG1	1.85	0.94
4:D:199:VAL:CG2	4:D:241:VAL:HG21	1.97	0.93
6:F:263:ARG:C	7:G:279:GLN:HE22	1.71	0.93
2:B:166:SER:OG	4:D:152:ASN:ND2	2.01	0.93
1:A:58:LYS:HZ3	4:D:506:SER:CB	1.75	0.93
2:B:166:SER:CB	4:D:152:ASN:HD21	1.80	0.93
2:B:80:VAL:HG11	4:D:65:TRP:CZ3	1.97	0.93
5:E:135:LEU:HB3	5:E:136:PRO:HD3	1.51	0.93
2:B:131:MET:HE1	3:C:85:VAL:HG21	1.50	0.93
2:B:175:MET:HG3	4:D:460:PRO:CG	1.98	0.93
4:D:175:PHE:CD1	4:D:193:LEU:HD11	2.03	0.93
7:G:130:ILE:HG22	7:G:131:LEU:H	1.27	0.93
2:B:2:SER:OG	2:B:28:ASP:OD1	1.88	0.92
2:B:443:ASP:CG	4:D:509:ARG:HH22	1.72	0.92
6:F:247:MET:CB	8:H:240:LYS:HZ1	1.79	0.92
6:F:247:MET:CE	8:H:243:PHE:HD1	1.81	0.92
1:A:71:ASP:HB3	3:C:114:ARG:HH22	1.16	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:38:GLU:O	7:G:42:THR:OG1	1.87	0.92
7:G:92:HIS:HE1	7:G:93:PHE:CE1	1.88	0.92
2:B:404:GLY:CA	4:D:459:TRP:CH2	2.52	0.92
5:E:130:PHE:HE2	6:F:263:ARG:O	1.46	0.92
2:B:402:GLU:OE2	4:D:158:ARG:NH1	2.01	0.92
2:B:181:PRO:HG3	2:B:189:SER:OG	1.70	0.92
1:A:189:TYR:CD1	3:C:271:MET:HE3	2.03	0.92
2:B:134:LYS:CD	3:C:85:VAL:HG13	2.00	0.92
4:D:197:ARG:HG2	4:D:201:LYS:HE3	1.49	0.91
2:B:407:VAL:CG2	4:D:459:TRP:CZ3	2.53	0.91
2:B:222:PHE:CE1	2:B:241:LEU:HD13	2.05	0.91
4:D:137:PHE:HE2	4:D:141:ARG:NH1	1.67	0.91
4:D:199:VAL:HG21	4:D:241:VAL:CG2	1.99	0.91
2:B:507:LEU:CD1	4:D:579:THR:HG22	2.01	0.91
2:B:35:ASP:HB3	4:D:30:MET:CE	2.01	0.91
1:A:281:SER:HB3	1:A:283:ARG:CD	1.96	0.90
6:F:313:GLN:HE21	8:H:282:HIS:CE1	1.90	0.90
2:B:132:CYS:SG	4:D:119:LEU:CD2	2.59	0.90
5:E:49:LEU:HD23	8:H:196:ASN:ND2	1.85	0.90
2:B:55:ASP:OD1	4:D:49:HIS:HE1	1.39	0.90
6:F:260:ALA:HB3	8:H:258:ARG:NH1	1.84	0.90
5:E:114:GLN:CD	7:G:277:PHE:HZ	1.38	0.90
7:G:312:ARG:NH1	8:H:323:ALA:HB2	1.85	0.90
2:B:263:GLN:NE2	2:B:346:ASN:ND2	2.19	0.90
1:A:1:MET:CE	1:A:28:THR:HG22	2.02	0.90
2:B:264:LEU:HD13	6:F:381:TRP:CH2	2.07	0.89
4:D:76:ARG:O	4:D:79:GLU:HB2	1.69	0.89
2:B:132:CYS:CB	4:D:119:LEU:HD21	2.02	0.89
3:C:4:THR:HG23	3:C:33:ILE:HD11	1.54	0.89
7:G:274:MET:HE2	8:H:280:GLN:CB	2.01	0.89
2:B:443:ASP:CG	4:D:509:ARG:NH2	2.26	0.89
2:B:500:LEU:HD21	4:D:571:LEU:CD1	2.03	0.89
7:G:92:HIS:CE1	7:G:93:PHE:CE1	2.60	0.89
7:G:131:LEU:O	7:G:132:GLU:C	2.04	0.89
1:A:145:THR:HG23	4:D:65:TRP:CZ2	2.07	0.89
2:B:424:LEU:CD2	4:D:484:ILE:CD1	2.50	0.89
3:C:5:LEU:HD12	3:C:22:LEU:CD1	2.01	0.89
5:E:77:ASP:OD2	6:F:238:ARG:NE	2.05	0.89
1:A:149:VAL:HG13	2:B:70:PRO:CG	2.02	0.88
4:D:122:GLU:HG3	4:D:512:ASN:HD21	1.35	0.88
5:E:106:ARG:NH1	7:G:271:MET:CA	2.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:241:TRP:CZ2	7:G:238:LEU:HD21	2.08	0.88
5:E:155:ILE:HG21	6:F:334:VAL:HG23	1.54	0.88
2:B:424:LEU:HD22	4:D:484:ILE:HD12	1.56	0.88
2:B:249:ASP:O	2:B:250:GLY:O	1.92	0.88
2:B:74:GLU:OE1	4:D:54:ARG:HG3	1.73	0.88
5:E:104:GLU:CD	5:E:124:GLU:OE2	2.12	0.88
5:E:181:GLU:CD	7:G:335:ARG:HH12	1.78	0.88
7:G:41:CYS:HA	7:G:47:ARG:NH1	1.89	0.88
1:A:235:LEU:HD11	3:C:313:ILE:HG22	1.56	0.88
4:D:509:ARG:NH1	4:D:521:PHE:CZ	2.38	0.87
2:B:507:LEU:HD12	4:D:579:THR:HG22	1.55	0.87
6:F:44:GLY:H	6:F:47:MET:HE2	1.37	0.87
6:F:224:ASP:OD2	8:H:216:LEU:HD21	1.75	0.87
4:D:528:VAL:HG13	4:D:546:MET:SD	2.15	0.87
3:C:236:ARG:NH2	4:D:579:THR:OG1	2.07	0.87
5:E:107:SER:HB2	7:G:276:PRO:HD2	1.55	0.87
6:F:173:LEU:CD1	7:G:118:VAL:CG2	2.47	0.87
6:F:206:MET:HE1	8:H:199:LYS:HG3	1.57	0.86
5:E:107:SER:CB	7:G:276:PRO:HD3	2.05	0.86
5:E:189:TRP:CZ3	8:H:340:ILE:HD11	2.06	0.86
2:B:483:ARG:NH2	4:D:549:GLN:HE22	1.72	0.86
8:H:257:THR:O	8:H:287:LYS:CE	2.23	0.86
1:A:58:LYS:HZ1	4:D:506:SER:HB2	1.39	0.86
2:B:97:ILE:CD1	4:D:82:GLN:CD	2.44	0.86
2:B:134:LYS:HD3	3:C:85:VAL:HG13	1.55	0.86
6:F:326:ARG:NH2	7:G:291:GLU:OE2	2.07	0.86
1:A:145:THR:CG2	4:D:69:LEU:HD11	2.05	0.86
1:A:148:LEU:HD13	2:B:80:VAL:HG21	1.58	0.86
8:H:259:HIS:C	8:H:291:GLU:CD	2.35	0.86
6:F:53:LYS:HE3	6:F:57:TYR:OH	1.75	0.86
2:B:97:ILE:CD1	4:D:82:GLN:HB3	2.00	0.86
4:D:352:HIS:CG	4:D:366:ARG:HE	1.94	0.86
2:B:138:LYS:CD	3:C:84:GLN:OE1	2.23	0.85
2:B:490:GLU:HA	4:D:560:ARG:HH22	1.41	0.85
3:C:63:ARG:HH12	4:D:535:ALA:HB1	1.39	0.85
3:C:129:ILE:CD1	4:D:489:LEU:HD13	2.06	0.85
4:D:662:THR:O	4:D:664:SER:N	2.07	0.85
1:A:283:ARG:O	1:A:284:ARG:N	2.09	0.85
3:C:227:VAL:HG22	3:C:230:ARG:HH21	1.41	0.85
4:D:46:ILE:HG23	4:D:50:ILE:HD12	1.58	0.85
5:E:148:TYR:OH	7:G:289:PHE:CD1	2.30	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LYS:HD2	3:C:84:GLN:NE2	1.69	0.84
5:E:181:GLU:CG	7:G:335:ARG:HH12	1.88	0.84
4:D:352:HIS:CD2	4:D:366:ARG:HE	1.95	0.84
6:F:247:MET:SD	8:H:240:LYS:CG	2.64	0.84
3:C:18:ASP:OD1	3:C:21:ASP:CG	2.15	0.84
4:D:352:HIS:CG	4:D:366:ARG:HH21	1.95	0.84
2:B:132:CYS:SG	4:D:119:LEU:HD21	2.16	0.84
4:D:189:GLU:OE1	4:D:197:ARG:NH1	2.10	0.84
2:B:507:LEU:CD1	4:D:579:THR:CG2	2.55	0.84
1:A:189:TYR:HD1	3:C:271:MET:CE	1.77	0.84
1:A:71:ASP:HB3	3:C:114:ARG:HH21	1.37	0.84
2:B:522:THR:OG1	4:D:593:GLU:OE2	1.95	0.83
3:C:229:LEU:CD2	4:D:571:LEU:HD12	2.07	0.83
4:D:298:ASN:ND2	4:D:300:SER:CB	2.40	0.83
7:G:249:THR:HG23	8:H:243:PHE:CD2	2.12	0.83
2:B:138:LYS:HD2	3:C:84:GLN:OE1	1.75	0.83
2:B:550:LEU:HD11	3:C:276:VAL:HG21	1.59	0.83
4:D:190:PRO:HD2	4:D:193:LEU:HD12	1.59	0.83
6:F:44:GLY:O	6:F:47:MET:HE2	1.77	0.83
2:B:131:MET:HE2	3:C:85:VAL:HG21	1.60	0.83
4:D:175:PHE:CE1	4:D:193:LEU:CD2	2.62	0.83
8:H:257:THR:O	8:H:287:LYS:NZ	2.11	0.83
7:G:41:CYS:HA	7:G:47:ARG:HH12	1.40	0.83
3:C:270:ARG:HD2	4:D:614:TYR:OH	1.79	0.83
2:B:490:GLU:CB	4:D:560:ARG:NH2	2.41	0.82
6:F:247:MET:HB2	8:H:240:LYS:HZ1	1.02	0.82
8:H:359:GLN:HG2	8:H:363:ASP:CG	1.98	0.82
2:B:30:LEU:CD2	4:D:34:LEU:HD23	2.09	0.82
1:A:128:LEU:HD22	4:D:97:ARG:HH21	1.42	0.82
1:A:77:LEU:HD22	3:C:154:LEU:CD2	2.10	0.82
2:B:402:GLU:OE2	4:D:158:ARG:NH2	2.12	0.82
1:A:171:LYS:HE2	1:A:175:ARG:NH2	1.94	0.82
2:B:84:PHE:HE2	4:D:65:TRP:CZ3	1.97	0.82
5:E:111:ARG:NH1	7:G:276:PRO:O	2.12	0.82
6:F:92:ARG:NH1	6:F:118:PHE:O	2.13	0.82
7:G:139:GLU:HG3	8:H:155:VAL:HG22	1.61	0.82
1:A:266:LEU:CD1	3:C:345:LEU:HG	2.09	0.82
2:B:97:ILE:CD1	4:D:82:GLN:CG	2.57	0.82
2:B:376:MET:HE1	4:D:211:HIS:HB2	1.60	0.82
6:F:230:LYS:HE3	8:H:222:LEU:HD23	1.60	0.82
1:A:148:LEU:HD11	2:B:80:VAL:HG22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:280:PHE:CD1	8:H:287:LYS:HG3	2.15	0.81
6:F:247:MET:HB2	8:H:240:LYS:HZ2	1.02	0.81
6:F:377:ARG:HH22	8:H:343:GLN:CD	1.83	0.81
6:F:377:ARG:HH22	8:H:343:GLN:CG	1.92	0.81
7:G:274:MET:SD	8:H:280:GLN:HB2	2.19	0.81
3:C:5:LEU:HD12	3:C:22:LEU:HD12	1.61	0.81
4:D:191:GLU:HG3	4:D:194:ARG:HH21	1.43	0.81
4:D:304:ASP:C	4:D:306:GLN:H	1.83	0.81
3:C:229:LEU:HD21	4:D:571:LEU:CD1	2.11	0.81
6:F:377:ARG:HH12	8:H:343:GLN:HG3	1.44	0.81
1:A:145:THR:OG1	4:D:65:TRP:CZ2	2.34	0.81
5:E:97:HIS:HE2	8:H:247:TYR:HH	0.84	0.81
1:A:172:VAL:HG13	3:C:253:ILE:HG21	1.61	0.81
5:E:104:GLU:OE1	5:E:124:GLU:CD	2.19	0.81
2:B:222:PHE:CD1	2:B:241:LEU:CD1	2.58	0.81
1:A:235:LEU:HD11	3:C:313:ILE:CG2	2.11	0.80
1:A:141:ARG:HG3	3:C:220:GLN:HE22	1.46	0.80
3:C:236:ARG:NH1	4:D:575:THR:HA	1.96	0.80
1:A:141:ARG:HG3	3:C:220:GLN:NE2	1.96	0.80
2:B:329:ILE:HD13	4:D:386:MET:SD	2.21	0.80
2:B:120:LYS:HZ1	3:C:175:PRO:HA	1.46	0.80
3:C:18:ASP:OD1	3:C:21:ASP:OD2	1.98	0.80
7:G:239:ARG:HG3	8:H:232:VAL:HG21	1.63	0.80
1:A:279:GLU:CB	1:A:280:PRO:CD	2.56	0.80
4:D:192:VAL:HG22	4:D:245:HIS:ND1	1.97	0.80
4:D:122:GLU:HG3	4:D:512:ASN:ND2	1.96	0.80
5:E:179:MET:HG2	8:H:329:ILE:HD11	1.63	0.80
1:A:124:VAL:HG21	2:B:110:GLN:NE2	1.97	0.79
7:G:249:THR:HG23	8:H:243:PHE:CG	2.17	0.79
4:D:453:GLN:HA	4:D:457:LEU:HD12	1.61	0.79
7:G:131:LEU:O	7:G:132:GLU:O	2.01	0.79
1:A:281:SER:OG	1:A:283:ARG:CZ	2.30	0.79
2:B:87:SER:O	2:B:89:VAL:N	2.16	0.79
2:B:500:LEU:HD21	4:D:571:LEU:HD13	1.62	0.79
5:E:104:GLU:CD	5:E:127:TYR:CE2	2.56	0.79
4:D:4:ARG:HG3	4:D:32:GLN:HE21	1.43	0.79
6:F:44:GLY:H	6:F:47:MET:CE	1.95	0.79
2:B:407:VAL:HG21	4:D:459:TRP:CE3	2.17	0.79
3:C:141:LEU:HG	3:C:142:PRO:HD2	1.65	0.78
6:F:326:ARG:HH11	8:H:295:PRO:HD3	1.45	0.78
4:D:211:HIS:CE1	4:D:215:ILE:CD1	2.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:C	3:C:114:ARG:HH21	1.86	0.78
2:B:80:VAL:HG13	4:D:65:TRP:CH2	2.15	0.78
2:B:97:ILE:HD12	4:D:82:GLN:CG	2.13	0.78
6:F:261:VAL:O	7:G:279:GLN:OE1	2.01	0.78
2:B:43:PHE:CZ	4:D:46:ILE:HD13	2.18	0.78
4:D:280:PRO:O	4:D:281:SER:C	2.09	0.78
5:E:106:ARG:O	7:G:273:PRO:HB3	1.84	0.78
5:E:181:GLU:CD	7:G:335:ARG:NH1	2.37	0.78
6:F:377:ARG:HH22	8:H:343:GLN:HG3	1.46	0.78
1:A:152:LYS:HZ1	2:B:73:ASP:CG	1.78	0.78
5:E:111:ARG:HH22	7:G:280:PHE:HB2	1.48	0.78
6:F:325:GLU:OE2	6:F:325:GLU:CA	2.26	0.78
2:B:35:ASP:HB3	4:D:30:MET:HE1	1.64	0.78
2:B:513:PRO:HG2	2:B:519:MET:CE	2.13	0.78
3:C:180:GLU:OE1	3:C:188:LYS:NZ	2.17	0.78
5:E:9:PRO:CB	6:F:197:GLN:OE1	2.32	0.78
6:F:241:TRP:HZ2	7:G:238:LEU:HD21	1.48	0.78
1:A:277:VAL:O	1:A:278:PRO:CA	2.31	0.78
4:D:117:GLN:O	4:D:119:LEU:N	2.17	0.78
1:A:279:GLU:HB3	1:A:280:PRO:CD	2.08	0.77
2:B:566:GLU:HA	2:B:569:LEU:HD12	1.66	0.77
6:F:263:ARG:C	7:G:279:GLN:CD	2.42	0.77
1:A:211:HIS:HA	4:D:630:VAL:HG23	1.65	0.77
2:B:96:ALA:C	2:B:98:GLU:N	2.34	0.77
2:B:399:VAL:HA	4:D:158:ARG:NH1	1.99	0.77
2:B:80:VAL:HG11	4:D:65:TRP:CZ2	2.18	0.77
7:G:274:MET:CE	8:H:280:GLN:CB	2.58	0.77
2:B:96:ALA:C	2:B:98:GLU:H	1.86	0.77
3:C:5:LEU:CD1	3:C:22:LEU:HD12	2.15	0.77
5:E:221:HIS:HB3	5:E:222:PRO:O	1.85	0.77
1:A:145:THR:HG23	4:D:65:TRP:HZ2	1.48	0.77
1:A:240:ASP:O	1:A:251:LYS:NZ	2.17	0.77
2:B:30:LEU:HD21	4:D:34:LEU:HD23	1.65	0.77
4:D:177:ALA:CA	4:D:256:ARG:NH2	2.46	0.77
2:B:522:THR:HG22	2:B:524:GLU:OE2	1.85	0.77
6:F:227:ILE:CA	8:H:223:ARG:HH22	1.97	0.77
1:A:152:LYS:HZ2	2:B:73:ASP:CG	1.79	0.77
2:B:196:GLN:O	2:B:197:LEU:HB2	1.85	0.77
5:E:9:PRO:HB3	6:F:197:GLN:OE1	1.85	0.77
6:F:247:MET:CB	8:H:240:LYS:HZ2	1.86	0.77
4:D:528:VAL:CG1	4:D:546:MET:SD	2.73	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:LYS:O	4:D:270:PHE:CD2	2.38	0.76
6:F:166:LYS:NZ	7:G:87:ASP:OD2	2.13	0.76
1:A:189:TYR:HA	3:C:271:MET:CE	2.15	0.76
2:B:94:GLU:CD	4:D:79:GLU:OE2	2.17	0.76
2:B:190:GLN:HE22	4:D:171:ARG:H	1.33	0.76
3:C:14:MET:SD	4:D:552:PHE:HA	2.26	0.76
2:B:94:GLU:OE1	4:D:79:GLU:OE2	2.04	0.76
2:B:451:GLN:HG3	2:B:463:ARG:HH12	1.50	0.76
2:B:513:PRO:HG2	2:B:519:MET:HE2	1.68	0.76
4:D:211:HIS:CE1	4:D:215:ILE:HD11	2.21	0.76
2:B:456:ASP:C	2:B:458:THR:H	1.88	0.76
2:B:289:TRP:CE2	2:B:293:ASN:ND2	2.52	0.76
4:D:177:ALA:CA	4:D:256:ARG:HH21	1.94	0.76
6:F:326:ARG:HH12	8:H:295:PRO:CG	1.99	0.76
1:A:148:LEU:HD13	2:B:80:VAL:HG23	1.68	0.76
5:E:102:LEU:HD22	7:G:255:ILE:CD1	2.15	0.76
2:B:507:LEU:HD12	4:D:579:THR:CG2	2.15	0.76
6:F:171:ASN:OD1	7:G:149:ASN:ND2	2.19	0.76
2:B:490:GLU:CG	4:D:560:ARG:CZ	2.64	0.75
6:F:9:LEU:HD22	6:F:124:PRO:HB3	1.68	0.75
2:B:131:MET:HE1	3:C:85:VAL:CG2	2.13	0.75
2:B:490:GLU:HG2	4:D:560:ARG:NH1	2.01	0.75
4:D:68:GLN:O	4:D:72:THR:OG1	2.04	0.75
5:E:121:LEU:CD2	8:H:276:LEU:HD21	2.16	0.75
5:E:148:TYR:OH	7:G:289:PHE:CE1	2.39	0.75
6:F:234:ILE:HG12	8:H:226:ILE:HD11	1.68	0.75
2:B:424:LEU:CD2	4:D:484:ILE:HD11	2.15	0.75
1:A:277:VAL:C	1:A:278:PRO:CA	2.55	0.75
6:F:377:ARG:NH2	8:H:343:GLN:HG3	2.02	0.75
2:B:376:MET:CE	4:D:211:HIS:HB2	2.15	0.75
1:A:277:VAL:HG12	1:A:278:PRO:HA	1.68	0.75
2:B:88:LYS:O	2:B:90:PRO:HD3	1.86	0.75
3:C:116:LEU:HD12	3:C:137:LEU:CD1	2.16	0.75
2:B:222:PHE:CE1	2:B:241:LEU:CD1	2.70	0.75
5:E:148:TYR:HH	7:G:289:PHE:HD1	1.28	0.75
7:G:274:MET:HE1	8:H:280:GLN:N	2.00	0.75
3:C:63:ARG:NH1	4:D:535:ALA:HB1	2.02	0.74
6:F:377:ARG:NH1	8:H:343:GLN:HG3	2.01	0.74
1:A:189:TYR:HA	3:C:271:MET:HE1	1.68	0.74
2:B:132:CYS:HG	4:D:119:LEU:HG	1.50	0.74
1:A:33:ILE:HG23	3:C:15:LEU:HD22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:TRP:CE2	4:D:20:LEU:HD13	2.21	0.74
5:E:107:SER:HA	7:G:273:PRO:CA	2.17	0.74
1:A:211:HIS:HA	4:D:630:VAL:CG2	2.17	0.74
3:C:121:VAL:CG1	3:C:122:PRO:HD2	2.17	0.74
1:A:145:THR:CG2	4:D:65:TRP:CZ2	2.70	0.74
1:A:141:ARG:HE	3:C:220:GLN:NE2	1.85	0.74
2:B:443:ASP:OD2	4:D:509:ARG:NH2	2.21	0.74
6:F:377:ARG:NH1	8:H:343:GLN:HB2	2.00	0.74
4:D:288:SER:O	4:D:289:GLU:N	2.20	0.74
5:E:114:GLN:NE2	8:H:284:ALA:HB2	2.03	0.74
6:F:247:MET:CE	8:H:243:PHE:CD1	2.70	0.74
6:F:359:ARG:HG3	8:H:328:GLN:CD	2.07	0.74
2:B:522:THR:HG23	4:D:590:TYR:HE2	1.53	0.74
2:B:193:PHE:O	2:B:196:GLN:HB2	1.87	0.74
2:B:287:LEU:HD21	4:D:343:HIS:HD2	1.52	0.73
2:B:166:SER:CB	4:D:152:ASN:ND2	2.50	0.73
2:B:42:TRP:CD2	4:D:20:LEU:HD13	2.23	0.73
5:E:141:PHE:CA	7:G:289:PHE:HZ	2.01	0.73
2:B:458:THR:O	2:B:460:LYS:N	2.20	0.73
6:F:92:ARG:NH1	6:F:119:LEU:HA	2.04	0.73
2:B:297:VAL:CG1	4:D:355:LEU:HD11	2.17	0.73
4:D:571:LEU:O	4:D:575:THR:HG23	1.88	0.73
3:C:116:LEU:CD1	3:C:137:LEU:HD11	2.19	0.73
4:D:199:VAL:HG22	4:D:237:MET:HG3	1.69	0.73
4:D:305:PRO:C	4:D:307:GLU:H	1.91	0.73
1:A:1:MET:HE3	1:A:28:THR:HG22	1.71	0.73
7:G:130:ILE:CG2	7:G:131:LEU:N	2.49	0.73
2:B:132:CYS:SG	4:D:119:LEU:CD1	2.76	0.72
4:D:601:MET:HE2	4:D:604:LEU:HD12	1.69	0.72
5:E:107:SER:CB	7:G:276:PRO:CD	2.57	0.72
6:F:247:MET:HE2	8:H:243:PHE:CD1	2.25	0.72
1:A:228:SER:HA	3:C:307:LEU:HD12	1.71	0.72
6:F:60:PHE:HE1	6:F:99:LEU:HD11	1.54	0.72
3:C:63:ARG:HH22	4:D:535:ALA:HB1	1.53	0.72
1:A:145:THR:CG2	4:D:65:TRP:HZ2	2.01	0.72
3:C:303:GLU:OE2	3:C:303:GLU:HA	1.88	0.72
6:F:287:ARG:HD3	6:F:321:LEU:HD21	1.71	0.72
2:B:84:PHE:CE2	4:D:65:TRP:CZ3	2.76	0.72
2:B:424:LEU:HD22	4:D:484:ILE:HD11	1.70	0.72
6:F:338:LEU:HD12	8:H:304:SER:HB3	1.71	0.72
1:A:138:THR:OG1	2:B:92:ILE:HD11	1.82	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:163:ASP:OD2	7:G:59:TYR:OH	2.03	0.72
7:G:124:THR:HG22	7:G:125:ILE:H	1.55	0.72
2:B:87:SER:C	2:B:89:VAL:H	1.93	0.71
3:C:129:ILE:CD1	4:D:489:LEU:CD1	2.68	0.71
6:F:257:VAL:HG11	8:H:255:ASP:HB2	1.72	0.71
1:A:99:CYS:CB	3:C:67:MET:HE2	2.20	0.71
1:A:172:VAL:HG13	3:C:253:ILE:CG2	2.20	0.71
4:D:175:PHE:HE1	4:D:193:LEU:CD2	2.02	0.71
3:C:133:ASP:OD1	3:C:136:ASP:CG	2.28	0.71
4:D:307:GLU:CG	7:G:324:ILE:HD11	2.19	0.71
2:B:77:LEU:HD23	2:B:81:LEU:HD11	1.71	0.71
2:B:266:TYR:CG	2:B:345:LEU:HD11	2.25	0.71
5:E:107:SER:CA	7:G:273:PRO:HA	2.21	0.71
2:B:402:GLU:OE2	4:D:158:ARG:NE	2.20	0.71
6:F:173:LEU:HD21	7:G:90:LEU:HD21	1.72	0.71
6:F:176:GLN:OE1	7:G:117:ASP:HB3	1.91	0.71
2:B:521:THR:HG22	3:C:251:ASP:OD2	1.89	0.71
5:E:108:LEU:HD22	8:H:254:LEU:HD11	1.72	0.71
1:A:113:ILE:HB	1:A:114:PRO:HD3	1.72	0.71
6:F:247:MET:HE2	8:H:243:PHE:HD1	1.54	0.71
