



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:07 AM UTC

PDB ID : 8AT3 / pdb_00008at3
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:

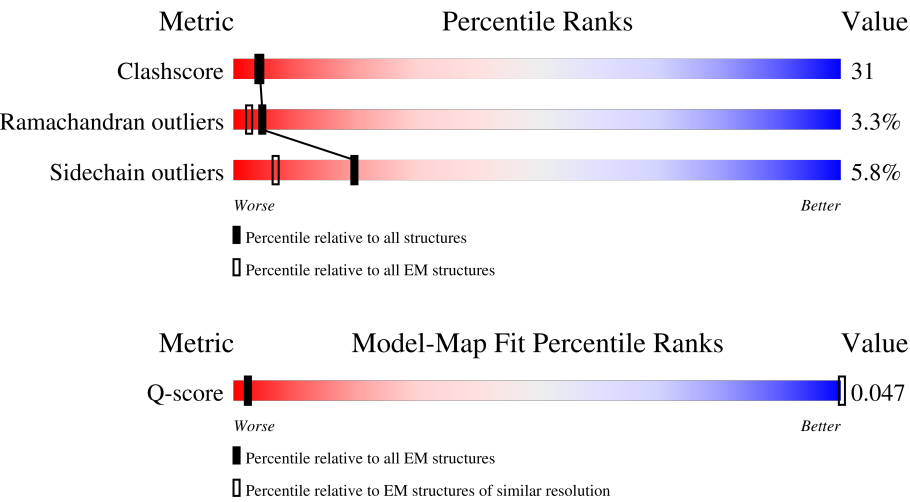
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3 (33.00 - 33.00)

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	31% 46%37%11%5%
2	B	597	27% 42%36%13%9%
3	C	353	26% 46%41%11%
4	D	666	30% 45%38%12%6%

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Mol	Chain	Length	Quality of chain
5	E	222	19%36%42%16%. .
6	F	978	5%17%15%6%.60%
7	G	348	17%35%40%17%6%. .
8	H	367	.25%21%9%45%

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		

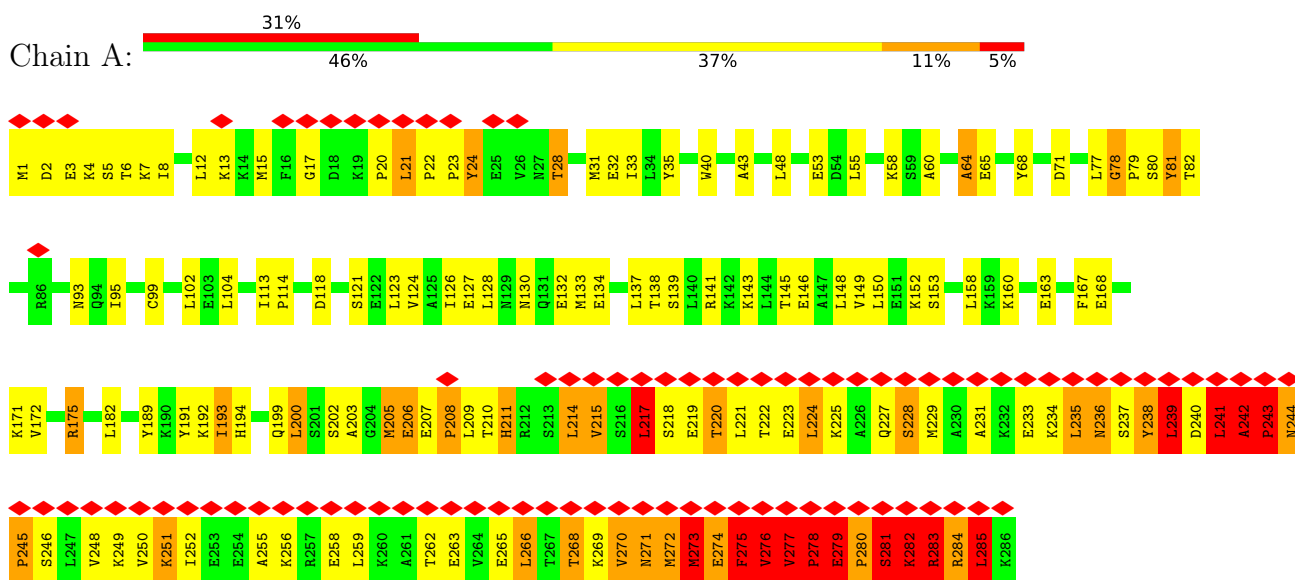
- Molecule 8 is a protein called HAUS augmin-like complex subunit 8.