1:A:64:ALA:HB1	4:D:492:VAL:CG1	2.21	0.71
1:A:145:THR:HG1	4:D:65:TRP:HZ2	1.37	0.71
6:F:28:GLY:HA2	6:F:38:LEU:HD11	1.73	0.70
1:A:133:MET:SD	3:C:217:LEU:HD22	2.31	0.70
1:A:71:ASP:CB	3:C:114:ARG:HH21	1.98	0.70
3:C:123:PRO:C	3:C:125:ASP:H	1.93	0.70
3:C:75:LEU:HD11	3:C:162:LEU:HD23	1.74	0.70
4:D:203:ARG:HB2	4:D:234:TRP:NE1	2.06	0.70
4:D:307:GLU:OE1	7:G:324:ILE:HD11	1.90	0.70
1:A:5:SER:HA	1:A:31:MET:HE1	1.74	0.70
2:B:347:MET:HB3	2:B:348:PRO:HD3	1.72	0.70
6:F:377:ARG:NH1	8:H:343:GLN:CG	2.48	0.70
2:B:120:LYS:NZ	3:C:171:SER:C	2.45	0.70
4:D:211:HIS:CE1	4:D:215:ILE:HD12	2.27	0.70
4:D:266:LYS:O	4:D:270:PHE:HD2	1.73	0.70
4:D:631:GLN:HB3	4:D:648:ARG:NH2	2.07	0.70
7:G:56:SER:OG	7:G:63:GLN:OE1	2.01	0.70
6:F:224:ASP:O	6:F:225:ARG:C	2.25	0.70
6:F:261:VAL:HG21	8:H:254:LEU:HD23	1.74	0.70
1:A:58:LYS:NZ	4:D:506:SER:HB2	1.96	0.70
2:B:94:GLU:HB3	4:D:79:GLU:OE1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:GLU:CD	4:D:197:ARG:HH12	1.95	0.70
4:D:298:ASN:HD21	4:D:300:SER:CB	1.93	0.70
4:D:317:GLN:HA	8:H:334:PHE:CE2	2.27	0.69
7:G:92:HIS:CE1	7:G:93:PHE:CD1	2.80	0.69
4:D:4:ARG:HG3	4:D:32:GLN:HE22	1.57	0.69
6:F:157:LEU:N	6:F:170:ARG:HH22	1.89	0.69
6:F:175:ARG:CZ	7:G:152:LEU:HD22	2.22	0.69
2:B:216:PHE:HE2	4:D:272:GLN:OE1	1.76	0.69
2:B:536:LEU:HD21	3:C:261:LYS:HG2	1.72	0.69
2:B:376:MET:HE1	4:D:211:HIS:CB	2.21	0.69
4:D:177:ALA:HB2	4:D:256:ARG:HH22	1.57	0.69
4:D:601:MET:CE	4:D:604:LEU:HD12	2.21	0.69
2:B:120:LYS:NZ	3:C:171:SER:OG	2.20	0.69
5:E:141:PHE:HB2	7:G:289:PHE:CZ	2.28	0.69
7:G:7:LEU:HD21	7:G:34:GLN:OE1	1.92	0.69
1:A:172:VAL:CG1	3:C:253:ILE:HG21	2.22	0.69
6:F:224:ASP:CG	6:F:227:ILE:HD11	2.12	0.69
2:B:205:LEU:HD22	4:D:259:LEU:HD21	1.75	0.69
1:A:138:THR:HG1	2:B:92:ILE:CD1	1.99	0.69
2:B:94:GLU:CB	4:D:79:GLU:OE1	2.40	0.69
2:B:80:VAL:CG1	4:D:65:TRP:CE3	2.75	0.68
7:G:37:TYR:OH	7:G:105:PRO:HG3	1.94	0.68
2:B:97:ILE:HD11	4:D:82:GLN:CG	2.22	0.68
4:D:177:ALA:CB	4:D:256:ARG:NH2	2.56	0.68
4:D:298:ASN:HB3	4:D:299:GLU:HB3	1.73	0.68
8:H:294:MET:HE3	8:H:298:ALA:CB	2.22	0.68
4:D:175:PHE:HE1	4:D:193:LEU:HD21	1.50	0.68
2:B:134:LYS:HD2	3:C:85:VAL:HG13	1.74	0.68
2:B:577:GLU:OE1	4:D:640:GLY:N	2.26	0.68
3:C:63:ARG:CZ	4:D:535:ALA:CB	2.71	0.68
5:E:179:MET:HG2	8:H:329:ILE:CD1	2.24	0.68
1:A:240:ASP:OD2	3:C:335:LYS:NZ	2.27	0.68
5:E:59:ILE:HG23	7:G:210:ILE:HD12	1.75	0.68
6:F:224:ASP:OD1	6:F:227:ILE:HD11	1.94	0.68
7:G:41:CYS:HA	7:G:108:GLN:OE1	1.93	0.68
1:A:12:LEU:HB3	1:A:21:LEU:CD2	2.23	0.68
2:B:97:ILE:CD1	4:D:82:GLN:CB	2.66	0.68
3:C:351:SER:O	3:C:353:PRO:HD2	1.94	0.68
1:A:279:GLU:HB2	1:A:280:PRO:HD3	1.75	0.67
7:G:130:ILE:CG2	7:G:131:LEU:H	2.00	0.67
2:B:334:LEU:HB3	2:B:335:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:16:MET:SD	6:F:130:LEU:HD23	2.33	0.67
6:F:377:ARG:HH11	8:H:343:GLN:HA	1.59	0.67
1:A:145:THR:CG2	4:D:69:LEU:CD1	2.57	0.67
5:E:73:LYS:NZ	7:G:220:GLU:OE2	2.26	0.67
5:E:137:LEU:HD23	7:G:285:LEU:HD23	1.75	0.67
2:B:216:PHE:CE2	4:D:272:GLN:OE1	2.47	0.67
2:B:456:ASP:C	2:B:458:THR:N	2.48	0.67
5:E:4:ALA:O	5:E:6:PRO:HD3	1.93	0.67
2:B:175:MET:CG	4:D:460:PRO:HG3	2.16	0.67
4:D:191:GLU:HG3	4:D:194:ARG:NH2	2.10	0.67
5:E:190:ARG:CZ	6:F:370:ILE:HG12	2.24	0.67
3:C:129:ILE:HD11	4:D:489:LEU:HD22	1.76	0.67
5:E:47:GLU:HG3	6:F:195:LYS:HZ3	1.59	0.67
5:E:114:GLN:NE2	7:G:277:PHE:CZ	2.63	0.67
6:F:259:ASP:HB3	6:F:263:ARG:NH2	2.10	0.67
2:B:536:LEU:HD22	3:C:261:LYS:HD3	1.77	0.67
6:F:227:ILE:HG12	8:H:223:ARG:HH22	1.60	0.67
4:D:304:ASP:C	4:D:306:GLN:N	2.45	0.67
4:D:195:ASP:O	4:D:199:VAL:HG23	1.95	0.67
4:D:189:GLU:CD	4:D:197:ARG:NH1	2.48	0.66
6:F:9:LEU:HD21	6:F:124:PRO:O	1.96	0.66
2:B:95:VAL:HG13	2:B:99:LYS:HB3	1.78	0.66
2:B:507:LEU:HD11	4:D:579:THR:HG22	1.77	0.66
4:D:190:PRO:CD	4:D:193:LEU:HD12	2.26	0.66
3:C:141:LEU:HD23	3:C:147:VAL:HG21	1.75	0.66
8:H:234:THR:HB	8:H:235:PRO:HD3	1.77	0.66
3:C:4:THR:CG2	3:C:33:ILE:HD11	2.26	0.66
3:C:116:LEU:HD12	3:C:137:LEU:HD12	1.75	0.66
4:D:211:HIS:NE2	4:D:215:ILE:HD11	2.10	0.66
5:E:60:ASN:CB	8:H:207:HIS:NE2	2.54	0.66
2:B:88:LYS:O	2:B:90:PRO:CD	2.43	0.66
2:B:84:PHE:CE2	4:D:65:TRP:CE3	2.77	0.66
4:D:289:GLU:C	4:D:291:ILE:H	1.98	0.66
5:E:97:HIS:CD2	8:H:247:TYR:HH	2.12	0.66
4:D:352:HIS:CG	4:D:366:ARG:NE	2.64	0.66
5:E:189:TRP:CZ2	8:H:340:ILE:HD13	2.31	0.66
1:A:241:LEU:HD22	1:A:248:VAL:HG13	1.78	0.66
1:A:266:LEU:O	1:A:270:VAL:HG23	1.96	0.65
2:B:319:THR:HG23	4:D:378:LEU:HD12	1.78	0.65
4:D:157:TYR:CE1	4:D:161:GLN:NE2	2.64	0.65
4:D:197:ARG:HD2	4:D:201:LYS:NZ	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:VAL:HG12	7:G:66:LEU:HD11	1.75	0.65
1:A:128:LEU:CD2	4:D:97:ARG:HH21	2.08	0.65
8:H:257:THR:O	8:H:287:LYS:HE2	1.94	0.65
1:A:12:LEU:CB	1:A:21:LEU:HD21	2.24	0.65
3:C:123:PRO:C	3:C:125:ASP:N	2.50	0.65
1:A:275:PHE:O	1:A:276:VAL:C	2.32	0.65
2:B:577:GLU:OE1	4:D:640:GLY:CA	2.45	0.65
1:A:215:VAL:HG21	4:D:629:PRO:HB2	1.79	0.65
6:F:227:ILE:HG12	8:H:223:ARG:NH2	2.11	0.65
7:G:301:THR:HG23	8:H:312:GLU:HB2	1.78	0.65
2:B:84:PHE:HE2	4:D:65:TRP:HE3	1.43	0.65
4:D:17:GLU:O	4:D:52:SER:HB3	1.96	0.65
6:F:377:ARG:HH12	8:H:343:GLN:HA	1.32	0.65
1:A:145:THR:CB	4:D:65:TRP:HZ2	2.10	0.65
2:B:30:LEU:CD2	4:D:34:LEU:CD2	2.74	0.65
2:B:42:TRP:CE2	4:D:20:LEU:CD1	2.80	0.65
2:B:87:SER:C	2:B:89:VAL:N	2.48	0.65
2:B:120:LYS:NZ	3:C:175:PRO:HA	2.11	0.65
7:G:123:ASP:O	7:G:124:THR:O	2.15	0.65
2:B:424:LEU:HD23	4:D:484:ILE:CD1	2.27	0.65
1:A:77:LEU:HD22	3:C:154:LEU:HD22	1.77	0.64
7:G:62:VAL:CG1	7:G:66:LEU:HD11	2.27	0.64
1:A:193:ILE:HG23	3:C:274:LEU:CD1	2.27	0.64
4:D:631:GLN:CB	4:D:648:ARG:NH2	2.60	0.64
2:B:70:PRO:O	4:D:66:TYR:OH	2.10	0.64
4:D:175:PHE:HD1	4:D:193:LEU:CD1	2.06	0.64
4:D:317:GLN:HG3	8:H:334:PHE:CD2	2.32	0.64
5:E:186:ILE:HG12	7:G:338:TYR:CZ	2.32	0.64
7:G:81:ILE:HG22	7:G:99:ILE:HD12	1.78	0.64
7:G:235:ILE:HD11	8:H:225:LEU:HD22	1.78	0.64
2:B:344:LEU:HD13	4:D:399:LYS:HD2	1.80	0.64
5:E:9:PRO:HB2	6:F:197:GLN:OE1	1.96	0.64
5:E:42:CYS:SG	6:F:187:LEU:HD23	2.37	0.64
2:B:36:LEU:CD2	4:D:34:LEU:HD21	2.28	0.64
2:B:132:CYS:SG	4:D:119:LEU:HD11	2.37	0.64
2:B:166:SER:HB3	4:D:152:ASN:ND2	2.13	0.64
2:B:453:LEU:HB3	2:B:471:VAL:HG12	1.80	0.64
5:E:60:ASN:HB3	8:H:207:HIS:CD2	2.33	0.64
5:E:141:PHE:CA	7:G:289:PHE:CZ	2.81	0.64
7:G:143:VAL:CG2	8:H:159:MET:CE	2.68	0.64
2:B:81:LEU:O	2:B:84:PHE:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:SER:O	2:B:196:GLN:C	2.33	0.64
3:C:133:ASP:OD1	3:C:136:ASP:OD2	2.16	0.64
1:A:1:MET:HE1	1:A:28:THR:HG22	1.78	0.64
1:A:277:VAL:O	1:A:278:PRO:N	2.31	0.63
3:C:86:ARG:CB	3:C:92:LEU:HD12	2.28	0.63
5:E:139:VAL:HG22	6:F:278:LEU:HD12	1.80	0.63
2:B:536:LEU:CD2	3:C:261:LYS:HD3	2.27	0.63
4:D:352:HIS:CG	4:D:366:ARG:NH2	2.63	0.63
4:D:631:GLN:HB2	4:D:648:ARG:HH22	1.61	0.63
8:H:359:GLN:O	8:H:363:ASP:HB2	1.98	0.63
2:B:588:GLU:OE2	4:D:650:ARG:NH2	2.30	0.63
1:A:266:LEU:HD12	3:C:345:LEU:CG	2.24	0.63
2:B:80:VAL:HG11	4:D:65:TRP:CE3	2.32	0.63
6:F:295:LEU:HD21	6:F:317:GLU:OE1	1.98	0.63
2:B:245:SER:O	2:B:246:PHE:C	2.32	0.63
2:B:483:ARG:NH2	4:D:549:GLN:NE2	2.37	0.63
4:D:485:CYS:SG	4:D:487:PRO:HD2	2.39	0.63
2:B:190:GLN:OE1	4:D:169:SER:O	2.16	0.63
2:B:507:LEU:HD21	4:D:582:LEU:HD23	1.79	0.63
5:E:64:LEU:HD13	8:H:211:ARG:HG3	1.80	0.63
4:D:317:GLN:HA	8:H:334:PHE:CD2	2.33	0.63
5:E:189:TRP:HZ3	8:H:340:ILE:HD12	1.50	0.63
2:B:570:TYR:CG	4:D:631:GLN:HG2	2.33	0.63
5:E:186:ILE:HG12	7:G:338:TYR:CE2	2.34	0.63
1:A:145:THR:OG1	4:D:65:TRP:HZ2	1.78	0.62
2:B:138:LYS:HG3	3:C:84:GLN:HE21	1.62	0.62
2:B:222:PHE:HD1	2:B:241:LEU:HD13	1.55	0.62
5:E:76:ALA:HB1	7:G:224:LEU:HD21	1.80	0.62
1:A:64:ALA:HB1	4:D:492:VAL:HG12	1.80	0.62
6:F:227:ILE:CG1	8:H:223:ARG:HH22	2.11	0.62
1:A:77:LEU:HD22	3:C:154:LEU:HD21	1.80	0.62
1:A:145:THR:HG23	4:D:65:TRP:CE2	2.34	0.62
4:D:185:SER:C	4:D:187:PHE:H	2.03	0.62
4:D:314:SER:OG	7:G:321:GLY:N	2.29	0.62
5:E:158:ILE:HD12	6:F:334:VAL:HG11	1.81	0.62
6:F:377:ARG:CZ	8:H:343:GLN:HG3	2.30	0.62
1:A:270:VAL:HG13	1:A:273:MET:HE3	1.80	0.62
2:B:35:ASP:CB	4:D:30:MET:CE	2.75	0.62
2:B:510:PHE:CE1	4:D:586:LEU:HB3	2.33	0.62
3:C:86:ARG:HB2	3:C:92:LEU:HD12	1.81	0.62
4:D:457:LEU:N	4:D:458:PRO:CD	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:LEU:HB3	7:G:217:LEU:HD23	1.82	0.62
5:E:189:TRP:HZ3	8:H:336:VAL:HG12	1.65	0.62
7:G:93:PHE:CE2	7:G:94:ASP:OD1	2.53	0.62
2:B:406:ILE:HD13	4:D:155:ILE:HD11	1.82	0.62
5:E:57:ALA:HB2	8:H:203:GLN:NE2	2.15	0.62
6:F:185:GLU:OE1	7:G:168:PRO:HB3	1.99	0.62
6:F:288:ILE:HD11	6:F:314:LEU:CD2	2.30	0.62
7:G:280:PHE:CZ	8:H:258:ARG:O	2.52	0.62
6:F:92:ARG:HH11	6:F:119:LEU:HA	1.61	0.62
2:B:193:PHE:HD2	2:B:196:GLN:HE22	1.48	0.62
5:E:179:MET:CG	8:H:329:ILE:CD1	2.77	0.61
2:B:536:LEU:HD21	3:C:261:LYS:CG	2.30	0.61
6:F:163:ASP:OD1	6:F:164:PRO:HD2	2.00	0.61
3:C:116:LEU:HD11	3:C:137:LEU:HD11	1.82	0.61
4:D:197:ARG:CD	4:D:201:LYS:HE3	2.30	0.61
3:C:129:ILE:HD13	4:D:489:LEU:CD1	2.30	0.61
2:B:74:GLU:CD	4:D:54:ARG:HG3	2.21	0.61
4:D:189:GLU:OE2	4:D:197:ARG:CZ	2.47	0.61
4:D:190:PRO:HG2	4:D:193:LEU:HD12	1.82	0.61
5:E:78:ILE:CD1	6:F:234:ILE:HG23	2.31	0.61
1:A:134:GLU:HG3	3:C:213:MET:SD	2.40	0.61
2:B:385:LEU:HD21	4:D:251:LEU:CD2	2.31	0.61
2:B:190:GLN:NE2	4:D:171:ARG:H	1.98	0.61
2:B:407:VAL:CB	4:D:459:TRP:HZ3	2.13	0.61
6:F:377:ARG:HH11	8:H:343:GLN:CA	2.07	0.61
2:B:88:LYS:O	2:B:90:PRO:N	2.33	0.61
2:B:293:ASN:O	2:B:297:VAL:HG23	2.01	0.61
5:E:9:PRO:CA	6:F:197:GLN:HE22	2.14	0.61
5:E:148:TYR:OH	7:G:289:PHE:HD1	1.76	0.61
3:C:167:PHE:HB3	3:C:185:ARG:NH2	2.16	0.61
4:D:535:ALA:HB1	4:D:537:GLU:OE2	2.00	0.61
5:E:59:ILE:HG23	7:G:210:ILE:CD1	2.31	0.61
6:F:116:SER:HA	6:F:119:LEU:HD12	1.83	0.61
6:F:247:MET:HE1	8:H:243:PHE:HD1	1.64	0.61
1:A:78:GLY:O	1:A:81:TYR:HD1	1.84	0.60
2:B:2:SER:OG	2:B:28:ASP:CG	2.39	0.60
5:E:21:LYS:NZ	7:G:159:SER:HA	2.16	0.60
5:E:175:LEU:HD21	7:G:328:CYS:SG	2.41	0.60
1:A:141:ARG:CG	3:C:220:GLN:HE22	2.14	0.60
6:F:377:ARG:NH2	8:H:343:GLN:CG	2.62	0.60
7:G:174:PRO:HB2	7:G:176:ASP:OD1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:598:VAL:HB	4:D:599:PRO:HD3	1.82	0.60
5:E:62:LYS:NZ	7:G:211:SER:OG	2.21	0.60
6:F:176:GLN:CD	7:G:117:ASP:HB3	2.22	0.60
2:B:77:LEU:HD21	4:D:61:GLY:C	2.21	0.60
5:E:141:PHE:HA	7:G:289:PHE:CZ	2.36	0.60
2:B:273:LEU:HA	4:D:330:LEU:HD13	1.84	0.60
2:B:385:LEU:HD21	4:D:251:LEU:HD21	1.84	0.60
3:C:63:ARG:NH2	4:D:535:ALA:HB1	2.11	0.60
3:C:116:LEU:CD1	3:C:137:LEU:CD1	2.78	0.60
4:D:157:TYR:CZ	4:D:161:GLN:NE2	2.69	0.60
5:E:97:HIS:CE1	6:F:255:VAL:HG13	2.37	0.60
5:E:104:GLU:HA	5:E:124:GLU:OE2	2.01	0.60
5:E:221:HIS:HB3	5:E:222:PRO:C	2.22	0.60
7:G:14:TYR:HB2	7:G:36:ILE:CG2	2.31	0.60
2:B:329:ILE:CD1	4:D:386:MET:SD	2.88	0.60
1:A:99:CYS:HB3	3:C:67:MET:CE	2.32	0.60
1:A:148:LEU:HD12	2:B:80:VAL:HG22	1.80	0.60
4:D:175:PHE:CD1	4:D:193:LEU:CD2	2.82	0.60
5:E:155:ILE:HG23	6:F:334:VAL:HG21	0.65	0.60
2:B:80:VAL:HG12	4:D:65:TRP:CE3	2.34	0.60
4:D:130:ARG:NH2	4:D:484:ILE:O	2.35	0.60
3:C:129:ILE:HD11	4:D:489:LEU:CD2	2.31	0.59
4:D:172:GLU:HB2	4:D:249:HIS:CE1	2.37	0.59
4:D:383:ASP:O	4:D:387:GLN:HG3	2.01	0.59
1:A:278:PRO:HB3	1:A:279:GLU:CG	2.09	0.59
2:B:91:ALA:C	2:B:93:GLU:N	2.56	0.59
2:B:96:ALA:O	2:B:99:LYS:N	2.34	0.59
7:G:14:TYR:CE1	7:G:18:GLN:NE2	2.70	0.59
1:A:33:ILE:HG23	3:C:15:LEU:CD2	2.31	0.59
1:A:93:ASN:OD1	3:C:68:ARG:NH1	2.36	0.59
1:A:207:GLU:N	1:A:208:PRO:CD	2.64	0.59
2:B:171:VAL:HG21	4:D:463:ILE:HD13	1.85	0.59
3:C:282:THR:HB	3:C:283:PRO:HD2	1.83	0.59
6:F:319:LEU:O	8:H:293:ILE:HD11	2.01	0.59
1:A:5:SER:HA	1:A:31:MET:CE	2.32	0.59
1:A:217:LEU:O	1:A:220:THR:OG1	2.17	0.59
4:D:422:LYS:O	4:D:426:HIS:CD2	2.54	0.59
2:B:263:GLN:NE2	2:B:346:ASN:HD21	1.98	0.59
2:B:490:GLU:CG	4:D:560:ARG:NH2	2.64	0.59
4:D:185:SER:OG	4:D:187:PHE:CE2	2.37	0.59
6:F:173:LEU:CD2	7:G:90:LEU:HD21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:HE	3:C:220:GLN:HE22	1.51	0.59
3:C:5:LEU:HD12	3:C:22:LEU:HD11	1.85	0.59
4:D:631:GLN:OE1	4:D:648:ARG:NH2	2.35	0.59
2:B:37:LYS:HB3	2:B:38:PRO:HD3	1.85	0.59
6:F:168:LEU:CD1	7:G:145:CYS:SG	2.91	0.59
5:E:148:TYR:HH	7:G:289:PHE:HE1	1.37	0.59
8:H:294:MET:HE3	8:H:298:ALA:HB2	1.84	0.59
3:C:5:LEU:CD1	3:C:22:LEU:CD1	2.76	0.58
6:F:9:LEU:HD22	6:F:124:PRO:CB	2.33	0.58
6:F:326:ARG:NH1	8:H:295:PRO:CG	2.62	0.58
7:G:59:TYR:CD1	7:G:62:VAL:CG2	2.66	0.58
5:E:72:GLU:OE1	8:H:218:ARG:NH1	2.36	0.58
5:E:141:PHE:CB	7:G:289:PHE:CZ	2.86	0.58
2:B:92:ILE:O	2:B:94:GLU:N	2.37	0.58
4:D:293:GLN:HB2	4:D:295:ARG:HD2	1.85	0.58
5:E:135:LEU:HB3	5:E:136:PRO:CD	2.29	0.58
2:B:195:SER:O	2:B:197:LEU:N	2.36	0.58
2:B:420:ARG:NE	4:D:477:GLU:OE1	2.29	0.58
5:E:78:ILE:HD11	6:F:234:ILE:HG23	1.85	0.58
5:E:111:ARG:HD2	7:G:276:PRO:HB2	1.84	0.58
1:A:141:ARG:CG	3:C:220:GLN:NE2	2.66	0.58
4:D:631:GLN:HB3	4:D:648:ARG:HH21	1.67	0.58
5:E:76:ALA:CB	7:G:224:LEU:HD21	2.33	0.58
2:B:344:LEU:HD22	2:B:347:MET:CE	2.34	0.58
2:B:344:LEU:HD22	2:B:347:MET:HE1	1.86	0.58
4:D:509:ARG:HD3	4:D:521:PHE:CZ	2.37	0.58
6:F:234:ILE:HG12	8:H:226:ILE:CD1	2.33	0.58
2:B:419:GLU:HB3	3:C:127:THR:HG21	1.86	0.58
5:E:139:VAL:HG22	6:F:278:LEU:CD1	2.34	0.58
6:F:60:PHE:CE1	6:F:99:LEU:HD11	2.36	0.58
1:A:280:PRO:CA	1:A:281:SER:N	2.67	0.57
2:B:490:GLU:HG2	4:D:560:ARG:NH2	2.19	0.57
4:D:631:GLN:CB	4:D:648:ARG:HH22	2.17	0.57
2:B:139:GLU:OE1	4:D:123:ARG:HD3	2.03	0.57
2:B:429:LEU:HB3	4:D:484:ILE:HG23	1.85	0.57
7:G:2:THR:HG21	7:G:37:TYR:CE1	2.38	0.57
2:B:171:VAL:HG11	4:D:463:ILE:HD12	1.86	0.57
4:D:185:SER:CB	4:D:187:PHE:CE2	2.88	0.57
2:B:97:ILE:HD12	4:D:82:GLN:NE2	2.17	0.57
4:D:306:GLN:C	4:D:307:GLU:O	2.43	0.57
7:G:142:VAL:HG13	8:H:163:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ILE:HD12	4:D:82:GLN:OE1	2.02	0.57
4:D:10:LEU:HD23	4:D:31:LEU:HD22	1.86	0.57
6:F:261:VAL:HG21	8:H:254:LEU:CD2	2.35	0.57
1:A:278:PRO:HG2	1:A:280:PRO:HD3	1.86	0.57
4:D:177:ALA:HB2	4:D:256:ARG:NH2	2.17	0.57
7:G:41:CYS:CA	7:G:47:ARG:NH1	2.65	0.57
7:G:249:THR:CG2	8:H:243:PHE:HB2	2.35	0.57
1:A:113:ILE:CG2	2:B:121:LEU:HD11	2.35	0.57
2:B:513:PRO:HG2	2:B:519:MET:HE3	1.84	0.57
3:C:128:SER:OG	3:C:132:LEU:O	2.12	0.57
4:D:601:MET:HE2	4:D:601:MET:HA	1.86	0.57
5:E:111:ARG:HH22	7:G:280:PHE:CB	2.17	0.57
1:A:113:ILE:HG21	2:B:121:LEU:HD11	1.87	0.57
4:D:215:ILE:CG2	4:D:419:LEU:HD11	2.35	0.57
5:E:166:ASP:OD1	6:F:340:TYR:OH	2.23	0.57
6:F:92:ARG:HH12	6:F:119:LEU:C	2.08	0.57
6:F:206:MET:HE3	8:H:199:LYS:CG	2.28	0.57
6:F:241:TRP:CH2	7:G:238:LEU:HD21	2.40	0.57
2:B:220:HIS:CE1	4:D:272:GLN:HB3	2.40	0.56
4:D:189:GLU:OE2	4:D:197:ARG:NH1	2.38	0.56
2:B:418:GLU:O	2:B:422:THR:HG23	2.05	0.56
6:F:326:ARG:HD2	8:H:293:ILE:HG23	1.86	0.56
1:A:171:LYS:HE2	1:A:175:ARG:HH21	1.67	0.56
2:B:138:LYS:HE3	3:C:84:GLN:CD	2.09	0.56
3:C:280:CYS:HB2	4:D:625:TRP:HD1	1.69	0.56
4:D:180:PRO:HG2	4:D:267:LYS:HZ1	1.70	0.56
4:D:197:ARG:HD2	4:D:201:LYS:CE	2.35	0.56
5:E:158:ILE:HD11	7:G:295:ILE:HG23	1.86	0.56
7:G:146:ILE:HG12	8:H:163:ILE:HG13	1.86	0.56
8:H:358:ARG:HH21	8:H:366:LEU:CD1	2.18	0.56
4:D:177:ALA:CB	4:D:256:ARG:HH22	2.17	0.56
6:F:259:ASP:HB3	6:F:263:ARG:HH21	1.71	0.56
4:D:179:ASP:OD1	4:D:180:PRO:HD2	2.05	0.56
4:D:193:LEU:HD23	4:D:253:ALA:CB	2.36	0.56
5:E:114:GLN:CD	7:G:277:PHE:CE1	2.60	0.56
1:A:228:SER:CA	3:C:307:LEU:HD12	2.36	0.56
4:D:289:GLU:C	4:D:291:ILE:N	2.58	0.56
2:B:383:GLU:OE2	4:D:203:ARG:NE	2.38	0.56
5:E:75:THR:O	5:E:79:THR:OG1	2.13	0.56
5:E:87:LYS:HD3	6:F:241:TRP:CE3	2.40	0.56
8:H:294:MET:CE	8:H:298:ALA:HB2	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:PHE:CE2	4:D:65:TRP:HZ3	2.23	0.56
2:B:178:PHE:HA	2:B:193:PHE:HE2	1.71	0.56
3:C:177:THR:HG22	3:C:188:LYS:HZ2	1.71	0.56
2:B:72:LEU:HB2	2:B:77:LEU:HD12	1.88	0.55
2:B:374:HIS:CE1	4:D:265:LEU:CD1	2.89	0.55
4:D:197:ARG:HD2	4:D:201:LYS:HE3	1.88	0.55
7:G:274:MET:HE1	8:H:280:GLN:H	1.71	0.55
4:D:307:GLU:CD	7:G:324:ILE:HD12	1.97	0.55
2:B:134:LYS:HD2	3:C:85:VAL:CG1	2.36	0.55
2:B:500:LEU:HD21	4:D:571:LEU:HD11	1.84	0.55
4:D:175:PHE:CD1	4:D:193:LEU:CD1	2.85	0.55
4:D:438:LYS:HE2	4:D:442:ARG:NH2	2.21	0.55
1:A:141:ARG:NE	3:C:220:GLN:HE22	2.04	0.55
2:B:193:PHE:HB3	2:B:392:GLU:OE1	2.07	0.55
3:C:63:ARG:NH1	4:D:535:ALA:CB	2.70	0.55
4:D:199:VAL:CG2	4:D:241:VAL:CG2	2.73	0.55
4:D:528:VAL:HG12	4:D:528:VAL:O	2.07	0.55
6:F:227:ILE:HG22	6:F:227:ILE:O	2.05	0.55
4:D:486:LEU:N	4:D:487:PRO:CD	2.70	0.55
6:F:359:ARG:CG	8:H:328:GLN:CD	2.70	0.55
2:B:96:ALA:O	2:B:98:GLU:N	2.38	0.55
2:B:264:LEU:CD1	6:F:381:TRP:CH2	2.87	0.55
6:F:192:TYR:CE1	7:G:172:PRO:CD	2.89	0.55
1:A:278:PRO:CG	1:A:279:GLU:CG	2.82	0.55
6:F:53:LYS:HE2	6:F:57:TYR:CZ	2.38	0.55
1:A:189:TYR:HA	3:C:271:MET:HE2	1.89	0.55
3:C:259:GLU:HG3	4:D:604:LEU:HD21	1.88	0.55
5:E:47:GLU:HG3	6:F:195:LYS:NZ	2.20	0.55
2:B:550:LEU:HD11	3:C:276:VAL:CG2	2.31	0.55
4:D:577:PRO:HG2	4:D:582:LEU:HD13	1.89	0.55
6:F:92:ARG:NH1	6:F:119:LEU:CA	2.70	0.55
7:G:7:LEU:O	7:G:11:VAL:HG23	2.07	0.55
4:D:190:PRO:CG	4:D:193:LEU:HD12	2.36	0.55
5:E:60:ASN:CB	8:H:207:HIS:CE1	2.66	0.55
2:B:41:ASP:O	2:B:45:SER:OG	2.25	0.54
3:C:129:ILE:HD13	4:D:489:LEU:HD11	1.89	0.54
5:E:10:VAL:HG13	6:F:193:GLN:OE1	2.07	0.54
6:F:135:ARG:HG3	8:H:168:LEU:CD2	2.36	0.54
6:F:175:ARG:HD3	7:G:121:TYR:OH	2.07	0.54
6:F:170:ARG:NE	7:G:89:MET:HG3	2.23	0.54
1:A:71:ASP:HB3	3:C:114:ARG:CZ	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:HD13	3:C:328:VAL:HG22	1.88	0.54
2:B:399:VAL:HA	4:D:158:ARG:HH12	1.71	0.54
4:D:213:ASP:OD2	4:D:227:ARG:NH2	2.40	0.54
3:C:115:LEU:HD23	4:D:490:LEU:HG	1.89	0.54
5:E:107:SER:HB2	7:G:276:PRO:CG	2.34	0.54
2:B:347:MET:HG3	4:D:406:LEU:CD1	2.38	0.54
3:C:95:GLU:HB3	3:C:153:ARG:HH12	1.73	0.54
6:F:157:LEU:CA	6:F:170:ARG:HH22	2.20	0.54
7:G:143:VAL:HG22	8:H:159:MET:HE1	1.82	0.54
2:B:121:LEU:HD12	3:C:172:PHE:CE2	2.42	0.54
2:B:205:LEU:HD22	4:D:259:LEU:CD2	2.38	0.54
1:A:244:ASN:OD1	1:A:245:PRO:HD2	2.08	0.54
4:D:298:ASN:HB2	4:D:299:GLU:N	2.22	0.54
5:E:49:LEU:HD23	8:H:196:ASN:HB3	1.90	0.54
1:A:55:LEU:HD22	3:C:59:LEU:HD22	1.90	0.54
2:B:374:HIS:CE1	4:D:261:SER:OG	2.61	0.54
2:B:522:THR:CG2	4:D:590:TYR:CE2	2.84	0.54
3:C:12:LEU:HB3	3:C:15:LEU:HD12	1.88	0.54
3:C:239:ALA:HB1	4:D:586:LEU:HD11	1.90	0.54
4:D:185:SER:CB	4:D:187:PHE:CD2	2.90	0.54
5:E:17:LEU:HD13	7:G:161:HIS:CE1	2.43	0.54
6:F:10:ALA:O	6:F:13:ARG:CG	2.39	0.54
6:F:157:LEU:HG	6:F:170:ARG:NH2	2.22	0.54
7:G:123:ASP:O	7:G:124:THR:C	2.42	0.54
2:B:77:LEU:HD23	2:B:81:LEU:CD1	2.37	0.54
2:B:195:SER:HA	2:B:389:TYR:HE1	1.72	0.54
2:B:197:LEU:O	2:B:198:LEU:HB2	2.08	0.54
2:B:573:PHE:O	4:D:639:ARG:HD2	2.08	0.54
7:G:16:ARG:NH2	7:G:120:GLN:OE1	2.41	0.54
2:B:157:ASN:HA	4:D:474:ILE:HD12	1.89	0.54
4:D:192:VAL:HG22	4:D:245:HIS:CG	2.42	0.54
2:B:264:LEU:HD13	6:F:381:TRP:HH2	1.69	0.53
3:C:224:TYR:N	3:C:225:PRO:HD2	2.23	0.53
2:B:490:GLU:CA	4:D:560:ARG:HH22	2.03	0.53
3:C:121:VAL:HG12	3:C:122:PRO:HD2	1.90	0.53
4:D:185:SER:C	4:D:187:PHE:N	2.61	0.53
2:B:80:VAL:O	2:B:83:THR:OG1	2.21	0.53
2:B:199:LEU:O	2:B:200:ASP:C	2.47	0.53
2:B:504:LEU:HD11	3:C:231:CYS:HB3	1.91	0.53
7:G:62:VAL:CG1	7:G:66:LEU:CD1	2.75	0.53
2:B:42:TRP:CD2	4:D:20:LEU:CD1	2.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:MET:HE3	4:D:554:ARG:HE	1.74	0.53
4:D:180:PRO:HG2	4:D:267:LYS:NZ	2.24	0.53
5:E:141:PHE:HB2	7:G:289:PHE:HZ	1.73	0.53
6:F:23:LEU:O	6:F:66:LYS:HE3	2.08	0.53
1:A:148:LEU:CD1	2:B:80:VAL:HG21	2.24	0.53
1:A:214:LEU:HB2	4:D:630:VAL:HG22	1.91	0.53
1:A:241:LEU:CD2	1:A:248:VAL:HG13	2.39	0.53
6:F:377:ARG:NH2	8:H:343:GLN:CD	2.60	0.53
7:G:142:VAL:HG13	8:H:163:ILE:CD1	2.38	0.53
2:B:121:LEU:HD12	3:C:172:PHE:HE2	1.73	0.53
4:D:317:GLN:HG3	8:H:334:PHE:HB2	1.91	0.53
7:G:345:SER:O	7:G:348:ASP:HB2	2.09	0.53
1:A:277:VAL:HG12	1:A:278:PRO:CA	2.36	0.53
2:B:454:ASP:O	2:B:456:ASP:N	2.39	0.53
4:D:63:LEU:O	4:D:67:GLN:HB2	2.08	0.53
2:B:536:LEU:CD2	3:C:261:LYS:CD	2.86	0.53
4:D:352:HIS:CD2	4:D:366:ARG:NE	2.71	0.53
6:F:338:LEU:HD12	8:H:304:SER:CB	2.37	0.53
2:B:195:SER:C	2:B:197:LEU:N	2.61	0.53
2:B:507:LEU:HD11	4:D:579:THR:CG2	2.33	0.53
2:B:588:GLU:CD	4:D:650:ARG:HH21	2.11	0.53
7:G:2:THR:HG21	7:G:37:TYR:CZ	2.44	0.53
2:B:120:LYS:HZ3	3:C:171:SER:C	2.12	0.53
4:D:572:GLN:O	4:D:575:THR:OG1	2.26	0.53
5:E:9:PRO:HA	6:F:197:GLN:HE22	1.74	0.53
6:F:283:LEU:HD23	6:F:321:LEU:HD13	1.91	0.53
7:G:131:LEU:C	7:G:132:GLU:O	2.46	0.53
1:A:64:ALA:HB1	4:D:492:VAL:HG11	1.88	0.52
4:D:651:TRP:O	4:D:655:VAL:HG23	2.08	0.52
5:E:181:GLU:CG	7:G:335:ARG:NH1	2.66	0.52
1:A:152:LYS:CE	2:B:73:ASP:OD1	2.57	0.52
2:B:194:LEU:HB3	2:B:392:GLU:OE2	2.08	0.52
6:F:326:ARG:NH1	8:H:295:PRO:HG3	2.24	0.52
6:F:6:ARG:C	6:F:8:HIS:H	2.12	0.52
1:A:171:LYS:CE	1:A:175:ARG:NH2	2.71	0.52
1:A:189:TYR:CG	3:C:271:MET:CE	2.92	0.52
2:B:349:ILE:HD13	4:D:316:ILE:HD12	1.91	0.52
2:B:349:ILE:CD1	4:D:316:ILE:HD12	2.40	0.52
2:B:220:HIS:O	2:B:367:ARG:NH1	2.43	0.52
3:C:121:VAL:HG13	3:C:122:PRO:HD2	1.89	0.52
3:C:141:LEU:CD2	3:C:147:VAL:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:THR:HG21	7:G:299:THR:HG21	1.92	0.52
7:G:150:GLU:HG2	8:H:166:GLN:NE2	2.24	0.52
7:G:327:LEU:CD1	8:H:326:PHE:CD1	2.93	0.52
1:A:138:THR:HG1	2:B:92:ILE:HD13	1.69	0.52
1:A:145:THR:HG23	4:D:65:TRP:NE1	2.25	0.52
2:B:90:PRO:O	2:B:92:ILE:N	2.43	0.52
5:E:141:PHE:CB	7:G:289:PHE:HZ	2.20	0.52
2:B:19:GLY:HA2	2:B:22:LEU:HD12	1.92	0.52
4:D:180:PRO:CG	4:D:267:LYS:NZ	2.73	0.52
4:D:348:ILE:HD11	4:D:373:LEU:HD21	1.91	0.52
5:E:110:GLN:HB2	7:G:273:PRO:O	2.10	0.52
6:F:240:MET:HE1	8:H:230:ASP:OD1	2.09	0.52
4:D:210:LEU:CD2	4:D:227:ARG:NH1	2.73	0.52
4:D:295:ARG:HA	4:D:299:GLU:N	2.25	0.52
6:F:173:LEU:HD11	7:G:118:VAL:HG21	1.87	0.52
2:B:7:PHE:CE1	2:B:11:LEU:HD11	2.45	0.52
2:B:178:PHE:HE1	2:B:396:HIS:CE1	2.28	0.52
2:B:374:HIS:CE1	4:D:265:LEU:HD12	2.45	0.52
1:A:171:LYS:HE2	1:A:175:ARG:CZ	2.40	0.51
3:C:116:LEU:HD12	3:C:137:LEU:HD11	1.83	0.51
5:E:141:PHE:N	7:G:289:PHE:HZ	2.08	0.51
1:A:24:TYR:HB3	3:C:31:VAL:HG21	1.92	0.51
2:B:490:GLU:C	4:D:560:ARG:NH2	2.59	0.51
5:E:104:GLU:CD	5:E:124:GLU:OE1	2.48	0.51
7:G:146:ILE:HG12	8:H:163:ILE:CG1	2.40	0.51
2:B:289:TRP:CZ2	2:B:293:ASN:ND2	2.76	0.51
8:H:259:HIS:O	8:H:291:GLU:HB3	2.10	0.51
5:E:87:LYS:HD3	6:F:241:TRP:CD2	2.44	0.51
7:G:327:LEU:HD11	8:H:326:PHE:CG	2.45	0.51
1:A:271:ASN:O	1:A:273:MET:N	2.44	0.51
4:D:80:GLU:HA	4:D:83:GLN:OE1	2.11	0.51
4:D:661:ALA:C	4:D:663:GLY:H	2.14	0.51
6:F:168:LEU:HD11	7:G:145:CYS:SG	2.50	0.51
6:F:234:ILE:HD11	8:H:222:LEU:HD21	1.93	0.51
2:B:84:PHE:CE2	4:D:65:TRP:HE3	2.25	0.51
7:G:219:GLU:O	7:G:222:VAL:HG23	2.10	0.51
1:A:48:LEU:HD22	3:C:52:LEU:HD22	1.90	0.51
2:B:83:THR:HG22	3:C:220:GLN:HG2	1.91	0.51
6:F:51:PRO:HA	6:F:121:PRO:O	2.11	0.51
1:A:227:GLN:HB3	3:C:307:LEU:HD11	1.93	0.51
5:E:127:TYR:CD2	7:G:275:GLY:HA3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:LEU:HD22	7:G:35:SER:HB3	1.93	0.51
2:B:80:VAL:HG11	4:D:65:TRP:CE2	2.45	0.51
2:B:95:VAL:HG12	2:B:100:LEU:HG	1.93	0.51
2:B:251:THR:C	2:B:253:GLU:N	2.63	0.51
4:D:214:SER:OG	4:D:426:HIS:HE1	1.94	0.51
1:A:152:LYS:NZ	2:B:73:ASP:OD1	2.40	0.50
3:C:351:SER:C	3:C:353:PRO:HD2	2.32	0.50
2:B:259:MET:CE	2:B:346:ASN:HB3	2.41	0.50
7:G:93:PHE:CE2	7:G:94:ASP:CG	2.85	0.50
4:D:197:ARG:HD2	4:D:201:LYS:HZ1	1.77	0.50
6:F:166:LYS:CE	7:G:84:LEU:HD12	2.40	0.50
6:F:260:ALA:HB3	8:H:258:ARG:HH11	1.69	0.50
8:H:241:ASP:HB2	8:H:242:PRO:HD3	1.92	0.50
6:F:170:ARG:NH2	7:G:89:MET:SD	2.82	0.50
2:B:361:GLN:HE22	4:D:413:ILE:HG23	1.77	0.50
1:A:1:MET:HE3	1:A:28:THR:CG2	2.41	0.50
1:A:152:LYS:HE3	2:B:73:ASP:OD1	2.11	0.50
5:E:79:THR:HG21	8:H:222:LEU:CD1	2.42	0.50
1:A:145:THR:CG2	4:D:69:LEU:HD13	2.29	0.50
1:A:207:GLU:N	1:A:208:PRO:HD2	2.27	0.50
2:B:36:LEU:HD21	4:D:34:LEU:CG	2.41	0.50
4:D:305:PRO:C	4:D:307:GLU:N	2.52	0.50
1:A:71:ASP:CA	3:C:114:ARG:HH21	2.25	0.50
2:B:384:LEU:HD13	4:D:199:VAL:HG11	1.94	0.50
5:E:135:LEU:CB	5:E:136:PRO:HD3	2.33	0.50
2:B:37:LYS:N	2:B:38:PRO:CD	2.75	0.49
2:B:402:GLU:CD	4:D:158:ARG:NH2	2.66	0.49
2:B:511:MET:C	2:B:513:PRO:HD3	2.33	0.49
6:F:192:TYR:CD2	8:H:188:ALA:HB1	2.47	0.49
2:B:190:GLN:HE22	4:D:171:ARG:N	2.05	0.49
4:D:172:GLU:HB2	4:D:249:HIS:NE2	2.26	0.49
4:D:525:TYR:OH	4:D:536:PRO:HA	2.13	0.49
5:E:219:ASN:O	5:E:221:HIS:N	2.45	0.49
7:G:62:VAL:O	7:G:66:LEU:HD12	2.12	0.49
7:G:239:ARG:HG3	8:H:232:VAL:CG2	2.39	0.49
2:B:430:LEU:O	2:B:431:SER:O	2.30	0.49
4:D:190:PRO:HG2	4:D:193:LEU:CD1	2.43	0.49
6:F:251:MET:HE3	8:H:247:TYR:CD1	2.47	0.49
3:C:303:GLU:OE2	3:C:303:GLU:CA	2.58	0.49
5:E:121:LEU:HD23	8:H:276:LEU:HD11	1.94	0.49
2:B:271:HIS:CE1	8:H:360:TRP:CE2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:ARG:HA	4:D:32:GLN:HE21	1.78	0.49
4:D:180:PRO:CG	4:D:267:LYS:HZ2	2.26	0.49
6:F:260:ALA:CB	8:H:258:ARG:HH11	2.13	0.49
2:B:243:VAL:HG12	2:B:243:VAL:O	2.12	0.49
5:E:190:ARG:CZ	6:F:370:ILE:CG1	2.91	0.49
6:F:60:PHE:HE1	6:F:99:LEU:CD1	2.24	0.49
1:A:284:ARG:O	1:A:285:LEU:N	2.38	0.49
2:B:374:HIS:CE1	4:D:265:LEU:HD11	2.48	0.49
4:D:575:THR:O	4:D:577:PRO:C	2.51	0.49
2:B:95:VAL:CG1	2:B:100:LEU:HG	2.43	0.49
3:C:92:LEU:HD23	3:C:97:ARG:N	2.27	0.49
5:E:190:ARG:NH1	6:F:370:ILE:CG1	2.76	0.49
1:A:150:LEU:CD2	2:B:504:LEU:HD21	2.43	0.49
5:E:42:CYS:SG	6:F:187:LEU:CD2	3.00	0.49
6:F:28:GLY:HA2	6:F:38:LEU:CD1	2.40	0.49
1:A:8:ILE:HD12	1:A:31:MET:HE3	1.95	0.48
3:C:36:CYS:N	3:C:37:PRO:HD2	2.28	0.48
5:E:106:ARG:NH1	7:G:272:SER:N	2.61	0.48
6:F:44:GLY:N	6:F:47:MET:HE2	2.18	0.48
1:A:40:TRP:CH2	3:C:43:GLY:HA3	2.48	0.48
2:B:374:HIS:HE1	4:D:261:SER:OG	1.95	0.48
2:B:407:VAL:HB	4:D:459:TRP:HZ3	1.77	0.48
4:D:307:GLU:OE1	7:G:324:ILE:CD1	2.53	0.48
4:D:590:TYR:CE1	4:D:594:LEU:HD11	2.48	0.48
4:D:594:LEU:O	4:D:599:PRO:HD3	2.13	0.48
2:B:36:LEU:HD21	4:D:34:LEU:HG	1.95	0.48
4:D:215:ILE:CG2	4:D:419:LEU:CD1	2.90	0.48
7:G:178:LYS:N	7:G:179:PRO:CD	2.76	0.48
2:B:37:LYS:N	2:B:38:PRO:HD2	2.28	0.48
2:B:83:THR:CG2	3:C:220:GLN:HG2	2.44	0.48
2:B:225:MET:O	2:B:226:SER:C	2.50	0.48
2:B:467:GLY:O	2:B:471:VAL:HG23	2.13	0.48
2:B:587:LEU:HD23	4:D:654:ALA:CB	2.42	0.48
4:D:528:VAL:HG12	4:D:546:MET:SD	2.53	0.48
7:G:294:SER:OG	8:H:305:PHE:HB2	2.13	0.48
3:C:218:GLU:OE1	4:D:556:GLN:HG3	2.13	0.48
3:C:324:PHE:O	3:C:328:VAL:HG23	2.13	0.48
5:E:38:LEU:HD11	6:F:180:LYS:HD3	1.95	0.48
6:F:209:GLU:OE1	8:H:210:LYS:NZ	2.36	0.48
2:B:35:ASP:HB3	4:D:30:MET:SD	2.53	0.48
2:B:402:GLU:HB2	4:D:158:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:LEU:CD2	4:D:571:LEU:HD11	2.43	0.48
2:B:264:LEU:HD13	6:F:381:TRP:CZ2	2.45	0.48
2:B:347:MET:CE	4:D:403:MET:SD	3.02	0.48
3:C:63:ARG:CZ	4:D:535:ALA:HB1	2.37	0.48
7:G:81:ILE:CG2	7:G:99:ILE:HD12	2.42	0.48
3:C:280:CYS:HB2	4:D:625:TRP:CD1	2.48	0.48
5:E:28:LEU:HD11	6:F:179:LEU:HD21	1.96	0.48
6:F:227:ILE:CB	8:H:223:ARG:HH22	2.27	0.48
6:F:261:VAL:HG22	8:H:258:ARG:HD2	1.96	0.48
6:F:283:LEU:CD2	6:F:321:LEU:HD13	2.44	0.48
7:G:14:TYR:HB2	7:G:36:ILE:HG21	1.94	0.48
1:A:211:HIS:O	1:A:215:VAL:HG23	2.14	0.48
2:B:347:MET:HE2	4:D:403:MET:SD	2.54	0.48
5:E:107:SER:HA	7:G:273:PRO:C	2.34	0.48
5:E:111:ARG:NH2	7:G:280:PHE:HB2	2.24	0.47
6:F:44:GLY:O	6:F:47:MET:CE	2.57	0.47
2:B:493:HIS:CE1	2:B:497:LEU:HD11	2.49	0.47
5:E:19:LEU:HD21	6:F:182:LEU:HD23	1.96	0.47
6:F:166:LYS:HE3	7:G:84:LEU:CD1	2.44	0.47
6:F:277:THR:HA	6:F:301:TYR:OH	2.15	0.47
2:B:89:VAL:O	2:B:90:PRO:C	2.50	0.47
2:B:132:CYS:HG	4:D:119:LEU:CD2	2.26	0.47
2:B:190:GLN:HG3	4:D:171:ARG:HH21	1.79	0.47
6:F:309:ILE:HG23	8:H:282:HIS:CD2	2.48	0.47
6:F:389:LEU:HD11	8:H:362:PHE:CE2	2.49	0.47
4:D:197:ARG:HG2	4:D:201:LYS:CE	2.32	0.47
7:G:13:LEU:HD22	7:G:116:LEU:HD12	1.96	0.47
7:G:124:THR:CG2	7:G:125:ILE:HG13	2.28	0.47
1:A:137:LEU:HD21	3:C:217:LEU:N	2.29	0.47
2:B:95:VAL:HA	2:B:99:LYS:HD2	1.97	0.47
2:B:266:TYR:CD2	2:B:345:LEU:HD11	2.49	0.47
5:E:178:GLU:OE2	7:G:331:MET:HE3	2.15	0.47
5:E:221:HIS:CB	5:E:222:PRO:O	2.61	0.47
7:G:235:ILE:HD11	8:H:225:LEU:CD2	2.44	0.47
3:C:99:PHE:CE1	3:C:157:GLN:OE1	2.67	0.47
4:D:486:LEU:HB2	4:D:487:PRO:HD3	1.96	0.47
6:F:9:LEU:HD22	6:F:124:PRO:CA	2.45	0.47
7:G:13:LEU:HD11	7:G:109:ILE:HG23	1.96	0.47
4:D:307:GLU:HB3	7:G:318:LYS:HE3	1.97	0.47
4:D:509:ARG:CD	4:D:521:PHE:CZ	2.98	0.47
4:D:663:GLY:O	4:D:665:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:VAL:CG2	8:H:159:MET:HE1	2.41	0.47
7:G:274:MET:CE	8:H:280:GLN:N	2.74	0.47
1:A:123:LEU:O	1:A:126:ILE:HG22	2.15	0.47
1:A:189:TYR:CG	3:C:271:MET:HE3	2.49	0.47
2:B:454:ASP:C	2:B:456:ASP:H	2.17	0.47
3:C:86:ARG:HB3	3:C:92:LEU:HD12	1.97	0.47
3:C:170:LEU:HD22	3:C:189:VAL:HG23	1.97	0.47
6:F:288:ILE:CD1	6:F:314:LEU:CD2	2.93	0.47
2:B:35:ASP:CB	4:D:30:MET:HE3	2.43	0.47
2:B:86:ILE:HG22	2:B:86:ILE:O	2.14	0.47
3:C:86:ARG:HB2	3:C:92:LEU:CD1	2.43	0.47
5:E:158:ILE:CD1	6:F:334:VAL:HG11	2.44	0.47
6:F:156:ALA:C	6:F:170:ARG:HH22	2.19	0.47
1:A:192:LYS:HD2	3:C:271:MET:SD	2.55	0.47
2:B:521:THR:HG23	3:C:247:GLN:CG	2.44	0.47
4:D:185:SER:HB2	4:D:187:PHE:CE2	2.50	0.47