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

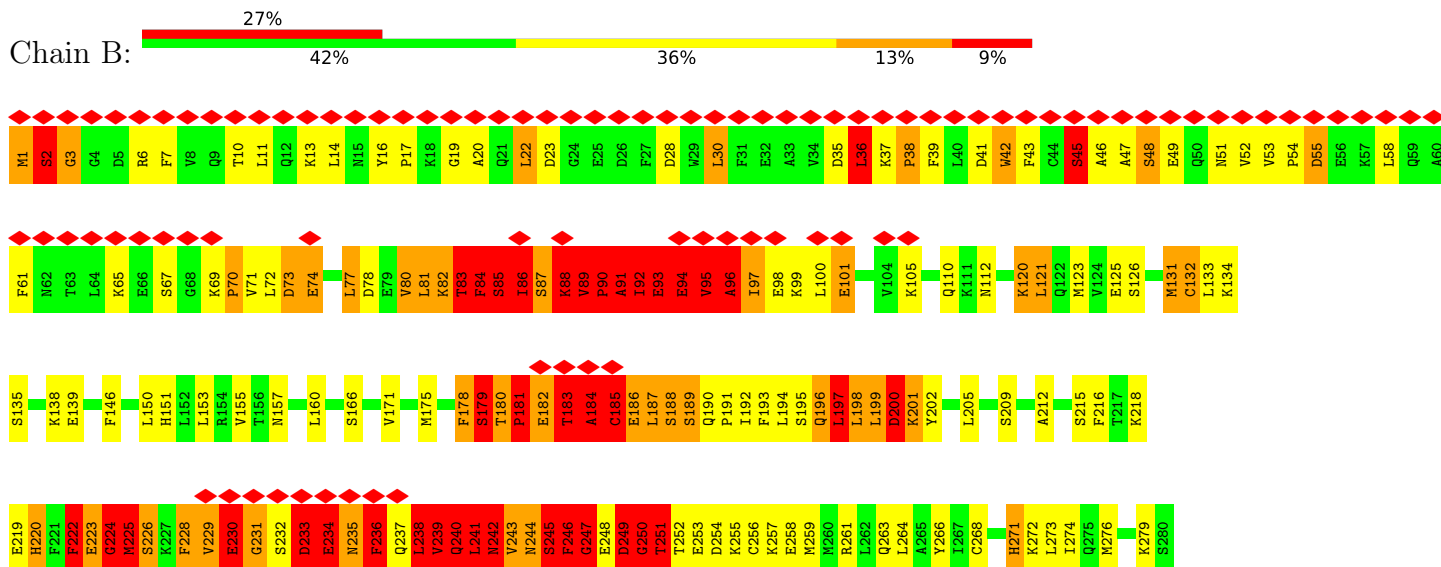
3 Residue-property plots

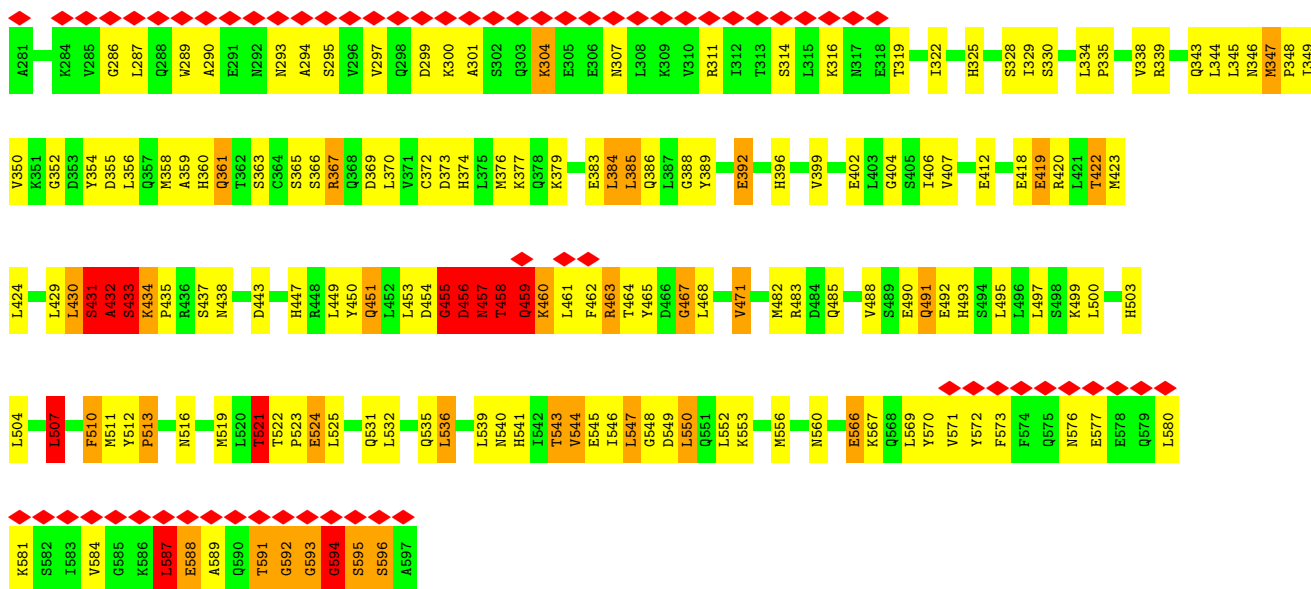
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