5:E:121:LEU:HD22	8:H:276:LEU:HD21	1.94	0.47
6:F:359:ARG:HG2	8:H:328:GLN:OE1	2.05	0.47
1:A:211:HIS:HB3	4:D:629:PRO:HG2	1.96	0.46
2:B:386:GLN:NE2	4:D:440:GLN:CD	2.69	0.46
6:F:251:MET:HE1	8:H:243:PHE:CE1	2.50	0.46
6:F:377:ARG:NH1	8:H:343:GLN:N	2.63	0.46
1:A:238:TYR:OH	3:C:325:GLU:OE1	2.33	0.46
1:A:242:ALA:C	1:A:244:ASN:H	2.19	0.46
2:B:577:GLU:OE1	4:D:640:GLY:HA2	2.15	0.46
2:B:449:LEU:HD23	2:B:468:LEU:HD21	1.97	0.46
5:E:189:TRP:CE3	8:H:340:ILE:HD11	2.50	0.46
6:F:5:SER:O	6:F:7:PRO:HD3	2.15	0.46
6:F:261:VAL:CG2	8:H:254:LEU:HD23	2.45	0.46
7:G:280:PHE:CE2	8:H:258:ARG:C	2.83	0.46
2:B:376:MET:HE3	4:D:211:HIS:HB2	1.96	0.46
3:C:67:MET:O	3:C:71:VAL:HG23	2.16	0.46
6:F:359:ARG:NE	8:H:321:GLU:OE1	2.47	0.46
7:G:93:PHE:CD2	7:G:94:ASP:OD1	2.69	0.46
1:A:1:MET:CE	1:A:28:THR:CG2	2.86	0.46
2:B:95:VAL:HG13	2:B:99:LYS:CB	2.45	0.46
2:B:500:LEU:CD2	4:D:571:LEU:CD1	2.85	0.46
4:D:117:GLN:O	4:D:118:ASP:C	2.54	0.46
4:D:355:LEU:O	4:D:362:SER:HB3	2.14	0.46
4:D:595:ASP:O	4:D:599:PRO:HG2	2.15	0.46
5:E:21:LYS:HZ2	7:G:159:SER:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:LEU:CD2	7:G:285:LEU:HD23	2.44	0.46
6:F:330:ASP:OD1	6:F:334:VAL:HG23	2.16	0.46
3:C:12:LEU:HD13	3:C:15:LEU:CD1	2.45	0.46
4:D:122:GLU:CG	4:D:512:ASN:HD21	2.15	0.46
4:D:661:ALA:C	4:D:663:GLY:N	2.69	0.46
5:E:155:ILE:N	5:E:156:PRO:CD	2.78	0.46
2:B:273:LEU:HD13	4:D:330:LEU:HA	1.98	0.46
2:B:457:ASN:O	2:B:459:GLN:N	2.47	0.46
5:E:102:LEU:HD23	7:G:255:ILE:HD12	1.86	0.46
6:F:47:MET:HG3	6:F:48:PHE:CD2	2.50	0.46
2:B:93:GLU:O	2:B:94:GLU:C	2.50	0.46
3:C:140:LEU:HD11	4:D:136:ALA:HB2	1.98	0.46
3:C:146:LEU:O	3:C:150:VAL:HG23	2.15	0.46
4:D:295:ARG:HH12	4:D:299:GLU:HG2	1.80	0.46
8:H:257:THR:HB	8:H:287:LYS:NZ	2.31	0.46
1:A:189:TYR:CA	3:C:271:MET:CE	2.92	0.46
2:B:220:HIS:HE1	4:D:272:GLN:HB3	1.80	0.46
2:B:465:TYR:HB3	4:D:520:ILE:HG21	1.99	0.46
2:B:536:LEU:HD11	3:C:262:SER:HB2	1.98	0.46
4:D:459:TRP:N	4:D:460:PRO:CD	2.78	0.46
5:E:69:LEU:HB3	7:G:217:LEU:CD2	2.46	0.46
7:G:47:ARG:CZ	7:G:101:GLY:HA2	2.46	0.46
1:A:78:GLY:O	1:A:81:TYR:CD1	2.68	0.45
2:B:30:LEU:HD23	4:D:34:LEU:HD23	1.96	0.45
2:B:330:SER:O	2:B:335:PRO:HD3	2.16	0.45
4:D:46:ILE:HA	4:D:50:ILE:HD12	1.99	0.45
7:G:123:ASP:C	7:G:124:THR:O	2.53	0.45
2:B:97:ILE:CD1	4:D:82:GLN:HG2	2.42	0.45
2:B:132:CYS:N	4:D:119:LEU:HD11	2.32	0.45
4:D:8:GLN:CG	4:D:28:GLU:OE1	2.44	0.45
4:D:203:ARG:HB2	4:D:234:TRP:CD1	2.51	0.45
6:F:16:MET:SD	6:F:130:LEU:CD2	3.02	0.45
2:B:339:ARG:CZ	8:H:363:ASP:O	2.65	0.45
2:B:404:GLY:HA2	4:D:459:TRP:CZ3	2.40	0.45
3:C:75:LEU:CD1	3:C:162:LEU:HD23	2.45	0.45
3:C:129:ILE:HD11	4:D:489:LEU:CD1	2.47	0.45
4:D:173:VAL:CG1	4:D:175:PHE:CZ	2.99	0.45
5:E:135:LEU:CB	5:E:136:PRO:CD	2.94	0.45
5:E:181:GLU:HG2	7:G:335:ARG:HH12	1.77	0.45
6:F:301:TYR:CE1	6:F:306:VAL:HG22	2.51	0.45
7:G:274:MET:CE	8:H:280:GLN:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:GLU:CD	4:D:113:GLU:OE2	2.46	0.45
2:B:407:VAL:CG2	4:D:459:TRP:CE3	2.90	0.45
2:B:453:LEU:HB3	2:B:471:VAL:CG1	2.47	0.45
2:B:458:THR:C	2:B:460:LYS:N	2.69	0.45
6:F:377:ARG:HH22	8:H:343:GLN:NE2	2.12	0.45
1:A:40:TRP:CH2	3:C:43:GLY:CA	2.99	0.45
2:B:521:THR:CG2	3:C:247:GLN:HE21	2.30	0.45
4:D:355:LEU:HD22	4:D:365:THR:HB	1.98	0.45
6:F:6:ARG:HD3	6:F:8:HIS:HD2	1.81	0.45
6:F:288:ILE:HD11	6:F:314:LEU:HD23	1.97	0.45
1:A:145:THR:OG1	4:D:65:TRP:CH2	2.63	0.45
2:B:263:GLN:HE21	2:B:346:ASN:ND2	2.06	0.45
3:C:28:PHE:CE1	3:C:32:LEU:HD11	2.52	0.45
5:E:148:TYR:HB3	7:G:292:LEU:HD13	1.98	0.45
7:G:178:LYS:HB3	7:G:179:PRO:HD3	1.99	0.45
7:G:235:ILE:CD1	8:H:225:LEU:CD2	2.95	0.45
1:A:121:SER:HB3	4:D:104:GLN:HE22	1.81	0.45
2:B:192:ILE:HG23	4:D:165:ILE:HG22	1.98	0.45
2:B:263:GLN:NE2	2:B:343:GLN:HA	2.32	0.45
6:F:64:PHE:CD1	6:F:98:TRP:CE3	3.05	0.45
6:F:297:MET:HE3	6:F:314:LEU:HG	1.99	0.45
5:E:104:GLU:OE1	5:E:124:GLU:CG	2.65	0.45
5:E:111:ARG:HD2	7:G:276:PRO:CB	2.46	0.45
7:G:41:CYS:CA	7:G:108:GLN:OE1	2.62	0.45
8:H:156:PRO:C	8:H:158:ASP:H	2.20	0.45
8:H:156:PRO:C	8:H:158:ASP:N	2.70	0.45
1:A:124:VAL:HG21	2:B:110:GLN:HE22	1.78	0.45
1:A:207:GLU:HB3	1:A:208:PRO:HD3	1.99	0.45
2:B:271:HIS:CE1	8:H:360:TRP:NE1	2.85	0.45
4:D:4:ARG:CG	4:D:32:GLN:HE21	2.21	0.45
7:G:274:MET:SD	8:H:280:GLN:CB	2.99	0.45
1:A:65:GLU:OE2	4:D:507:ILE:HD12	2.17	0.44
2:B:74:GLU:OE1	4:D:54:ARG:CG	2.56	0.44
4:D:199:VAL:HG22	4:D:237:MET:CG	2.44	0.44
5:E:104:GLU:CD	5:E:126:SER:OG	2.53	0.44
6:F:170:ARG:NE	7:G:89:MET:SD	2.81	0.44
7:G:2:THR:CG2	7:G:37:TYR:CZ	2.99	0.44
7:G:14:TYR:HB2	7:G:36:ILE:HG23	1.98	0.44
4:D:289:GLU:O	4:D:291:ILE:HG12	2.17	0.44
6:F:166:LYS:HE2	7:G:84:LEU:HD12	1.98	0.44
7:G:135:SER:O	7:G:136:HIS:C	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:294:MET:SD	8:H:298:ALA:CB	3.05	0.44
5:E:49:LEU:CD2	8:H:196:ASN:HD22	2.10	0.44
6:F:170:ARG:HE	7:G:89:MET:CE	2.30	0.44
7:G:124:THR:HG22	7:G:125:ILE:N	2.26	0.44
7:G:139:GLU:O	7:G:143:VAL:HG23	2.16	0.44
7:G:146:ILE:CG1	8:H:163:ILE:HG13	2.47	0.44
8:H:358:ARG:HH21	8:H:366:LEU:HD13	1.81	0.44
1:A:211:HIS:CG	4:D:629:PRO:HD2	2.53	0.44
2:B:447:HIS:ND1	2:B:463:ARG:HD2	2.33	0.44
5:E:114:GLN:NE2	7:G:277:PHE:CE1	2.85	0.44
6:F:84:ASP:OD1	6:F:87:ARG:HD2	2.16	0.44
6:F:138:MET:HE2	8:H:172:TYR:CG	2.52	0.44
1:A:13:LYS:HG3	1:A:21:LEU:HD11	2.00	0.44
1:A:33:ILE:CG2	3:C:15:LEU:HD22	2.42	0.44
4:D:170:GLN:HG3	4:D:171:ARG:HE	1.82	0.44
4:D:572:GLN:HA	4:D:575:THR:OG1	2.18	0.44
5:E:121:LEU:HD23	8:H:276:LEU:HD21	1.97	0.44
1:A:278:PRO:HB2	1:A:279:GLU:HG3	1.43	0.44
2:B:540:ASN:O	2:B:544:VAL:HG23	2.18	0.44
3:C:63:ARG:NH1	4:D:537:GLU:CD	2.67	0.44
4:D:215:ILE:HG21	4:D:419:LEU:HD11	1.99	0.44
5:E:88:HIS:HB2	7:G:238:LEU:HD12	1.98	0.44
5:E:149:ILE:HG23	6:F:325:GLU:HG3	1.99	0.44
1:A:99:CYS:HB3	3:C:67:MET:HE1	2.00	0.44
2:B:319:THR:HG23	4:D:378:LEU:CD1	2.46	0.44
4:D:352:HIS:CG	4:D:366:ARG:CZ	3.01	0.44
6:F:170:ARG:NE	7:G:89:MET:CG	2.81	0.44
6:F:330:ASP:OD1	6:F:334:VAL:N	2.50	0.44
7:G:298:PHE:HB2	8:H:308:ILE:HD13	2.00	0.44
1:A:152:LYS:CE	2:B:73:ASP:CG	2.83	0.44
4:D:173:VAL:HG21	4:D:249:HIS:CG	2.53	0.44
1:A:145:THR:HG23	4:D:65:TRP:HE1	1.82	0.44
2:B:205:LEU:CD2	4:D:259:LEU:HD21	2.46	0.44
3:C:12:LEU:CB	3:C:15:LEU:HD12	2.47	0.44
3:C:266:PHE:CD2	4:D:611:HIS:CD2	3.06	0.44
5:E:107:SER:N	7:G:273:PRO:HA	2.32	0.44
6:F:170:ARG:HE	7:G:89:MET:CG	2.31	0.44
3:C:129:ILE:HD11	4:D:489:LEU:HD13	1.97	0.43
1:A:95:ILE:HG13	3:C:166:CYS:SG	2.58	0.43
1:A:145:THR:CB	4:D:69:LEU:HD11	2.47	0.43
2:B:407:VAL:HG23	4:D:459:TRP:CZ3	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:280:CYS:CB	4:D:625:TRP:HD1	2.31	0.43
5:E:97:HIS:ND1	6:F:255:VAL:HG13	2.32	0.43
7:G:340:ALA:O	7:G:344:SER:OG	2.34	0.43
2:B:97:ILE:CD1	4:D:82:GLN:OE1	2.63	0.43
4:D:17:GLU:OE2	4:D:17:GLU:HA	2.18	0.43
4:D:590:TYR:CE1	4:D:594:LEU:CD1	3.01	0.43
3:C:227:VAL:HG22	3:C:230:ARG:NH2	2.20	0.43
1:A:271:ASN:C	1:A:273:MET:N	2.69	0.43
7:G:176:ASP:OD1	7:G:176:ASP:N	2.50	0.43
2:B:588:GLU:OE1	4:D:650:ARG:NE	2.48	0.43
4:D:293:GLN:HE21	4:D:295:ARG:HB2	1.84	0.43
6:F:244:ILE:HD12	8:H:233:LEU:HD22	2.01	0.43
6:F:341:LEU:HD21	7:G:298:PHE:HE2	1.83	0.43
2:B:43:PHE:CZ	4:D:46:ILE:CD1	2.97	0.43
2:B:220:HIS:CE1	4:D:272:GLN:CB	3.00	0.43
2:B:322:ILE:HD13	4:D:379:ARG:HG3	2.00	0.43
5:E:189:TRP:HH2	8:H:340:ILE:HD12	1.61	0.43
1:A:215:VAL:CG2	4:D:629:PRO:HB2	2.47	0.43
1:A:270:VAL:O	1:A:273:MET:HB2	2.19	0.43
3:C:270:ARG:HD2	4:D:614:TYR:CZ	2.53	0.43
5:E:111:ARG:NH2	7:G:280:PHE:CD2	2.86	0.43
6:F:165:GLN:NE2	7:G:60:PRO:HD2	2.34	0.43
2:B:406:ILE:CD1	4:D:155:ILE:HD11	2.47	0.43
2:B:431:SER:O	2:B:433:SER:N	2.51	0.43
2:B:456:ASP:O	2:B:458:THR:N	2.51	0.43
2:B:571:VAL:HG13	3:C:288:VAL:HG21	2.01	0.43
3:C:8:VAL:HG13	3:C:12:LEU:HD12	1.99	0.43
3:C:36:CYS:N	3:C:37:PRO:CD	2.82	0.43
1:A:158:LEU:HD13	3:C:238:ALA:HB2	2.00	0.43
2:B:190:GLN:CD	4:D:170:GLN:HA	2.39	0.43
7:G:137:SER:C	7:G:139:GLU:H	2.22	0.43
7:G:280:PHE:CE2	8:H:258:ARG:HA	2.54	0.43
1:A:99:CYS:CB	3:C:67:MET:CE	2.89	0.42
2:B:80:VAL:HG11	4:D:65:TRP:CD2	2.54	0.42
2:B:81:LEU:HA	2:B:84:PHE:HD2	1.83	0.42
3:C:4:THR:HG23	3:C:33:ILE:CD1	2.35	0.42
4:D:285:LYS:HD3	4:D:287:PHE:CZ	2.54	0.42
4:D:457:LEU:O	4:D:460:PRO:HD2	2.19	0.42
5:E:21:LYS:HZ3	7:G:159:SER:HA	1.83	0.42
5:E:166:ASP:OD1	6:F:344:LYS:HE3	2.18	0.42
4:D:525:TYR:CZ	4:D:539:VAL:CG2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:ARG:O	5:E:124:GLU:OE1	2.36	0.42
4:D:291:ILE:H	4:D:291:ILE:HG12	1.65	0.42
6:F:84:ASP:OD1	6:F:87:ARG:CG	2.68	0.42
7:G:178:LYS:N	7:G:179:PRO:HD2	2.34	0.42
1:A:133:MET:SD	3:C:217:LEU:CD2	3.05	0.42
3:C:180:GLU:CD	3:C:184:LEU:HD23	2.40	0.42
4:D:442:ARG:O	4:D:446:VAL:HG23	2.19	0.42
5:E:78:ILE:HG13	5:E:79:THR:HG23	2.01	0.42
5:E:137:LEU:HD23	7:G:285:LEU:HB3	2.02	0.42
1:A:71:ASP:CA	3:C:114:ARG:NH2	2.78	0.42
1:A:172:VAL:HG21	3:C:250:ILE:HG23	2.01	0.42
4:D:67:GLN:O	4:D:71:HIS:HB2	2.20	0.42
4:D:76:ARG:HA	4:D:79:GLU:OE2	2.19	0.42
4:D:659:GLN:O	4:D:664:SER:O	2.37	0.42
5:E:179:MET:CG	8:H:329:ILE:HD12	2.48	0.42
6:F:168:LEU:HD12	7:G:145:CYS:SG	2.60	0.42
2:B:89:VAL:C	2:B:90:PRO:O	2.58	0.42
4:D:352:HIS:CB	4:D:366:ARG:NH2	2.37	0.42
5:E:88:HIS:CD2	7:G:237:SER:HG	2.38	0.42
5:E:189:TRP:CZ3	8:H:336:VAL:HG12	2.50	0.42
6:F:166:LYS:HE2	7:G:87:ASP:HB2	2.02	0.42
1:A:8:ILE:HD12	1:A:31:MET:CE	2.50	0.42
1:A:266:LEU:HD21	3:C:344:MET:CE	2.49	0.42
2:B:274:ILE:CD1	4:D:392:LEU:HD11	2.50	0.42
5:E:130:PHE:HZ	6:F:263:ARG:O	1.92	0.42
6:F:192:TYR:CE1	7:G:172:PRO:HD3	2.54	0.42
3:C:285:LYS:HZ1	4:D:628:GLN:HE22	1.66	0.42
4:D:46:ILE:CG2	4:D:50:ILE:HD12	2.38	0.42
6:F:261:VAL:CG2	8:H:258:ARG:HD2	2.50	0.42
7:G:150:GLU:HG2	8:H:166:GLN:HE21	1.84	0.42
2:B:289:TRP:NE1	2:B:293:ASN:ND2	2.68	0.42
2:B:587:LEU:HD23	4:D:654:ALA:HB3	2.02	0.42
3:C:70:GLU:OE2	3:C:70:GLU:HA	2.20	0.42
4:D:6:LEU:HD11	4:D:44:LYS:HE3	2.01	0.42
5:E:94:MET:HG2	7:G:245:PHE:HE2	1.83	0.42
6:F:280:ILE:HA	6:F:281:PRO:HD3	1.80	0.42
2:B:450:TYR:HB3	2:B:463:ARG:NH1	2.35	0.42
3:C:142:PRO:CB	3:C:146:LEU:HD23	2.50	0.42
3:C:285:LYS:NZ	4:D:628:GLN:HE22	2.18	0.42
6:F:166:LYS:HE3	7:G:84:LEU:HD12	2.01	0.42
7:G:139:GLU:HG3	8:H:155:VAL:CG2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:TYR:CD1	4:D:631:GLN:HG2	2.55	0.41
3:C:12:LEU:HD13	3:C:15:LEU:HD12	2.02	0.41
3:C:285:LYS:NZ	4:D:628:GLN:NE2	2.67	0.41
5:E:145:LEU:HD22	6:F:284:LEU:HD13	2.01	0.41
6:F:206:MET:CE	8:H:199:LYS:CG	2.76	0.41
6:F:377:ARG:HH11	8:H:343:GLN:N	2.17	0.41
7:G:183:ALA:HB1	7:G:187:LEU:HD12	2.02	0.41
7:G:188:GLN:O	7:G:192:THR:OG1	2.35	0.41
2:B:30:LEU:HD11	4:D:39:CYS:SG	2.60	0.41
2:B:570:TYR:HA	4:D:644:LEU:HD11	2.02	0.41
3:C:185:ARG:O	3:C:189:VAL:HG23	2.20	0.41
4:D:75:GLN:O	4:D:79:GLU:HG3	2.20	0.41
4:D:46:ILE:HG23	4:D:50:ILE:CD1	2.40	0.41
6:F:176:GLN:NE2	7:G:117:ASP:HB3	2.34	0.41
6:F:392:CYS:HA	6:F:393:PRO:HD3	1.81	0.41
7:G:60:PRO:N	7:G:61:PRO:CD	2.83	0.41
6:F:227:ILE:O	6:F:227:ILE:CG2	2.68	0.41
1:A:149:VAL:HG13	2:B:70:PRO:HG3	1.97	0.41
2:B:276:MET:HE2	4:D:334:GLN:HE21	1.85	0.41
2:B:430:LEU:C	2:B:431:SER:O	2.58	0.41
2:B:543:THR:OG1	3:C:269:LEU:HD12	2.20	0.41
4:D:10:LEU:HD11	4:D:43:TRP:CE3	2.54	0.41
4:D:173:VAL:HG23	4:D:249:HIS:CE1	2.56	0.41
4:D:203:ARG:HD3	4:D:234:TRP:CE2	2.56	0.41
5:E:58:GLU:HG2	7:G:207:LEU:HD11	2.02	0.41
5:E:182:VAL:HG23	7:G:335:ARG:NH2	2.35	0.41
6:F:251:MET:CE	8:H:247:TYR:CD1	3.03	0.41
7:G:9:ALA:HB3	7:G:109:ILE:HD13	2.01	0.41
1:A:236:ASN:HA	1:A:239:LEU:HD12	2.02	0.41
6:F:84:ASP:OD1	6:F:87:ARG:HG3	2.21	0.41
6:F:157:LEU:HG	6:F:170:ARG:HH21	1.84	0.41
2:B:301:ALA:O	4:D:361:VAL:HG11	2.21	0.41
3:C:4:THR:O	3:C:8:VAL:HG23	2.20	0.41
4:D:197:ARG:O	4:D:201:LYS:HG3	2.20	0.41
5:E:179:MET:HG3	8:H:329:ILE:CD1	2.50	0.41
7:G:318:LYS:HG3	7:G:324:ILE:HG12	2.02	0.41
2:B:276:MET:CE	4:D:334:GLN:HG2	2.51	0.41
3:C:236:ARG:NH1	4:D:574:ASN:O	2.54	0.41
4:D:352:HIS:HB3	4:D:366:ARG:CZ	2.40	0.41
6:F:168:LEU:HD11	7:G:145:CYS:CB	2.51	0.41
1:A:99:CYS:HB2	3:C:67:MET:HE2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:HG23	3:C:274:LEU:HD12	2.02	0.41
2:B:93:GLU:C	2:B:94:GLU:O	2.58	0.41
2:B:97:ILE:O	2:B:101:GLU:HG3	2.20	0.41
2:B:385:LEU:CD1	4:D:254:LEU:HD13	2.51	0.41
2:B:432:ALA:C	2:B:433:SER:O	2.57	0.41
3:C:36:CYS:O	3:C:39:LEU:O	2.38	0.41
4:D:34:LEU:O	4:D:39:CYS:HB3	2.21	0.41
4:D:175:PHE:CE1	4:D:193:LEU:CG	3.03	0.41
4:D:525:TYR:CE2	4:D:539:VAL:HG21	2.55	0.41
5:E:134:LEU:HD22	7:G:278:PHE:HD1	1.85	0.41
5:E:139:VAL:HG13	6:F:278:LEU:HD12	2.02	0.41
5:E:207:CYS:O	5:E:208:ILE:C	2.58	0.41
6:F:6:ARG:HA	6:F:7:PRO:HD2	1.51	0.41
6:F:157:LEU:HA	6:F:170:ARG:HH22	1.86	0.41
7:G:40:LEU:O	7:G:47:ARG:NH1	2.53	0.41
1:A:99:CYS:HB3	3:C:67:MET:HE2	1.91	0.41
6:F:44:GLY:H	6:F:47:MET:HE1	1.83	0.41
6:F:227:ILE:CA	8:H:223:ARG:NH2	2.62	0.41
6:F:263:ARG:CA	7:G:279:GLN:HE22	2.31	0.41
7:G:9:ALA:HB1	7:G:109:ILE:HG21	2.03	0.41
4:D:289:GLU:HA	4:D:290:PRO:HD3	1.19	0.40
5:E:179:MET:HG3	8:H:329:ILE:HD12	2.03	0.40
7:G:139:GLU:CG	8:H:155:VAL:HG22	2.41	0.40
1:A:211:HIS:ND1	4:D:630:VAL:HG23	2.36	0.40
2:B:229:VAL:HG12	2:B:229:VAL:O	2.21	0.40
2:B:347:MET:HG3	4:D:406:LEU:HD11	2.04	0.40
2:B:347:MET:CG	4:D:406:LEU:HD11	2.51	0.40
2:B:521:THR:HG23	3:C:247:GLN:NE2	2.37	0.40
1:A:175:ARG:NH1	3:C:254:ASN:OD1	2.44	0.40
2:B:273:LEU:CA	4:D:330:LEU:HD13	2.51	0.40
4:D:219:VAL:O	4:D:221:PRO:HD3	2.21	0.40
5:E:78:ILE:HD13	6:F:234:ILE:HG23	2.02	0.40
5:E:181:GLU:CB	7:G:335:ARG:HH12	2.33	0.40
7:G:274:MET:CE	8:H:280:GLN:CA	2.99	0.40
1:A:104:LEU:O	3:C:63:ARG:NH2	2.47	0.40
2:B:160:LEU:HB2	4:D:145:CYS:SG	2.61	0.40
3:C:5:LEU:HD13	3:C:22:LEU:HD12	2.00	0.40
4:D:172:GLU:C	4:D:173:VAL:HG23	2.41	0.40
1:A:4:LYS:HG2	1:A:35:TYR:CE2	2.56	0.40
2:B:78:ASP:O	2:B:82:LYS:HG3	2.22	0.40
2:B:85:SER:C	2:B:87:SER:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:LEU:O	2:B:201:LYS:N	2.55	0.40
4:D:120:ASN:C	4:D:122:GLU:H	2.25	0.40
7:G:127:SER:C	7:G:129:VAL:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	284/286 (99%)	273 (96%)	4 (1%)	7 (2%)	5	32
2	B	595/597 (100%)	542 (91%)	18 (3%)	35 (6%)	1	17
3	C	351/353 (99%)	338 (96%)	7 (2%)	6 (2%)	9	42
4	D	662/666 (99%)	622 (94%)	19 (3%)	21 (3%)	4	26
5	E	213/222 (96%)	203 (95%)	5 (2%)	5 (2%)	6	34
6	F	383/978 (39%)	365 (95%)	9 (2%)	9 (2%)	6	34
7	G	335/348 (96%)	311 (93%)	9 (3%)	15 (4%)	2	22
8	H	199/367 (54%)	197 (99%)	1 (0%)	1 (0%)	29	69
All	All	3022/3817 (79%)	2851 (94%)	72 (2%)	99 (3%)	6	26

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	MET
1	A	277	VAL
1	A	278	PRO
1	A	279	GLU
1	A	282	LYS
1	A	283	ARG
2	B	88	LYS

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Mol	Chain	Res	Type
2	B	92	ILE
2	B	93	GLU
2	B	95	VAL
2	B	97	ILE
2	B	197	LEU
2	B	234	GLU
2	B	236	PHE
2	B	238	LEU
2	B	240	GLN
2	B	241	LEU
2	B	243	VAL
2	B	250	GLY
2	B	431	SER
2	B	432	ALA
2	B	457	ASN
2	B	459	GLN
2	B	594	GLY
3	C	118	ALA
3	C	119	ASP
3	C	122	PRO
3	C	124	SER
3	C	352	LEU
4	D	118	ASP
4	D	173	VAL
4	D	178	VAL
4	D	186	THR
4	D	217	SER
4	D	284	LEU
4	D	288	SER
4	D	304	ASP
4	D	305	PRO
4	D	306	GLN
4	D	308	THR
4	D	663	GLY
4	D	665	ARG
5	E	2	MET
5	E	3	ALA
6	F	5	SER
6	F	7	PRO
7	G	124	THR
7	G	130	ILE
7	G	132	GLU

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Mol	Chain	Res	Type
7	G	134	LEU
7	G	138	THR
7	G	185	GLU
7	G	197	GLY
7	G	228	VAL
7	G	230	ASP
7	G	231	GLY
8	H	157	GLU
2	B	3	GLY
2	B	91	ALA
2	B	184	ALA
2	B	242	ASN
2	B	248	GLU
2	B	252	THR
2	B	455	GLY
2	B	592	GLY
4	D	119	LEU
4	D	170	GLN
4	D	177	ALA
4	D	286	GLU
4	D	290	PRO
4	D	300	SER
5	E	4	ALA
5	E	220	LEU
6	F	2	GLN
6	F	296	GLN
7	G	123	ASP
1	A	243	PRO
2	B	94	GLU
2	B	187	LEU
2	B	200	ASP
4	D	278	LYS
6	F	228	SER
6	F	337	ASP
7	G	2	THR
2	B	199	LEU
2	B	233	ASP
7	G	122	PRO
6	F	148	ALA
6	F	333	GLY
7	G	125	ILE
5	E	5	ASN