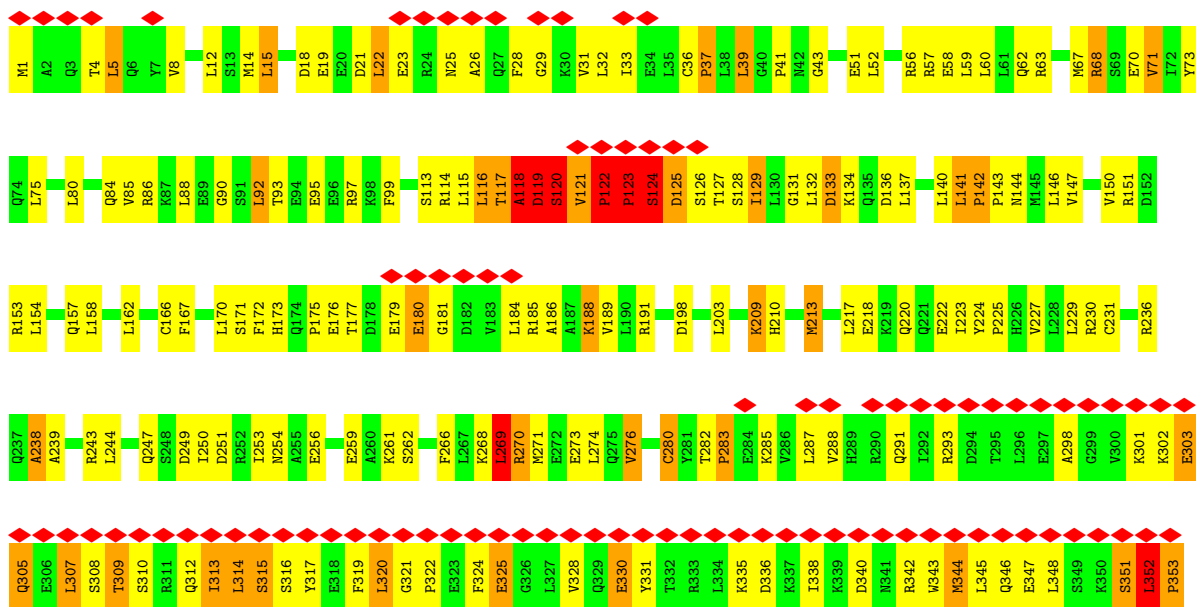


• Molecule 2: HAUS augmin-like complex subunit 3



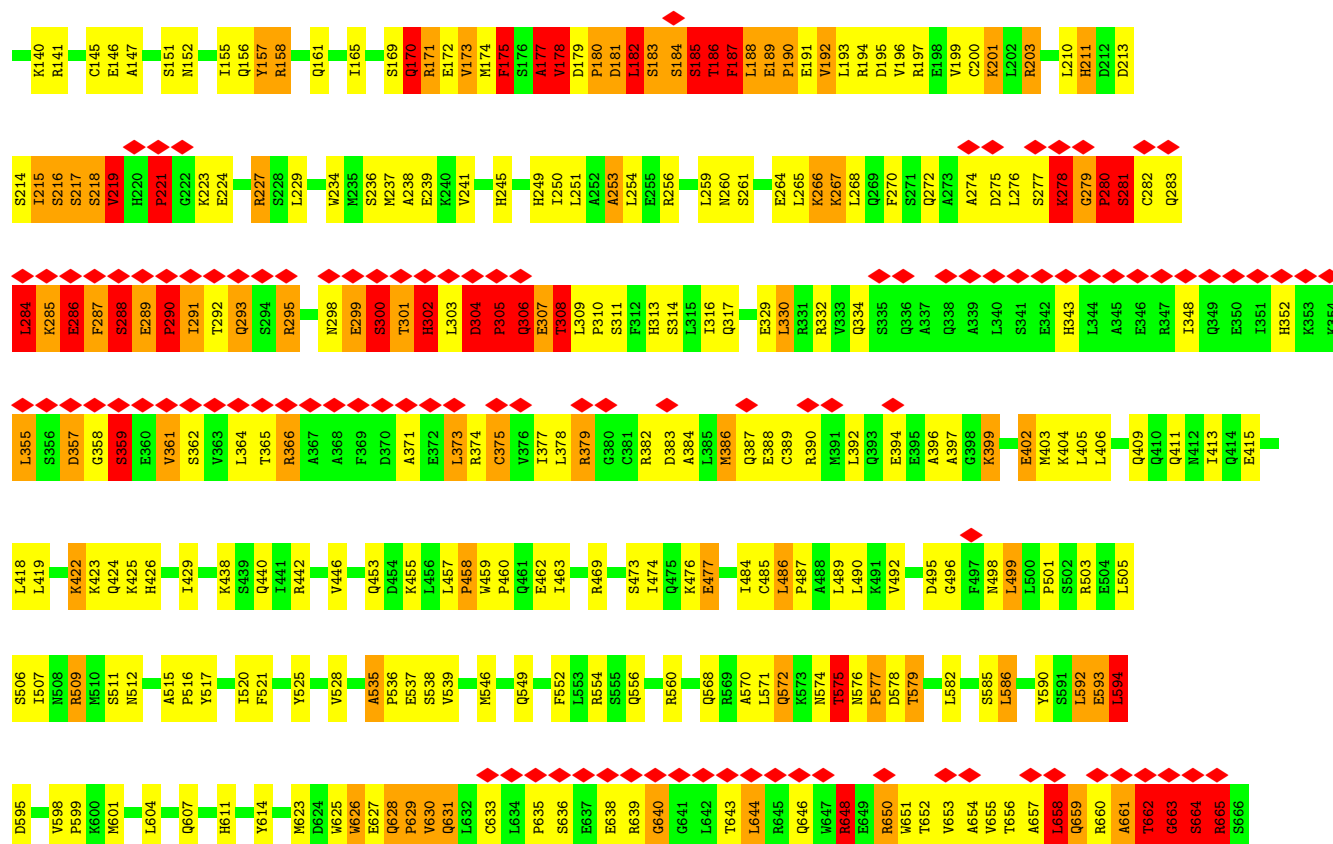


• Molecule 3: HAUS augmin like complex subunit 4 L homeolog

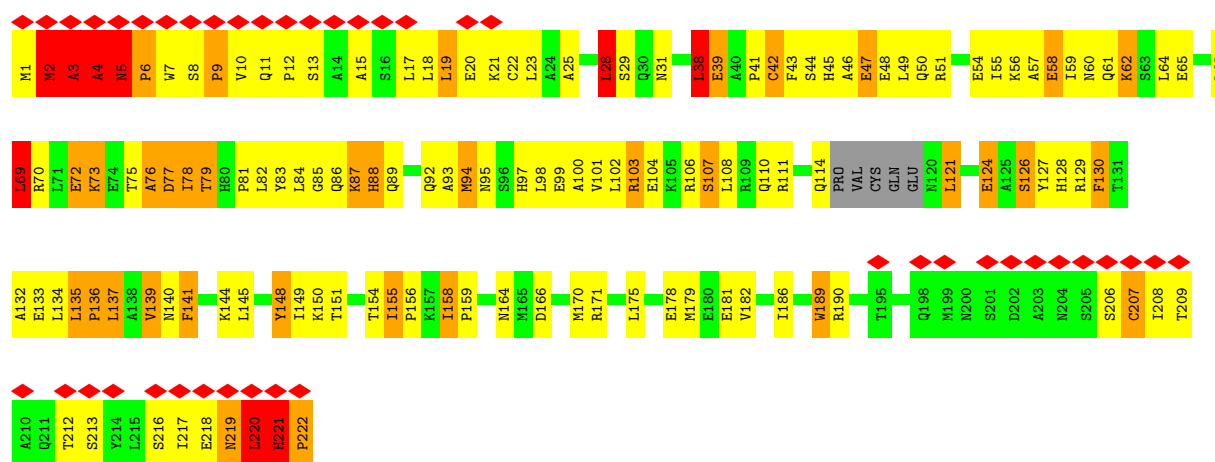


• Molecule 4: HAUS augmin-like complex subunit 5

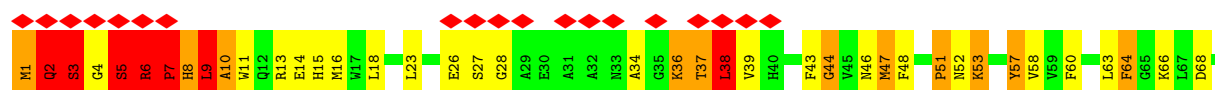


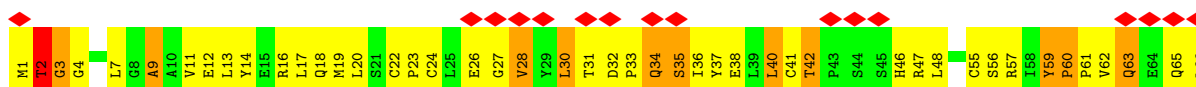


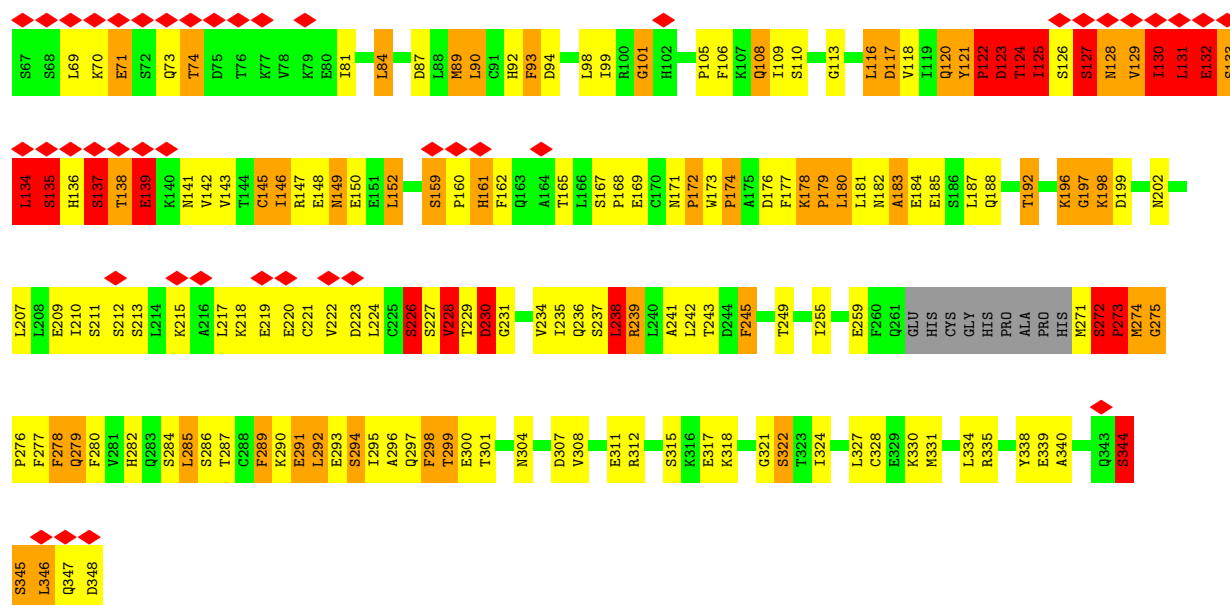
• Molecule 5: HAUS augmin like complex subunit 2 L homeolog



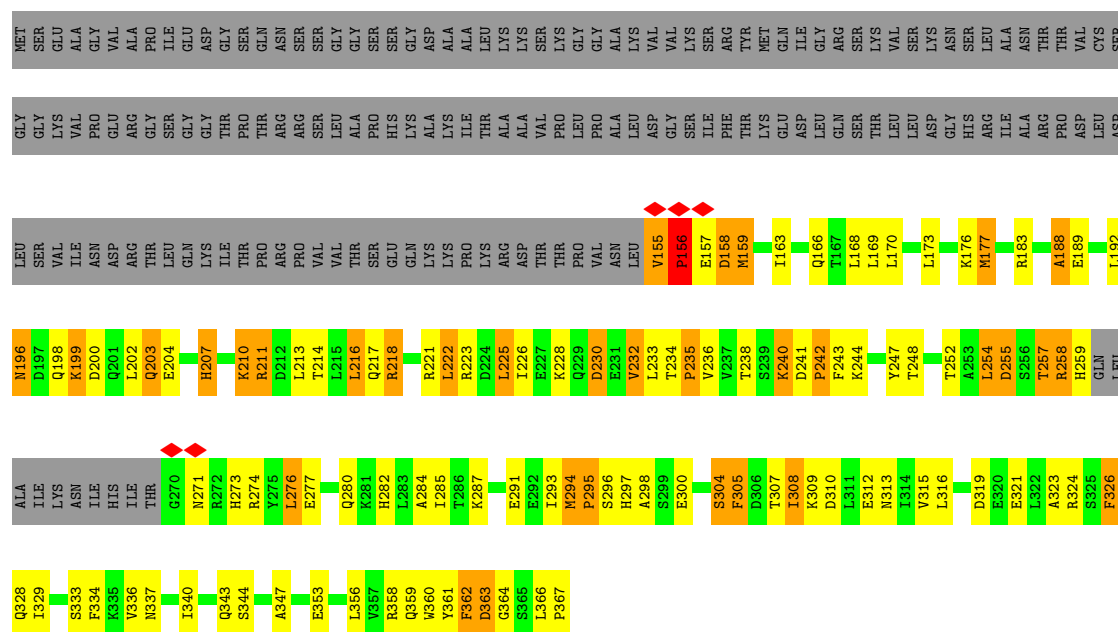
• Molecule 6: HAUS augmin like complex subunit 6 L homeolog







• Molecule 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 ($\text{\AA}$)	601.6, 601.6, 601.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	2.23	77/2309 (3.3%)	2.16	109/3102 (3.5%)
2	B	1.73	160/4836 (3.3%)	1.97	186/6496 (2.9%)
3	C	1.44	69/2920 (2.4%)	1.82	93/3925 (2.4%)
4	D	1.62	151/5502 (2.7%)	1.82	187/7397 (2.5%)
5	E	2.05	83/1743 (4.8%)	1.58	48/2359 (2.0%)
6	F	1.87	131/3229 (4.1%)	1.73	107/4333 (2.5%)
7	G	1.86	117/2736 (4.3%)	1.92	105/3698 (2.8%)
8	H	1.70	62/1692 (3.7%)	1.47	41/2278 (1.8%)
All	All	1.79	850/24967 (3.4%)	1.85	876/33588 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (850) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	288	SER	C-N	29.39	1.78	1.32
1	A	280	PRO	C-N	29.15	1.75	1.33
2	B	223	GLU	C-N	28.89	1.81	1.33
1	A	276	VAL	C-N	28.16	1.65	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ARG	C-N	28.05	1.69	1.33
1	A	283	ARG	C-N	26.69	1.70	1.33
1	A	272	MET	C-N	-25.19	0.96	1.33
2	B	392	GLU	C-N	-23.22	1.03	1.33
2	B	591	THR	C-N	22.69	1.66	1.33
6	F	34	ALA	C-N	20.48	1.59	1.33
3	C	319	PHE	C-N	20.02	1.66	1.33
1	A	277	VAL	C-N	19.69	1.79	1.33
1	A	274	GLU	C-N	19.09	1.58	1.33
1	A	273	MET	C-N	19.03	1.57	1.33
1	A	282	LYS	C-N	18.68	1.59	1.33
2	B	560	ASN	C-N	16.79	1.57	1.34
1	A	269	LYS	C-N	-16.03	1.12	1.33
2	B	593	GLY	C-N	15.93	1.56	1.33
6	F	1	MET	C-N	-15.66	1.11	1.33
4	D	659	GLN	C-N	15.01	1.54	1.33
2	B	592	GLY	C-N	-14.86	1.11	1.33
4	D	72	THR	C-N	14.77	1.52	1.33
4	D	69	LEU	C-N	14.28	1.51	1.33
4	D	402	GLU	C-N	-14.20	1.14	1.33
7	G	315	SER	C-N	14.12	1.53	1.33
1	A	229	MET	C-N	-13.99	1.15	1.34
6	F	213	LEU	C-N	-13.93	1.15	1.33
2	B	455	GLY	C-N	13.93	1.52	1.33
5	E	86	GLN	C-N	-13.79	1.15	1.34
2	B	587	LEU	C-N	13.76	1.53	1.33
5	E	133	GLU	C-N	-13.71	1.15	1.34
6	F	146	ALA	C-N	-13.66	1.15	1.33
4	D	495	ASP	C-N	13.59	1.52	1.33
6	F	262	VAL	C-N	-13.55	1.14	1.33
7	G	234	VAL	C-N	-13.55	1.16	1.33
1	A	265	GLU	C-N	-13.46	1.15	1.34
1	A	206	GLU	C-N	-13.38	1.15	1.33
2	B	73	ASP	C-N	-13.21	1.16	1.33
6	F	44	GLY	C-N	-13.19	1.18	1.33
5	E	69	LEU	C-N	-13.18	1.16	1.33
6	F	258	VAL	C-N	-13.09	1.16	1.33
4	D	289	GLU	C-N	-13.04	1.03	1.33
7	G	345	SER	C-N	12.94	1.51	1.34
4	D	227	ARG	C-N	-12.89	1.17	1.33
1	A	268	THR	C-N	-12.89	1.16	1.33
1	A	2	ASP	C-N	12.87	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	215	SER	C-N	-12.78	1.18	1.33
7	G	289	PHE	C-N	-12.70	1.16	1.33
7	G	226	SER	C-N	12.65	1.51	1.33
1	A	239	LEU	C-N	12.64	1.53	1.33
6	F	222	LYS	C-N	12.56	1.49	1.33
7	G	275	GLY	C-N	-12.55	1.18	1.34
2	B	6	ARG	C-N	-12.52	1.18	1.33
7	G	27	GLY	C-N	12.52	1.52	1.33
5	E	73	LYS	C-N	-12.50	1.16	1.33
4	D	177	ALA	C-N	-12.43	1.16	1.33
3	C	291	GLN	C-N	-12.37	1.19	1.34
4	D	180	PRO	C-N	12.24	1.50	1.33
6	F	209	GLU	C-N	-12.20	1.18	1.33
2	B	589	ALA	C-N	-12.16	1.17	1.33
6	F	106	VAL	C-N	12.15	1.51	1.33
2	B	17	PRO	N-CD	-12.09	1.30	1.47
4	D	180	PRO	N-CD	-12.01	1.30	1.47
8	H	300	GLU	C-N	-12.00	1.18	1.33
2	B	150	LEU	C-N	11.98	1.49	1.33
4	D	221	PRO	N-CD	-11.96	1.31	1.47
7	G	141	ASN	C-N	-11.94	1.18	1.33
5	E	6	PRO	N-CD	-11.91	1.31	1.47
2	B	513	PRO	N-CD	-11.91	1.31	1.47
8	H	333	SER	C-N	-11.89	1.18	1.33
7	G	161	HIS	C-N	-11.88	1.18	1.33
8	H	196	ASN	C-N	-11.82	1.18	1.33
1	A	270	VAL	C-N	11.81	1.49	1.33
1	A	82	THR	C-N	11.81	1.46	1.33
5	E	58	GLU	C-N	-11.80	1.19	1.33
7	G	122	PRO	N-CD	-11.79	1.31	1.47
7	G	122	PRO	C-N	-11.79	1.17	1.33
5	E	82	LEU	C-N	-11.76	1.17	1.34
4	D	576	ASN	C-N	11.75	1.56	1.34
5	E	9	PRO	N-CD	-11.74	1.31	1.47
8	H	367	PRO	N-CD	-11.73	1.31	1.47
4	D	21	PRO	N-CD	-11.72	1.31	1.47
1	A	245	PRO	N-CD	-11.71	1.31	1.47
4	D	313	HIS	C-N	-11.65	1.17	1.34
6	F	253	LYS	C-N	-11.64	1.18	1.33
4	D	652	THR	C-N	11.61	1.48	1.33
7	G	196	LYS	C-N	11.60	1.50	1.33
1	A	22	PRO	N-CD	-11.59	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	26	PRO	N-CD	-11.56	1.31	1.47
6	F	202	GLN	C-N	-11.54	1.19	1.33
2	B	594	GLY	C-N	-11.47	1.17	1.33
2	B	54	PRO	N-CD	-11.46	1.31	1.47
3	C	314	LEU	C-N	-11.46	1.18	1.34
7	G	71	GLU	C-N	11.42	1.49	1.33
2	B	90	PRO	N-CD	-11.41	1.31	1.47
5	E	222	PRO	N-CD	-11.39	1.31	1.47
7	G	130	ILE	C-N	11.39	1.49	1.33
2	B	222	PHE	C-N	-11.37	1.18	1.33
1	A	208	PRO	N-CD	-11.35	1.31	1.47
6	F	260	ALA	C-N	-11.32	1.19	1.33
5	E	93	ALA	C-N	-11.25	1.18	1.34
5	E	15	ALA	C-N	-11.25	1.19	1.33
3	C	124	SER	C-N	11.20	1.48	1.33