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Mol	Chain	Res	Type
2	B	181	PRO
2	B	239	VAL
2	B	89	VAL
2	B	90	PRO
3	C	123	PRO
7	G	273	PRO
4	D	280	PRO
6	F	6	ARG

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 PDB entries followed by that with respect to all EM entries.

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	260/260 (100%)	248 (95%)	12 (5%)	27	52
2	B	541/541 (100%)	506 (94%)	35 (6%)	17	42
3	C	326/326 (100%)	312 (96%)	14 (4%)	29	53
4	D	605/605 (100%)	570 (94%)	35 (6%)	20	45
5	E	190/195 (97%)	176 (93%)	14 (7%)	13	38
6	F	343/882 (39%)	327 (95%)	16 (5%)	26	51
7	G	313/320 (98%)	295 (94%)	18 (6%)	20	45
8	H	192/328 (58%)	184 (96%)	8 (4%)	30	54
All	All	2770/3457 (80%)	2618 (94%)	152 (6%)	25	47

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	28	THR
1	A	153	SER
1	A	200	LEU
1	A	217	LEU
1	A	218	SER
1	A	220	THR

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	239	LEU
1	A	246	SER
1	A	262	THR
1	A	268	THR
2	B	30	LEU
2	B	36	LEU
2	B	45	SER
2	B	48	SER
2	B	58	LEU
2	B	77	LEU
2	B	83	THR
2	B	94	GLU
2	B	121	LEU
2	B	131	MET
2	B	179	SER
2	B	180	THR
2	B	183	THR
2	B	185	CYS
2	B	188	SER
2	B	196	GLN
2	B	197	LEU
2	B	198	LEU
2	B	200	ASP
2	B	225	MET
2	B	226	SER
2	B	228	PHE
2	B	238	LEU
2	B	246	PHE
2	B	251	THR
2	B	385	LEU
2	B	437	SER
2	B	456	ASP
2	B	491	GLN
2	B	495	LEU
2	B	507	LEU
2	B	536	LEU
2	B	547	LEU
2	B	550	LEU
2	B	591	THR
3	C	60	LEU
3	C	92	LEU

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Mol	Chain	Res	Type
3	C	120	SER
3	C	141	LEU
3	C	158	LEU
3	C	176	GLU
3	C	218	GLU
3	C	269	LEU
3	C	303	GLU
3	C	309	THR
3	C	314	LEU
3	C	315	SER
3	C	330	GLU
3	C	352	LEU
4	D	1	MET
4	D	64	LEU
4	D	69	LEU
4	D	72	THR
4	D	77	THR
4	D	83	GLN
4	D	122	GLU
4	D	164	GLU
4	D	170	GLN
4	D	171	ARG
4	D	174	MET
4	D	182	LEU
4	D	183	SER
4	D	186	THR
4	D	229	LEU
4	D	291	ILE
4	D	292	THR
4	D	293	GLN
4	D	295	ARG
4	D	299	GLU
4	D	302	HIS
4	D	359	SER
4	D	375	CYS
4	D	402	GLU
4	D	405	LEU
4	D	499	LEU
4	D	503	ARG
4	D	575	THR
4	D	579	THR
4	D	592	LEU

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Mol	Chain	Res	Type
4	D	636	SER
4	D	648	ARG
4	D	658	LEU
4	D	662	THR
4	D	664	SER
5	E	9	PRO
5	E	18	LEU
5	E	28	LEU
5	E	38	LEU
5	E	69	LEU
5	E	70	ARG
5	E	121	LEU
5	E	206	SER
5	E	207	CYS
5	E	209	THR
5	E	212	THR
5	E	213	SER
5	E	220	LEU
5	E	221	HIS
6	F	3	SER
6	F	9	LEU
6	F	37	THR
6	F	38	LEU
6	F	114	VAL
6	F	173	LEU
6	F	187	LEU
6	F	219	LEU
6	F	224	ASP
6	F	278	LEU
6	F	283	LEU
6	F	293	HIS
6	F	325	GLU
6	F	331	CYS
6	F	338	LEU
6	F	360	HIS
7	G	2	THR
7	G	19	MET
7	G	31	THR
7	G	46	HIS
7	G	48	LEU
7	G	74	THR
7	G	124	THR

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Mol	Chain	Res	Type
7	G	127	SER
7	G	134	LEU
7	G	135	SER
7	G	138	THR
7	G	180	LEU
7	G	192	THR
7	G	226	SER
7	G	229	THR
7	G	230	ASP
7	G	322	SER
7	G	344	SER
8	H	202	LEU
8	H	204	GLU
8	H	213	LEU
8	H	216	LEU
8	H	254	LEU
8	H	356	LEU
8	H	363	ASP
8	H	367	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	114	HIS
2	B	190	GLN
2	B	263	GLN
2	B	346	ASN
2	B	361	GLN
2	B	374	HIS
2	B	386	GLN
2	B	493	HIS
3	C	220	GLN
3	C	247	GLN
4	D	32	GLN
4	D	49	HIS
4	D	68	GLN
4	D	104	GLN
4	D	152	ASN
4	D	161	GLN
4	D	170	GLN
4	D	211	HIS
4	D	334	GLN