1	A	17	GLY	C-N	11.19	1.50	1.33
4	D	280	PRO	N-CD	-11.19	1.32	1.47
3	C	113	SER	C-N	-11.15	1.17	1.33
3	C	283	PRO	N-CD	-11.11	1.32	1.47
3	C	22	LEU	C-N	11.06	1.49	1.33
3	C	313	ILE	C-N	-11.04	1.19	1.34
6	F	329	TYR	C-N	11.01	1.47	1.33
6	F	7	PRO	N-CD	-11.00	1.32	1.47
3	C	353	PRO	N-CD	-10.99	1.32	1.47
5	E	41	PRO	N-CD	-10.94	1.32	1.47
4	D	290	PRO	N-CD	-10.92	1.32	1.47
6	F	292	MET	C-N	10.91	1.49	1.34
5	E	61	GLN	C-N	-10.90	1.19	1.33
4	D	501	PRO	C-N	-10.88	1.19	1.34
3	C	322	PRO	N-CD	-10.87	1.32	1.47
4	D	650	ARG	C-N	-10.86	1.20	1.33
3	C	122	PRO	N-CD	-10.86	1.32	1.47
6	F	175	ARG	C-N	-10.84	1.20	1.33
5	E	95	ASN	C-N	-10.83	1.20	1.33
6	F	121	PRO	C-N	-10.83	1.17	1.33
2	B	367	ARG	C-N	-10.80	1.20	1.33
4	D	496	GLY	C-N	10.79	1.48	1.33
8	H	361	TYR	C-N	10.78	1.50	1.33
6	F	195	LYS	C-N	-10.78	1.19	1.33
2	B	191	PRO	N-CD	-10.76	1.32	1.47
2	B	181	PRO	N-CD	-10.74	1.32	1.47
6	F	380	GLU	C-N	-10.73	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	223	LYS	C-N	-10.70	1.19	1.33
1	A	222	THR	C-N	-10.70	1.19	1.33
7	G	299	THR	C-N	-10.69	1.20	1.33
5	E	51	ARG	C-N	-10.68	1.20	1.33
2	B	233	ASP	C-N	10.68	1.48	1.33
5	E	78	ILE	C-N	-10.67	1.18	1.33
5	E	22	CYS	C-N	-10.63	1.19	1.33
5	E	88	HIS	C-N	-10.63	1.19	1.33
6	F	51	PRO	C-N	-10.62	1.17	1.33
6	F	256	ASP	C-N	-10.61	1.20	1.33
8	H	297	HIS	C-N	-10.56	1.20	1.33
4	D	18	MET	C-N	10.54	1.46	1.33
8	H	218	ARG	C-N	-10.54	1.19	1.34
5	E	136	PRO	C-N	-10.54	1.20	1.33
7	G	129	VAL	C-N	10.50	1.48	1.33
7	G	287	THR	C-N	-10.49	1.20	1.33
8	H	319	ASP	C-N	-10.46	1.20	1.33
4	D	311	SER	C-N	-10.45	1.19	1.33
7	G	290	LYS	C-N	-10.43	1.20	1.33
6	F	173	LEU	C-N	-10.42	1.20	1.33
2	B	516	ASN	C-N	-10.39	1.19	1.33
5	E	128	HIS	C-N	-10.39	1.20	1.33
5	E	25	ALA	C-N	10.37	1.47	1.33
2	B	363	SER	C-N	-10.35	1.19	1.33
3	C	213	MET	C-N	-10.35	1.20	1.33
4	D	83	GLN	C-N	10.35	1.47	1.33
4	D	182	LEU	C-N	-10.34	1.21	1.33
4	D	224	GLU	C-N	10.34	1.47	1.33
4	D	305	PRO	N-CD	-10.32	1.33	1.47
7	G	278	PHE	C-N	-10.31	1.20	1.33
6	F	148	ALA	C-N	10.31	1.50	1.33
6	F	82	PRO	N-CD	-10.26	1.33	1.47
6	F	390	GLY	C-N	10.22	1.47	1.33
6	F	27	SER	C-N	10.13	1.46	1.33
7	G	347	GLN	C-N	10.12	1.47	1.33
5	E	72	GLU	C-N	-10.10	1.20	1.33
7	G	23	PRO	N-CD	-10.10	1.33	1.47
7	G	117	ASP	C-N	-10.06	1.21	1.33
7	G	159	SER	C-N	10.04	1.45	1.34
7	G	237	SER	C-N	-10.01	1.20	1.33
5	E	11	GLN	C-N	-9.99	1.20	1.33
1	A	81	TYR	C-N	9.96	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	90	LEU	C-N	9.95	1.46	1.33
5	E	137	LEU	C-N	-9.95	1.20	1.33
4	D	635	PRO	N-CD	-9.87	1.33	1.47
6	F	121	PRO	N-CD	-9.85	1.33	1.47
6	F	251	MET	C-N	-9.85	1.21	1.33
3	C	123	PRO	N-CD	-9.82	1.33	1.47
4	D	357	ASP	C-N	9.82	1.47	1.33
4	D	53	HIS	C-N	-9.78	1.21	1.33
4	D	653	VAL	C-N	-9.74	1.20	1.33
8	H	364	GLY	C-N	9.73	1.48	1.33
2	B	70	PRO	N-CD	-9.71	1.34	1.47
8	H	156	PRO	N-CD	-9.68	1.34	1.47
6	F	205	ASP	C-N	-9.65	1.20	1.33
4	D	661	ALA	C-N	-9.63	1.20	1.33
7	G	311	GLU	C-N	-9.62	1.20	1.34
7	G	98	LEU	C-N	-9.61	1.22	1.33
4	D	638	GLU	C-N	-9.58	1.20	1.33
6	F	279	ASN	C-N	-9.57	1.24	1.33
7	G	279	GLN	C-N	-9.56	1.21	1.33
5	E	81	PRO	C-N	-9.54	1.21	1.33
4	D	90	CYS	C-N	9.50	1.46	1.33
5	E	9	PRO	C-N	-9.45	1.21	1.33
7	G	89	MET	C-N	-9.45	1.20	1.33
6	F	206	MET	C-N	-9.43	1.21	1.33
2	B	3	GLY	C-N	-9.42	1.22	1.33
1	A	278	PRO	N-CD	-9.42	1.34	1.47
7	G	113	GLY	C-N	-9.38	1.21	1.33
4	D	646	GLN	C-N	-9.36	1.21	1.33
6	F	197	GLN	C-N	-9.35	1.22	1.33
6	F	223	VAL	C-N	9.35	1.47	1.33
3	C	144	ASN	C-N	9.34	1.46	1.34
8	H	222	LEU	C-N	-9.34	1.21	1.33
7	G	145	CYS	C-N	-9.31	1.22	1.33
6	F	246	GLN	C-N	-9.30	1.21	1.33
8	H	295	PRO	N-CD	-9.26	1.34	1.47
4	D	572	GLN	C-N	9.23	1.46	1.34
7	G	63	GLN	C-N	9.23	1.46	1.34
6	F	237	THR	C-N	-9.21	1.21	1.33
2	B	250	GLY	C-N	-9.21	1.21	1.33
6	F	393	PRO	N-CD	-9.21	1.34	1.47
6	F	68	ASP	C-N	-9.19	1.21	1.33
1	A	245	PRO	C-N	9.19	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	209	GLU	C-N	-9.19	1.22	1.33
7	G	286	SER	C-N	-9.18	1.22	1.33
4	D	396	ALA	C-N	9.18	1.46	1.33
4	D	644	LEU	C-N	-9.16	1.22	1.33
5	E	62	LYS	C-N	-9.15	1.22	1.33
6	F	191	GLU	C-N	-9.15	1.22	1.33
6	F	257	VAL	C-N	-9.14	1.22	1.33
2	B	360	HIS	C-N	-9.13	1.21	1.33
4	D	158	ARG	C-N	-9.11	1.22	1.33
7	G	317	GLU	C-N	9.11	1.46	1.33
8	H	344	SER	C-N	-9.10	1.22	1.33
4	D	662	THR	C-N	9.07	1.46	1.33
4	D	511	SER	C-N	9.06	1.47	1.33