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Mol	Chain	Res	Type
4	D	343	HIS
4	D	352	HIS
4	D	426	HIS
4	D	542	HIS
4	D	549	GLN
4	D	628	GLN
4	D	631	GLN
5	E	114	GLN
6	F	313	GLN
7	G	18	GLN
7	G	92	HIS
7	G	161	HIS
7	G	279	GLN
8	H	196	ASN
8	H	207	HIS
8	H	282	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	18
6	F	17
4	D	14
2	B	13
1	A	13
7	G	9
8	H	7
3	C	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	298:ASN	C	299:GLU	N	4.29
1	B	223:GLU	C	224:GLY	N	1.81
1	A	277:VAL	C	278:PRO	N	1.79
1	D	288:SER	C	289:GLU	N	1.78
1	A	280:PRO	C	281:SER	N	1.75
1	A	283:ARG	C	284:ARG	N	1.70
1	A	284:ARG	C	285:LEU	N	1.69
1	B	591:THR	C	592:GLY	N	1.66
1	C	319:PHE	C	320:LEU	N	1.66
1	A	276:VAL	C	277:VAL	N	1.65
1	B	367:ARG	C	368:GLN	N	1.20
1	C	213:MET	C	214:ARG	N	1.20
1	D	221:PRO	C	222:GLY	N	1.20
1	D	638:GLU	C	639:ARG	N	1.20
1	D	650:ARG	C	651:TRP	N	1.20
1	D	661:ALA	C	662:THR	N	1.20
1	E	51:ARG	C	52:ILE	N	1.20
1	E	72:GLU	C	73:LYS	N	1.20
1	E	95:ASN	C	96:SER	N	1.20
1	E	128:HIS	C	129:ARG	N	1.20
1	E	136:PRO	C	137:LEU	N	1.20
1	E	137:LEU	C	138:ALA	N	1.20
1	F	173:LEU	C	174:ALA	N	1.20
1	F	175:ARG	C	176:GLN	N	1.20
1	G	287:THR	C	288:CYS	N	1.20
1	G	299:THR	C	300:GLU	N	1.20
1	H	297:HIS	C	298:ALA	N	1.20
1	H	319:ASP	C	320:GLU	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	222:THR	C	223:GLU	N	1.19
1	A	242:ALA	C	243:PRO	N	1.19
1	B	363:SER	C	364:CYS	N	1.19
1	B	516:ASN	C	517:THR	N	1.19
1	C	291:GLN	C	292:ILE	N	1.19
1	C	313:ILE	C	314:LEU	N	1.19
1	D	223:LYS	C	224:GLU	N	1.19
1	D	311:SER	C	312:PHE	N	1.19
1	D	501:PRO	C	502:SER	N	1.19
1	E	15:ALA	C	16:SER	N	1.19
1	E	22:CYS	C	23:LEU	N	1.19
1	E	58:GLU	C	59:ILE	N	1.19
1	E	61:GLN	C	62:LYS	N	1.19
1	E	88:HIS	C	89:GLN	N	1.19
1	F	80:TRP	C	81:PRO	N	1.19
1	F	195:LYS	C	196:ALA	N	1.19
1	F	202:GLN	C	203:ILE	N	1.19
1	F	260:ALA	C	261:VAL	N	1.19
1	F	380:GLU	C	381:TRP	N	1.19
1	G	120:GLN	C	121:TYR	N	1.19
1	H	218:ARG	C	219:GLU	N	1.19
1	B	6:ARG	C	7:PHE	N	1.18
1	B	215:SER	C	216:PHE	N	1.18
1	B	222:PHE	C	223:GLU	N	1.18
1	C	314:LEU	C	315:SER	N	1.18
1	E	78:ILE	C	79:THR	N	1.18
1	E	93:ALA	C	94:MET	N	1.18
1	F	44:GLY	C	45:VAL	N	1.18
1	F	209:GLU	C	210:HIS	N	1.18
1	F	253:LYS	C	254:GLU	N	1.18
1	G	141:ASN	C	142:VAL	N	1.18
1	G	161:HIS	C	162:PHE	N	1.18
1	G	275:GLY	C	276:PRO	N	1.18
1	H	196:ASN	C	197:ASP	N	1.18
1	H	300:GLU	C	301:ASN	N	1.18
1	H	333:SER	C	334:PHE	N	1.18
1	B	589:ALA	C	590:GLN	N	1.17
1	B	594:GLY	C	595:SER	N	1.17
1	C	113:SER	C	114:ARG	N	1.17
1	D	227:ARG	C	228:SER	N	1.17
1	D	313:HIS	C	314:SER	N	1.17
1	E	82:LEU	C	83:TYR	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	51:PRO	C	52:ASN	N	1.17
1	F	121:PRO	C	122:GLY	N	1.17
1	G	122:PRO	C	123:ASP	N	1.17
1	A	268:THR	C	269:LYS	N	1.16
1	B	73:ASP	C	74:GLU	N	1.16
1	D	177:ALA	C	178:VAL	N	1.16
1	E	69:LEU	C	70:ARG	N	1.16
1	E	73:LYS	C	74:GLU	N	1.16
1	F	258:VAL	C	259:ASP	N	1.16
1	G	234:VAL	C	235:ILE	N	1.16
1	G	289:PHE	C	290:LYS	N	1.16
1	A	206:GLU	C	207:GLU	N	1.15
1	A	229:MET	C	230:ALA	N	1.15
1	A	265:GLU	C	266:LEU	N	1.15
1	E	133:GLU	C	134:LEU	N	1.15
1	F	213:LEU	C	214:GLN	N	1.15
1	H	155:VAL	C	156:PRO	N	1.15
1	D	402:GLU	C	403:MET	N	1.14
1	E	86:GLN	C	87:LYS	N	1.14
1	F	146:ALA	C	147:ASP	N	1.14
1	F	262:VAL	C	263:ARG	N	1.14
1	A	269:LYS	C	270:VAL	N	1.12
1	B	592:GLY	C	593:GLY	N	1.11
1	F	1:MET	C	2:GLN	N	1.11
1	B	392:GLU	C	393:LEU	N	1.03
1	D	289:GLU	C	290:PRO	N	1.03
1	A	272:MET	C	273:MET	N	0.96

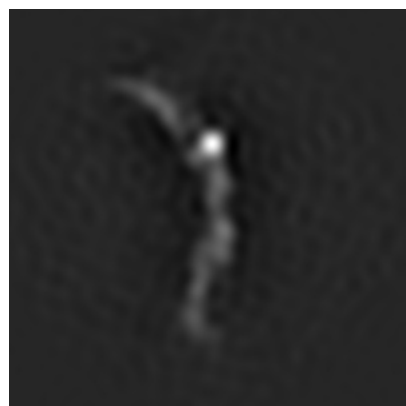
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15632. These allow visual inspection of the internal detail of the map and identification of artifacts.

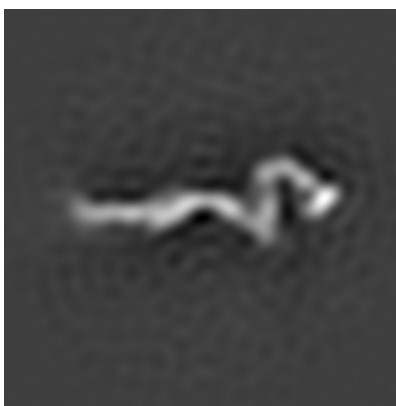
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

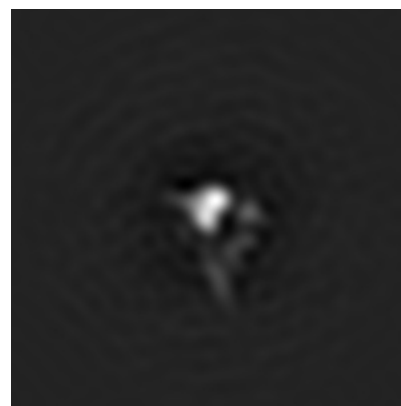
6.1.1 Primary map



X

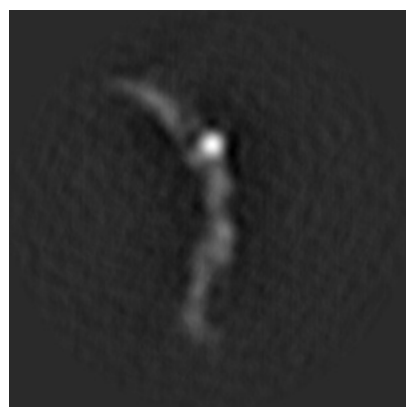


Y

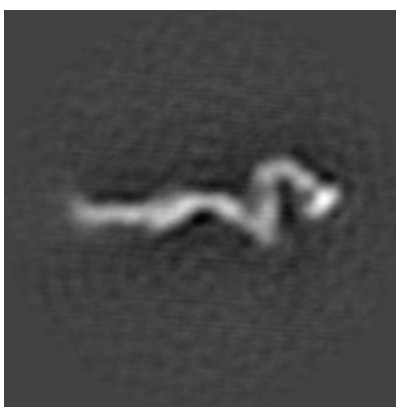


Z

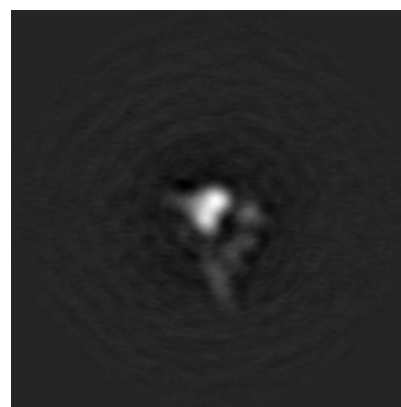
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

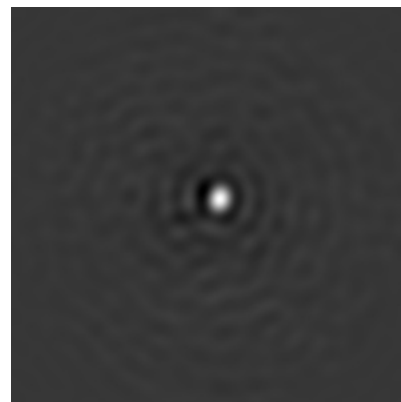
6.2.1 Primary map



X Index: 128

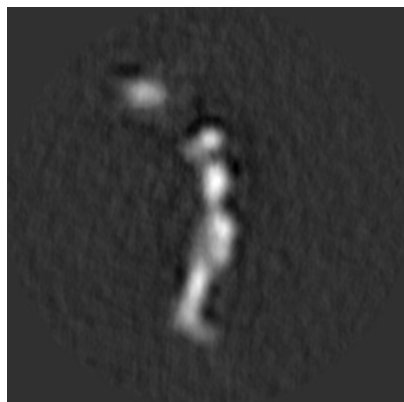


Y Index: 128

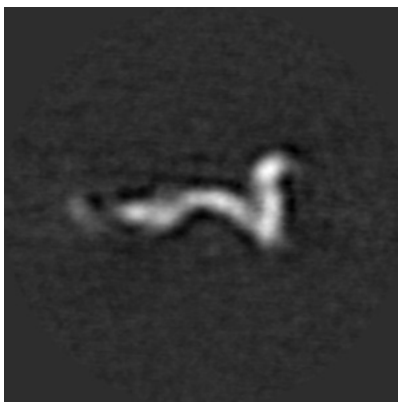


Z Index: 128

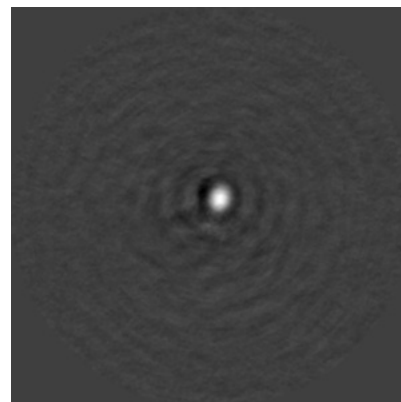
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 127

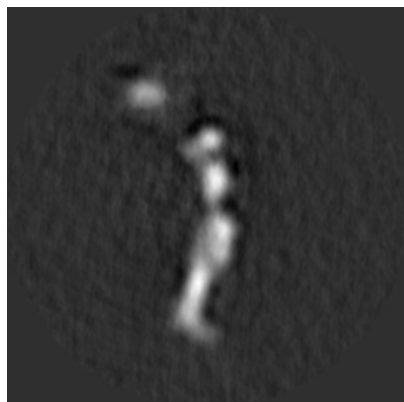


Y Index: 132

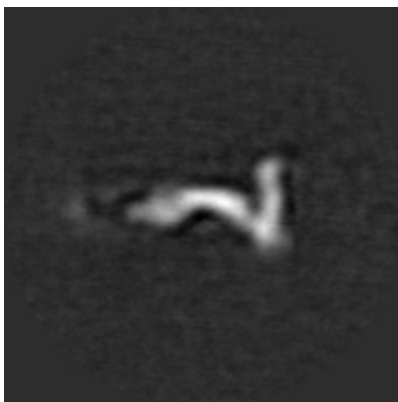


Z Index: 169

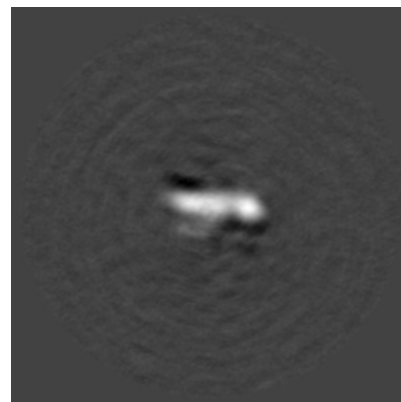
6.3.2 Raw map



X Index: 127



Y Index: 132



Z Index: 169

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

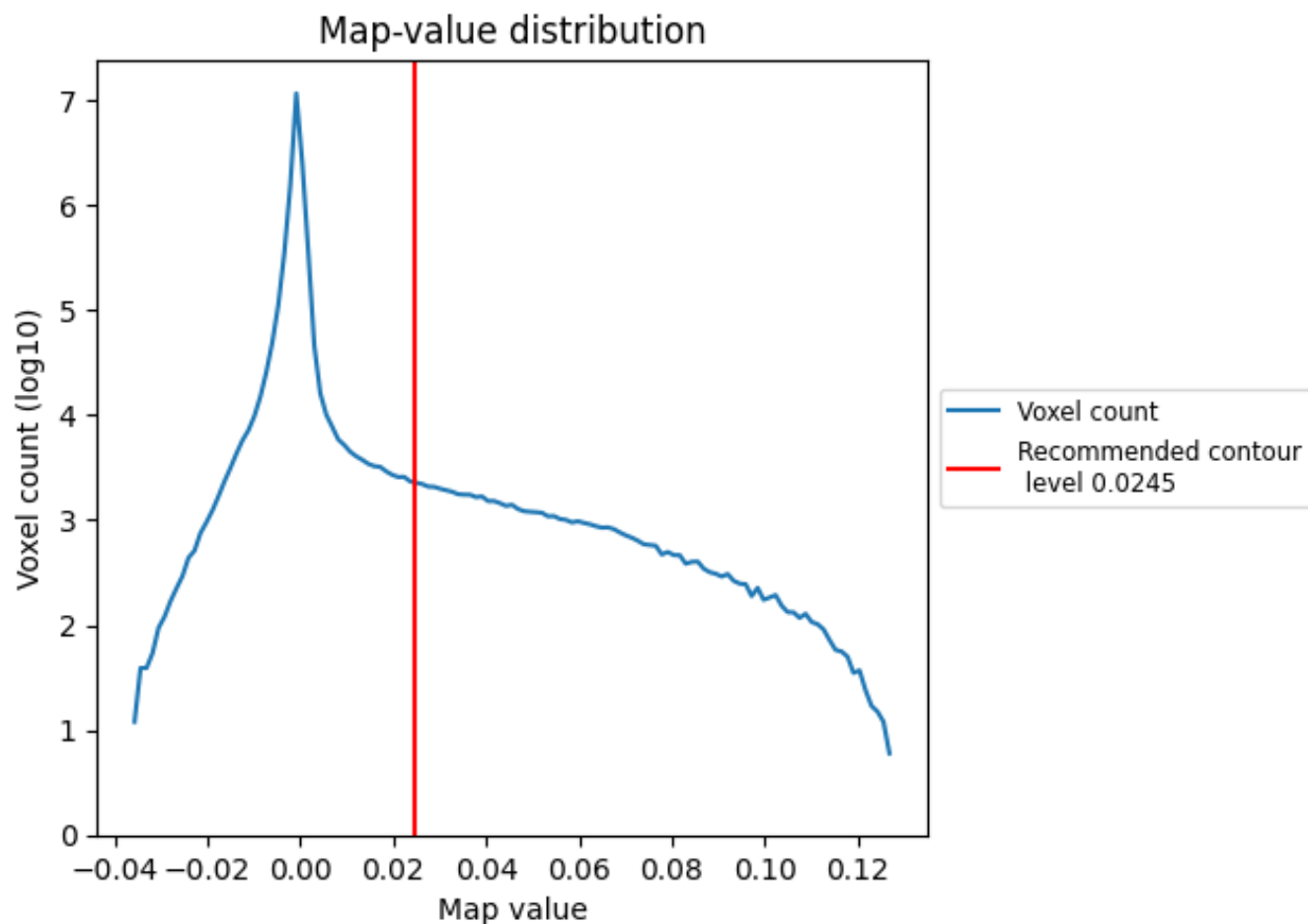
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