4	D	221	PRO	C-N	-9.02	1.20	1.33
6	F	276	ALA	C-N	9.02	1.46	1.33
5	E	47	GLU	C-N	-9.01	1.22	1.33
6	F	306	VAL	C-N	-9.01	1.21	1.33
7	G	282	HIS	C-N	-9.01	1.22	1.33
7	G	213	SER	C-N	-9.00	1.21	1.33
2	B	422	THR	C-N	-8.99	1.21	1.33
5	E	65	GLU	C-N	-8.98	1.22	1.33
4	D	276	LEU	C-N	8.97	1.46	1.33
5	E	23	LEU	C-N	8.96	1.46	1.34
1	A	20	PRO	N-CD	-8.95	1.35	1.47
5	E	140	ASN	C-N	-8.93	1.21	1.33
7	G	124	THR	C-N	8.93	1.45	1.33
5	E	85	GLY	C-N	-8.92	1.22	1.33
8	H	242	PRO	C-N	-8.92	1.22	1.33
3	C	88	LEU	C-N	8.89	1.47	1.33
6	F	103	SER	C-N	8.88	1.46	1.33
8	H	207	HIS	C-N	-8.87	1.22	1.33
5	E	94	MET	C-N	-8.87	1.22	1.33
2	B	219	GLU	C-N	-8.86	1.21	1.33
5	E	98	LEU	C-N	-8.83	1.22	1.33
2	B	461	LEU	C-N	8.82	1.45	1.33
6	F	194	ARG	C-N	-8.81	1.22	1.33
5	E	54	GLU	C-N	-8.80	1.22	1.33
6	F	224	ASP	C-N	-8.80	1.22	1.33
3	C	331	TYR	C-N	-8.76	1.22	1.33
6	F	108	ALA	C-N	-8.76	1.20	1.33
3	C	118	ALA	C-N	8.73	1.46	1.33
1	A	235	LEU	C-N	8.73	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	LEU	C-N	8.72	1.45	1.33
4	D	87	LYS	C-N	8.71	1.45	1.33
8	H	236	VAL	C-N	-8.69	1.23	1.33
1	A	78	GLY	C-N	-8.69	1.24	1.34
2	B	65	LYS	C-N	8.65	1.45	1.34
1	A	243	PRO	N-CD	-8.62	1.35	1.47
6	F	363	LYS	C-N	8.56	1.46	1.33
6	F	384	LYS	C-N	-8.56	1.20	1.33
2	B	17	PRO	C-N	8.54	1.44	1.33
2	B	10	THR	C-N	-8.53	1.22	1.33
7	G	152	LEU	C-N	-8.52	1.22	1.33
4	D	238	ALA	C-N	-8.51	1.23	1.33
1	A	64	ALA	C-N	-8.51	1.22	1.33
5	E	84	LEU	C-N	-8.50	1.22	1.33
4	D	577	PRO	N-CD	-8.49	1.35	1.47
7	G	181	LEU	C-N	8.49	1.46	1.33
4	D	16	GLU	C-N	-8.49	1.21	1.33
2	B	45	SER	C-N	-8.48	1.21	1.33
2	B	258	GLU	C-N	-8.48	1.22	1.33
4	D	388	GLU	C-N	-8.48	1.22	1.33
5	E	126	SER	C-N	-8.46	1.22	1.33
4	D	278	LYS	C-N	-8.45	1.20	1.33
6	F	172	LYS	C-N	-8.45	1.22	1.33
1	A	53	GLU	C-N	-8.45	1.22	1.33
7	G	108	GLN	C-N	-8.43	1.23	1.33
6	F	281	PRO	N-CD	-8.43	1.35	1.47
7	G	322	SER	C-N	8.41	1.44	1.33
2	B	38	PRO	N-CD	-8.40	1.35	1.47
5	E	50	GLN	C-N	-8.40	1.22	1.33
5	E	151	THR	C-N	-8.39	1.23	1.33
1	A	280	PRO	N-CD	-8.38	1.36	1.47
4	D	640	GLY	C-N	8.36	1.45	1.33
5	E	164	ASN	C-N	-8.36	1.23	1.33
5	E	2	MET	C-N	-8.35	1.22	1.33
1	A	241	LEU	C-N	8.33	1.46	1.33
1	A	221	LEU	C-N	-8.33	1.23	1.33
6	F	15	HIS	C-N	-8.33	1.23	1.33
8	H	274	ARG	C-N	-8.33	1.23	1.33
3	C	19	GLU	C-N	8.32	1.45	1.34
7	G	73	GLN	C-N	-8.32	1.23	1.33
2	B	184	ALA	C-N	8.32	1.44	1.33
2	B	181	PRO	C-N	8.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	288	ILE	C-N	8.31	1.45	1.33
5	E	68	LEU	C-N	-8.30	1.22	1.33
7	G	221	CYS	C-N	8.30	1.44	1.33
2	B	314	SER	C-N	-8.29	1.23	1.33
2	B	543	THR	C-N	-8.28	1.23	1.33
7	G	285	LEU	C-N	-8.27	1.23	1.33
8	H	159	MET	C-N	-8.26	1.23	1.33
1	A	263	GLU	C-N	8.22	1.44	1.33
6	F	9	LEU	C-N	8.18	1.44	1.33
3	C	270	ARG	C-N	-8.16	1.23	1.33
2	B	286	GLY	C-N	-8.14	1.22	1.33
5	E	29	SER	C-N	-8.14	1.23	1.34
3	C	116	LEU	C-N	8.13	1.45	1.33
4	D	46	ILE	C-N	-8.13	1.24	1.33
4	D	498	ASN	C-N	8.12	1.45	1.33
6	F	186	ASN	C-N	-8.12	1.23	1.33
2	B	218	LYS	C-N	-8.09	1.22	1.34
2	B	247	GLY	C-N	8.09	1.45	1.33
7	G	148	GLU	C-N	-8.09	1.23	1.33
4	D	594	LEU	C-N	8.07	1.45	1.33
2	B	61	PHE	C-N	8.07	1.44	1.33
5	E	103	ARG	C-N	8.06	1.42	1.33
4	D	5	SER	C-N	-8.05	1.23	1.33
4	D	377	ILE	C-N	-8.05	1.23	1.33
8	H	155	VAL	C-N	-8.04	1.15	1.33
2	B	311	ARG	C-N	-8.02	1.24	1.33
6	F	176	GLN	C-N	-8.02	1.23	1.33
1	A	275	PHE	C-N	-8.01	1.22	1.33
4	D	216	SER	C-N	7.99	1.44	1.33
6	F	111	PRO	N-CD	-7.99	1.36	1.47
1	A	259	LEU	C-N	7.97	1.44	1.33
4	D	21	PRO	C-N	-7.96	1.23	1.34
6	F	164	PRO	C-N	-7.95	1.23	1.33
2	B	365	SER	C-N	-7.91	1.23	1.33
3	C	191	ARG	C-N	-7.91	1.23	1.33
7	G	160	PRO	N-CD	-7.89	1.36	1.47
4	D	415	GLU	C-N	-7.88	1.23	1.33
2	B	151	HIS	C-N	7.88	1.44	1.33
4	D	101	HIS	C-N	7.87	1.44	1.33
2	B	492	GLU	C-N	-7.87	1.24	1.33
5	E	100	ALA	C-N	-7.86	1.24	1.33
4	D	657	ALA	C-N	-7.85	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	236	GLN	C-N	-7.84	1.23	1.33
6	F	179	LEU	C-N	-7.83	1.24	1.33
4	D	665	ARG	C-N	-7.82	1.22	1.33
6	F	74	GLU	C-N	7.81	1.43	1.33
4	D	81	GLU	C-N	7.80	1.44	1.33
4	D	660	ARG	C-N	7.79	1.43	1.33
8	H	177	MET	C-N	-7.79	1.24	1.33
4	D	264	GLU	C-N	-7.79	1.23	1.33
8	H	221	ARG	C-N	-7.79	1.23	1.33
6	F	81	PRO	N-CD	-7.76	1.36	1.47
7	G	26	GLU	C-N	-7.75	1.22	1.33
6	F	198	LEU	C-N	-7.75	1.23	1.33
3	C	346	GLN	C-N	-7.74	1.23	1.34
4	D	371	ALA	C-N	7.74	1.44	1.33
2	B	183	THR	C-N	7.73	1.44	1.33