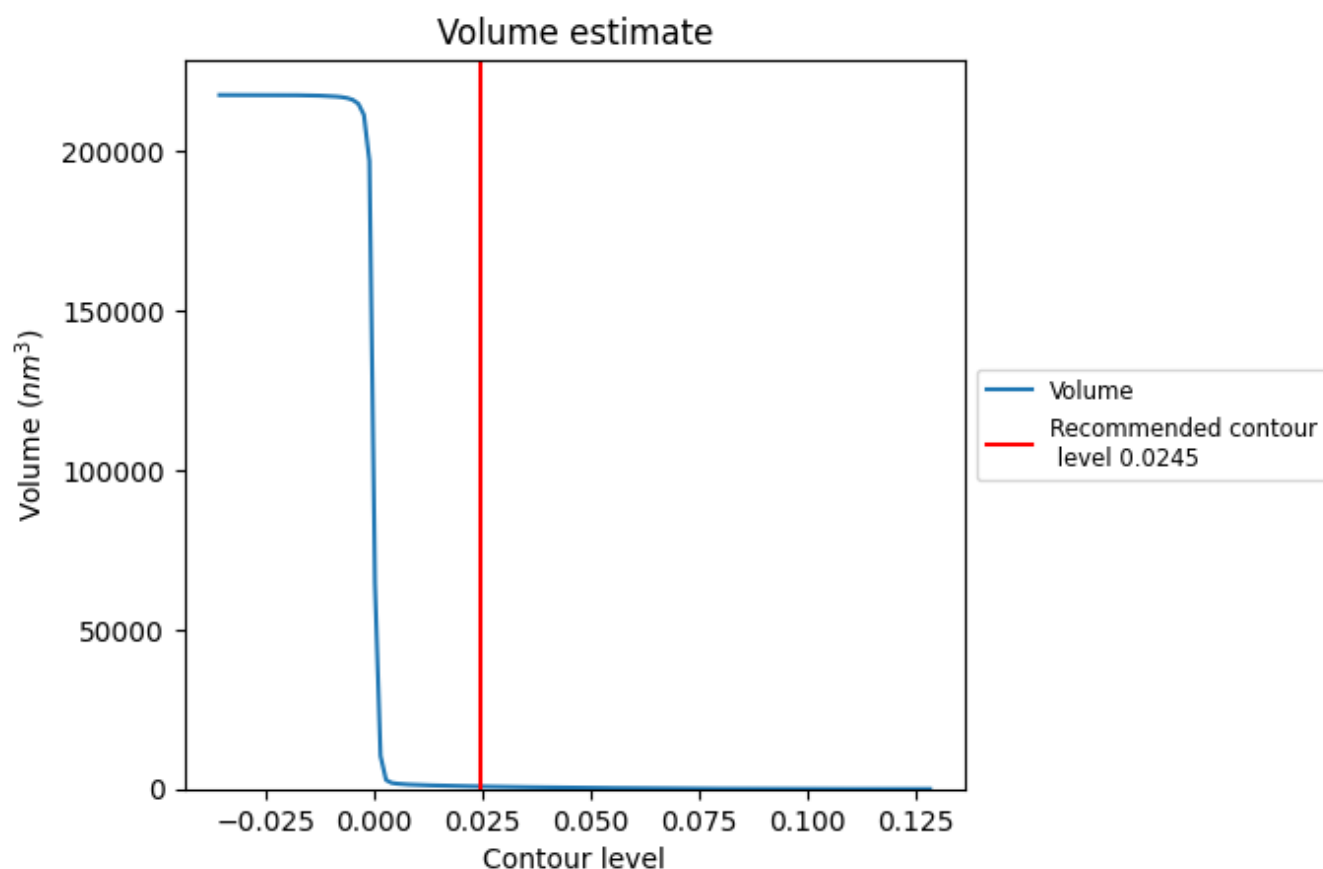
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

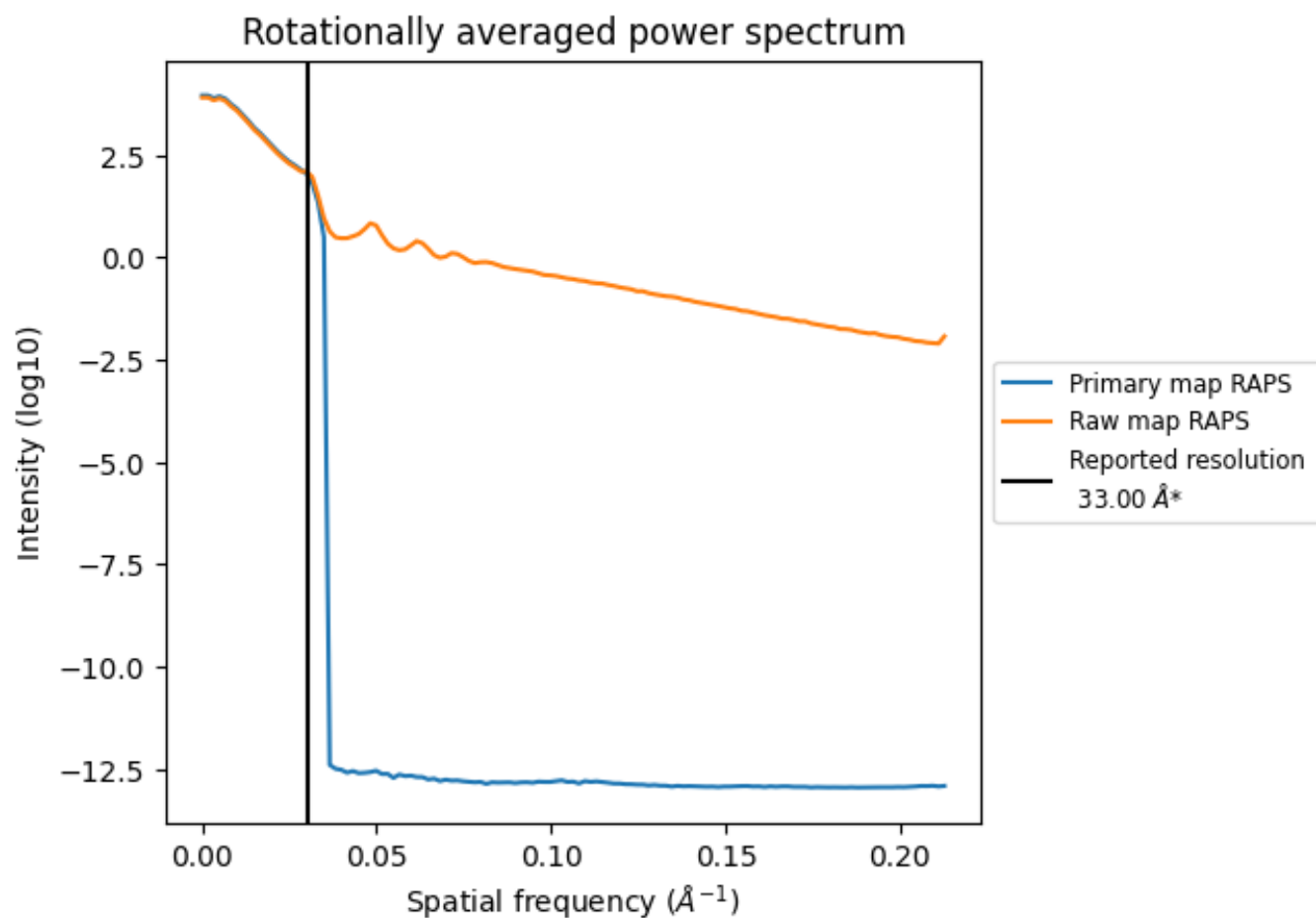
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 788 nm^3 ; this corresponds to an approximate mass of 712 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

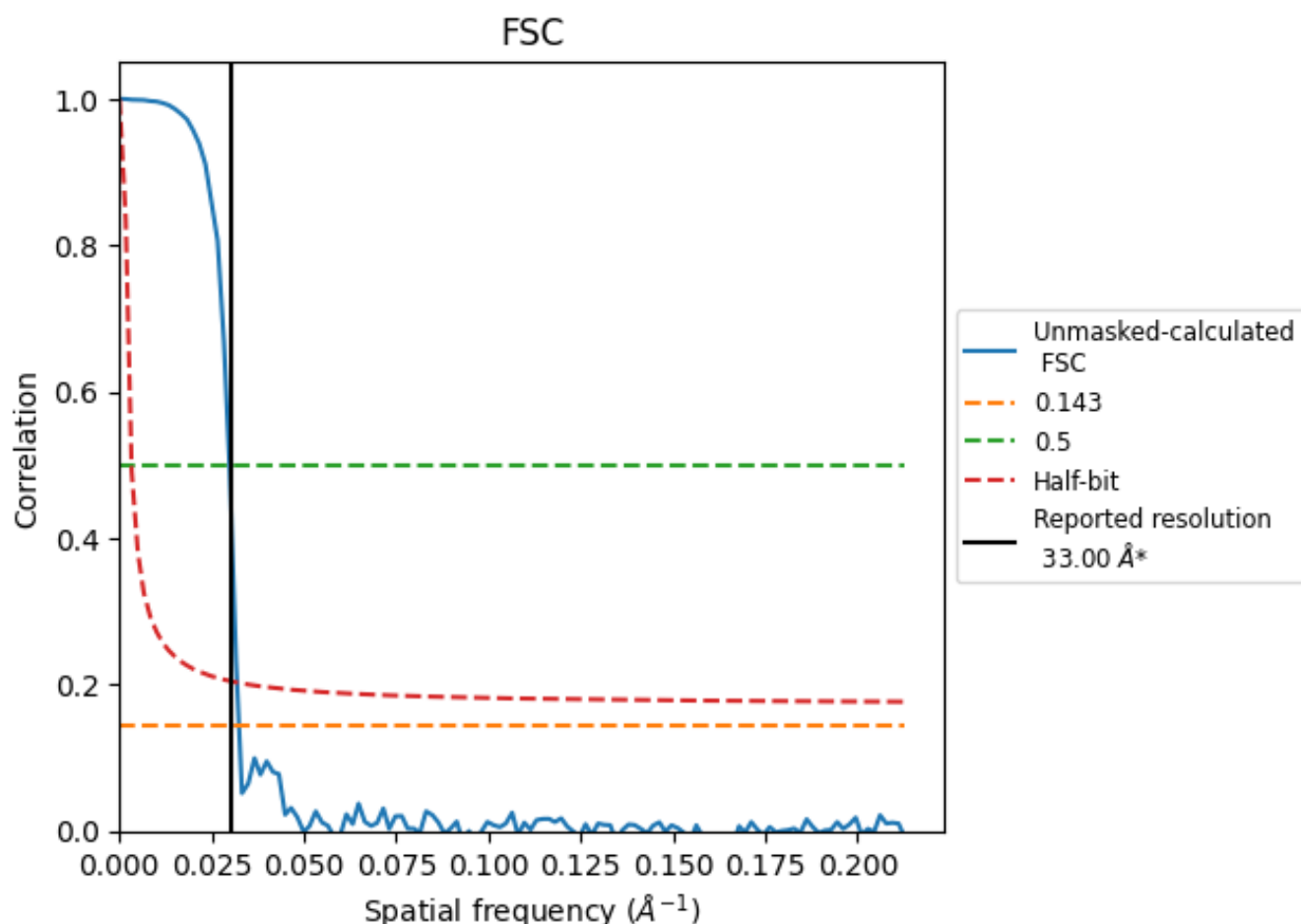


*Reported resolution corresponds to spatial frequency of 0.030 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.030 \AA^{-1}

8.2 Resolution estimates [i](#)

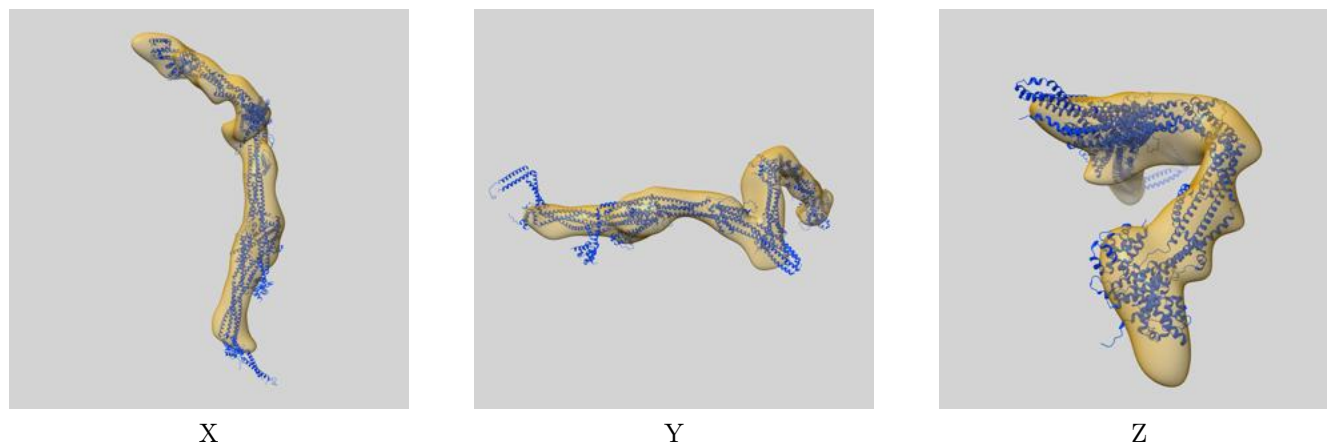
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	33.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	30.86	33.56	31.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

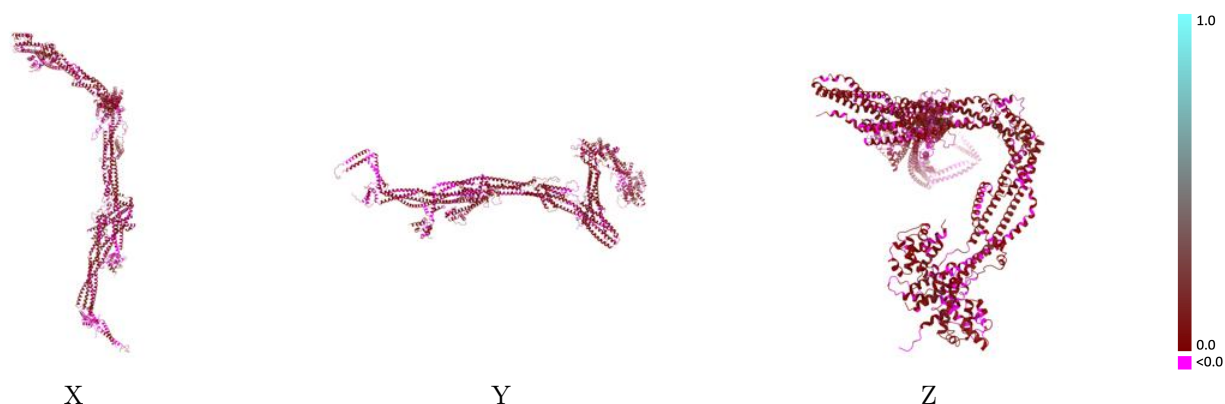
This section contains information regarding the fit between EMDB map EMD-15632 and PDB model 8AT3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



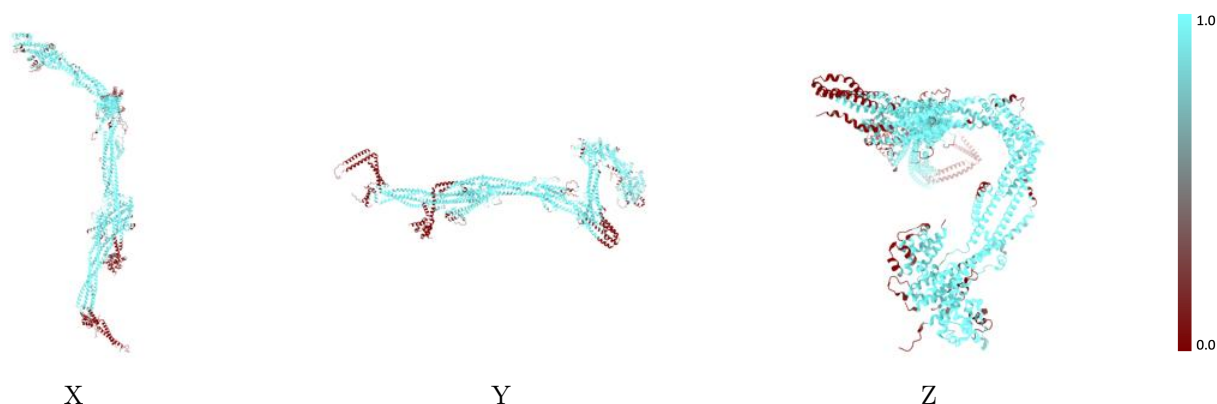
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



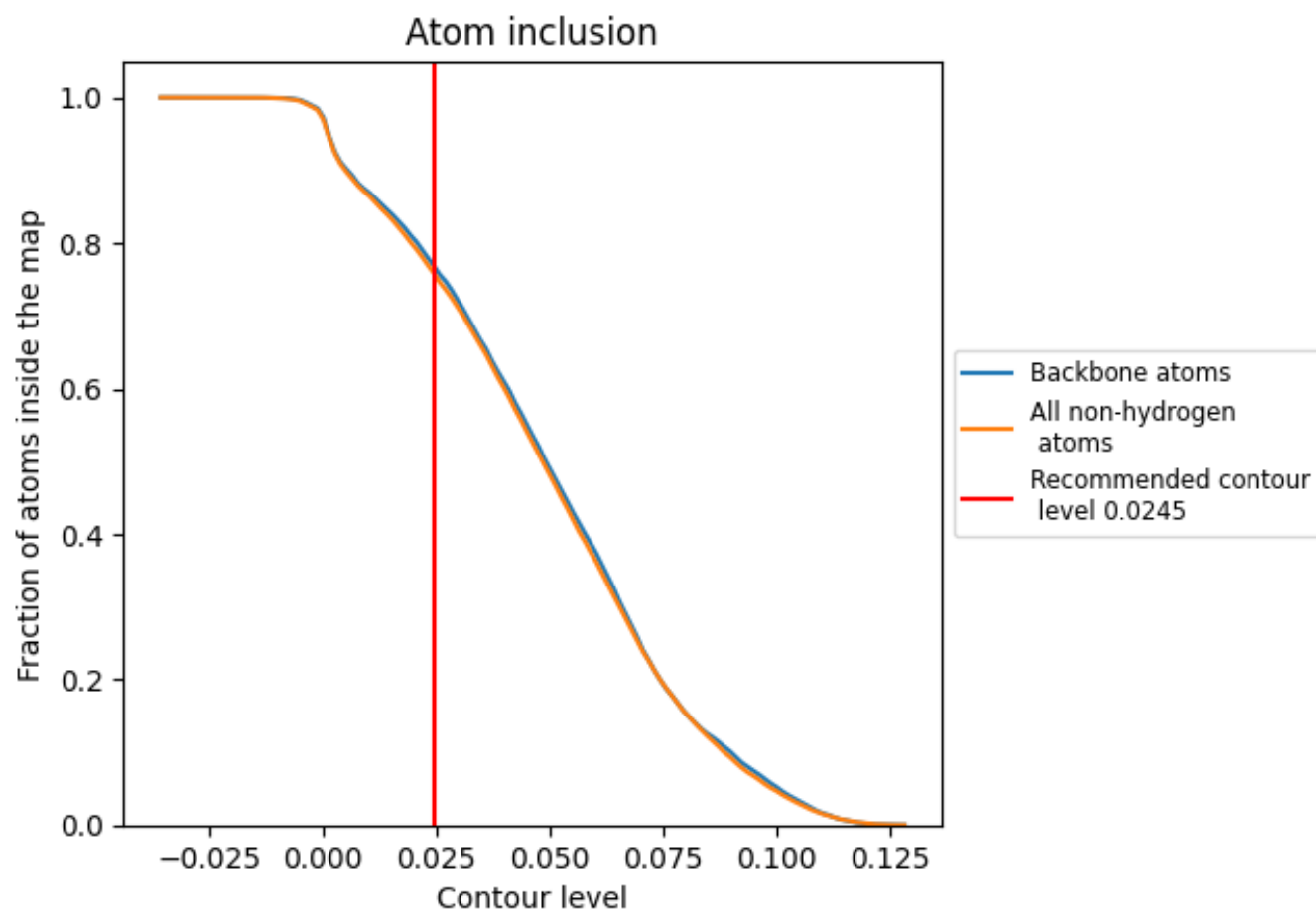
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0245).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7585	<div><div></div></div> 0.0470
A	<div><div></div></div> 0.6828	<div><div></div></div> 0.0420
B	<div><div></div></div> 0.7179	<div><div></div></div> 0.0420
C	<div><div></div></div> 0.7318	<div><div></div></div> 0.0500
D	<div><div></div></div> 0.6881	<div><div></div></div> 0.0430
E	<div><div></div></div> 0.7950	<div><div></div></div> 0.0480
F	<div><div></div></div> 0.8465	<div><div></div></div> 0.0400
G	<div><div></div></div> 0.8081	<div><div></div></div> 0.0510
H	<div><div></div></div> 0.9677	<div><div></div></div> 0.0890

1.0

0.0

<0.0