2	B	356	LEU	C-N	-7.73	1.24	1.33
6	F	177	LYS	C-N	-7.73	1.23	1.33
7	G	259	GLU	C-N	7.73	1.44	1.33
5	E	12	PRO	N-CD	-7.72	1.36	1.47
7	G	296	ALA	C-N	-7.72	1.23	1.33
6	F	80	TRP	C-N	-7.71	1.19	1.34
2	B	242	ASN	C-N	-7.70	1.23	1.33
3	C	41	PRO	N-CD	-7.70	1.36	1.47
2	B	384	LEU	C-N	-7.70	1.24	1.33
5	E	8	SER	C-N	-7.69	1.22	1.33
4	D	250	ILE	C-N	-7.68	1.23	1.33
1	A	256	LYS	C-N	7.66	1.44	1.33
2	B	462	PHE	C-N	7.66	1.44	1.33
2	B	42	TRP	C-N	-7.65	1.24	1.33
2	B	224	GLY	C-N	-7.64	1.22	1.33
1	A	200	LEU	C-N	-7.63	1.23	1.33
7	G	238	LEU	C-N	-7.63	1.24	1.33
6	F	185	GLU	C-N	-7.62	1.24	1.33
4	D	192	VAL	C-N	-7.60	1.24	1.33
7	G	174	PRO	N-CD	-7.60	1.37	1.47
8	H	225	LEU	C-N	-7.60	1.24	1.33
8	H	252	THR	C-N	-7.56	1.23	1.33
6	F	63	LEU	C-N	7.53	1.43	1.33
2	B	36	LEU	C-N	-7.52	1.22	1.33
6	F	98	TRP	C-N	-7.51	1.24	1.33
3	C	352	LEU	C-N	7.50	1.46	1.34
1	A	219	GLU	C-N	-7.50	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	169	ALA	C-N	-7.49	1.24	1.33
2	B	435	PRO	C-N	-7.48	1.23	1.33
5	E	141	PHE	C-N	-7.48	1.24	1.33
8	H	240	LYS	C-N	-7.48	1.23	1.33
4	D	424	GLN	C-N	-7.47	1.24	1.33
2	B	435	PRO	N-CD	-7.46	1.37	1.47
3	C	151	ARG	C-N	7.45	1.44	1.33
2	B	369	ASP	C-N	-7.44	1.23	1.33
2	B	595	SER	C-N	7.44	1.44	1.33
4	D	309	LEU	C-N	-7.41	1.23	1.33
4	D	196	VAL	C-N	-7.41	1.24	1.33
7	G	30	LEU	C-N	-7.39	1.22	1.33
4	D	23	GLN	C-N	-7.39	1.23	1.33
2	B	503	HIS	C-N	-7.38	1.24	1.33
1	A	224	LEU	C-N	7.37	1.43	1.33
4	D	47	ILE	C-N	-7.37	1.23	1.33
6	F	385	TRP	C-N	-7.36	1.24	1.33
2	B	212	ALA	C-N	-7.34	1.24	1.33
7	G	346	LEU	C-N	-7.34	1.23	1.33
2	B	352	GLY	C-N	-7.34	1.24	1.33
5	E	139	VAL	C-N	-7.34	1.24	1.33
8	H	170	LEU	C-N	-7.33	1.24	1.33
4	D	215	ILE	C-N	7.31	1.45	1.33
6	F	249	LYS	C-N	-7.31	1.23	1.33
7	G	32	ASP	C-N	7.31	1.45	1.33
5	E	46	ALA	C-N	-7.30	1.24	1.33
6	F	365	GLU	C-N	-7.29	1.24	1.33
4	D	17	GLU	C-N	7.28	1.44	1.33
7	G	139	GLU	C-N	7.28	1.43	1.33
2	B	234	GLU	C-N	7.25	1.43	1.33
3	C	315	SER	C-N	7.25	1.43	1.33
2	B	457	ASN	C-N	7.25	1.43	1.33
5	E	89	GLN	C-N	-7.24	1.24	1.33
5	E	129	ARG	C-N	-7.24	1.24	1.34
7	G	106	PHE	C-N	-7.22	1.24	1.33
7	G	17	LEU	C-N	-7.22	1.24	1.33
6	F	359	ARG	C-N	7.22	1.43	1.33
8	H	307	THR	C-N	-7.22	1.24	1.33
1	A	102	LEU	C-N	7.22	1.43	1.33
2	B	361	GLN	C-N	-7.21	1.24	1.33
5	E	170	MET	C-N	-7.21	1.24	1.33
8	H	200	ASP	C-N	-7.21	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	ASP	C-N	7.20	1.44	1.33
7	G	55	CYS	C-N	7.20	1.43	1.34
4	D	186	THR	C-N	-7.19	1.23	1.33
2	B	23	ASP	C-N	-7.19	1.22	1.33
4	D	425	LYS	C-N	-7.19	1.24	1.33
2	B	458	THR	C-N	-7.16	1.23	1.33
4	D	389	CYS	C-N	7.16	1.43	1.33
5	E	135	LEU	C-N	-7.16	1.24	1.34
8	H	310	ASP	C-N	-7.15	1.24	1.33
8	H	242	PRO	N-CD	-7.15	1.37	1.47
4	D	593	GLU	C-N	-7.14	1.24	1.34
2	B	463	ARG	C-N	7.13	1.43	1.33
2	B	71	VAL	C-N	7.11	1.43	1.33
4	D	330	LEU	C-N	-7.10	1.24	1.33
8	H	217	GLN	C-N	-7.10	1.23	1.33
7	G	241	ALA	C-N	-7.07	1.24	1.33
7	G	293	GLU	C-N	-7.06	1.24	1.33
4	D	305	PRO	C-N	-7.05	1.23	1.33
4	D	277	SER	C-N	-7.05	1.23	1.33
6	F	298	ASP	C-N	-7.00	1.24	1.33
2	B	82	LYS	C-N	-7.00	1.23	1.33
1	A	205	MET	C-N	7.00	1.42	1.33
2	B	225	MET	C-N	-7.00	1.24	1.33
2	B	279	LYS	C-N	-6.99	1.25	1.33
4	D	373	LEU	C-N	-6.98	1.24	1.33
5	E	130	PHE	C-N	-6.98	1.24	1.33
1	A	182	LEU	C-N	-6.97	1.24	1.33
8	H	362	PHE	C-N	6.96	1.43	1.33
2	B	338	VAL	C-N	-6.94	1.24	1.33
7	G	300	GLU	C-N	-6.93	1.25	1.33
3	C	223	ILE	C-N	-6.93	1.23	1.33
5	E	87	LYS	C-N	-6.93	1.24	1.33
6	F	184	LYS	C-N	-6.92	1.24	1.33
3	C	325	GLU	C-N	6.91	1.43	1.33
6	F	392	CYS	C-N	-6.88	1.25	1.33
4	D	592	LEU	C-N	-6.88	1.24	1.33
3	C	309	THR	C-N	-6.87	1.25	1.33
7	G	93	PHE	C-N	6.87	1.42	1.33
4	D	476	LYS	C-N	-6.85	1.24	1.33
2	B	220	HIS	C-N	-6.84	1.24	1.33
7	G	171	ASN	C-N	-6.84	1.27	1.33
8	H	230	ASP	C-N	-6.84	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	GLU	C-N	-6.83	1.24	1.33
6	F	78	TYR	C-N	-6.82	1.22	1.33
2	B	240	GLN	C-N	-6.82	1.24	1.33
4	D	76	ARG	C-N	6.82	1.42	1.33
8	H	198	GLN	C-N	-6.80	1.25	1.33
6	F	382	GLU	C-N	6.78	1.43	1.33
2	B	46	ALA	C-N	-6.77	1.23	1.33
8	H	308	ILE	C-N	-6.77	1.25	1.33
5	E	132	ALA	C-N	-6.77	1.23	1.33
6	F	58	VAL	C-N	-6.76	1.25	1.33
6	F	116	SER	C-N	6.75	1.41	1.34
2	B	512	TYR	C-N	-6.75	1.24	1.34
4	D	300	SER	C-N	6.74	1.42	1.33
7	G	292	LEU	C-N	-6.73	1.25	1.33
1	A	143	LYS	C-N	-6.72	1.25	1.33
1	A	231	ALA	C-N	6.72	1.43	1.33
2	B	580	LEU	C-N	6.72	1.42	1.33
4	D	82	GLN	C-N	-6.71	1.25	1.33
5	E	48	GLU	C-N	-6.70	1.25	1.33
3	C	134	LYS	C-N	-6.69	1.24	1.34
8	H	353	GLU	C-N	-6.69	1.25	1.34
2	B	300	LYS	C-N	-6.69	1.24	1.33
8	H	192	LEU	C-N	-6.65	1.25	1.33
3	C	310	SER	C-N	-6.63	1.24	1.34
7	G	291	GLU	C-N	-6.63	1.25	1.33
4	D	85	ARG	C-N	-6.62	1.25	1.33
4	D	94	LEU	C-N	6.62	1.42	1.33
8	H	315	VAL	C-N	-6.62	1.25	1.33
3	C	179	GLU	C-N	6.62	1.42	1.33
3	C	37	PRO	N-CD	-6.60	1.38	1.47
4	D	633	CYS	C-N	6.60	1.42	1.33
2	B	434	LYS	C-N	6.60	1.49	1.33
7	G	308	VAL	C-N	-6.60	1.25	1.33
7	G	223	ASP	C-N	-6.59	1.24	1.33
2	B	20	ALA	C-N	6.59	1.43	1.33
6	F	312	VAL	C-N	-6.59	1.25	1.33
7	G	42	THR	C-N	-6.58	1.26	1.33
4	D	422	LYS	C-N	-6.58	1.25	1.33
5	E	150	LYS	C-N	-6.58	1.25	1.33
7	G	120	GLN	C-N	-6.58	1.20	1.33
2	B	228	PHE	C-N	-6.57	1.26	1.34
2	B	255	LYS	C-N	6.57	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	129	ILE	C-N	-6.57	1.24	1.33
3	C	142	PRO	C-N	-6.56	1.25	1.33
7	G	182	ASN	C-N	-6.55	1.25	1.33
4	D	366	ARG	C-N	-6.55	1.25	1.33
7	G	184	GLU	C-N	-6.55	1.24	1.33
5	E	79	THR	C-N	-6.54	1.22	1.33
5	E	92	GLN	C-N	-6.52	1.25	1.33
6	F	293	HIS	C-N	-6.52	1.24	1.33
6	F	43	PHE	C-N	6.50	1.42	1.32
4	D	375	CYS	C-N	6.49	1.42	1.33
2	B	572	TYR	C-N	-6.48	1.25	1.33
4	D	361	VAL	C-N	6.47	1.42	1.33
6	F	18	LEU	C-N	-6.45	1.25	1.33
4	D	516	PRO	N-CD	-6.45	1.38	1.47
4	D	623	MET	C-N	-6.45	1.25	1.33
1	A	15	MET	C-N	6.45	1.43	1.33
5	E	83	TYR	C-N	-6.43	1.25	1.34
2	B	14	LEU	C-N	6.43	1.43	1.33
4	D	32	GLN	C-N	6.43	1.42	1.33
6	F	226	LYS	C-N	6.43	1.41	1.34
6	F	255	VAL	C-N	-6.43	1.25	1.33
1	A	7	LYS	C-N	-6.43	1.25	1.33
3	C	90	GLY	C-N	6.41	1.42	1.33
8	H	228	LYS	C-N	-6.40	1.24	1.33
7	G	304	ASN	C-N	-6.40	1.25	1.33
2	B	370	LEU	C-N	-6.39	1.25	1.33
3	C	249	ASP	C-N	-6.39	1.25	1.33
4	D	477	GLU	C-N	-6.39	1.25	1.33
4	D	286	GLU	C-N	-6.38	1.25	1.33
7	G	183	ALA	C-N	6.38	1.42	1.33
7	G	57	ARG	C-N	-6.38	1.25	1.33
6	F	241	TRP	C-N	-6.37	1.25	1.33
7	G	149	ASN	C-N	-6.37	1.25	1.33
6	F	52	ASN	C-N	-6.36	1.25	1.33
8	H	337	ASN	C-N	-6.35	1.25	1.33
5	E	144	LYS	C-N	-6.34	1.25	1.33
6	F	245	MET	C-N	-6.34	1.25	1.33
6	F	96	CYS	C-N	6.34	1.42	1.33
8	H	277	GLU	C-N	6.34	1.42	1.33
2	B	372	CYS	C-N	-6.33	1.25	1.33
4	D	44	LYS	C-N	-6.32	1.25	1.33
1	A	258	GLU	C-N	-6.32	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	524	GLU	C-N	-6.31	1.25	1.33
5	E	148	TYR	C-N	-6.31	1.25	1.33
3	C	186	ALA	C-N	6.31	1.42	1.33
7	G	33	PRO	N-CD	-6.29	1.39	1.47
7	G	284	SER	C-N	-6.29	1.25	1.33
8	H	309	LYS	C-N	-6.27	1.25	1.33
2	B	316	LYS	C-N	6.27	1.42	1.33
3	C	51	GLU	C-N	-6.27	1.25	1.33
4	D	332	ARG	C-N	-6.27	1.25	1.33
2	B	523	PRO	N-CD	-6.26	1.39	1.47
2	B	377	LYS	C-N	-6.26	1.25	1.33
8	H	248	THR	C-N	-6.26	1.25	1.33
4	D	48	ARG	C-N	-6.25	1.25	1.33
7	G	35	SER	C-N	6.25	1.41	1.33
2	B	83	THR	C-N	6.25	1.42	1.33
2	B	521	THR	C-N	6.24	1.44	1.33
4	D	19	GLY	C-N	6.22	1.44	1.33
3	C	203	LEU	C-N	6.22	1.42	1.33
4	D	409	GLN	C-N	-6.22	1.25	1.33
1	A	215	VAL	C-N	-6.21	1.25	1.33
2	B	525	LEU	C-N	-6.21	1.25	1.33
3	C	93	THR	C-N	-6.21	1.25	1.33
4	D	98	ALA	C-N	6.21	1.42	1.33
1	A	23	PRO	N-CD	-6.20	1.39	1.47
8	H	203	GLN	C-N	-6.19	1.25	1.33
3	C	188	LYS	C-N	-6.18	1.26	1.33
2	B	48	SER	C-N	-6.18	1.25	1.34
5	E	44	SER	C-N	-6.17	1.25	1.33
4	D	157	TYR	C-N	-6.17	1.25	1.33
4	D	42	ILE	C-N	-6.16	1.25	1.34
4	D	382	ARG	C-N	6.16	1.42	1.33
4	D	310	PRO	N-CD	-6.16	1.39	1.47
5	E	7	TRP	C-N	6.15	1.43	1.33
4	D	45	PHE	C-N	-6.15	1.26	1.33
1	A	249	LYS	C-N	6.15	1.41	1.33
2	B	91	ALA	C-N	-6.15	1.25	1.33
7	G	242	LEU	C-N	-6.14	1.26	1.33
4	D	268	LEU	C-N	-6.14	1.25	1.33
6	F	278	LEU	C-N	6.14	1.42	1.33
6	F	248	LEU	C-N	-6.13	1.25	1.33
4	D	364	LEU	C-N	6.12	1.42	1.33
4	D	658	LEU	C-N	-6.12	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	294	MET	C-N	6.12	1.41	1.33
6	F	134	ALA	C-N	-6.11	1.26	1.33
7	G	65	GLN	C-N	-6.11	1.24	1.33
8	H	276	LEU	C-N	6.11	1.42	1.33
2	B	74	GLU	C-N	6.10	1.41	1.33
2	B	120	LYS	C-N	-6.10	1.25	1.33
3	C	142	PRO	N-CD	-6.09	1.39	1.47
5	E	99	GLU	C-N	-6.08	1.25	1.33
2	B	423	MET	C-N	-6.08	1.25	1.33
2	B	510	PHE	C-N	-6.06	1.24	1.33
6	F	315	LEU	C-N	-6.06	1.25	1.33
7	G	178	LYS	C-N	6.06	1.41	1.33
2	B	239	VAL	C-N	-6.06	1.25	1.33
3	C	58	GLU	C-N	-6.06	1.26	1.33
1	A	242	ALA	C-N	-6.04	1.19	1.33
7	G	12	GLU	C-N	-6.04	1.26	1.33
4	D	429	ILE	C-N	-6.03	1.26	1.33
3	C	209	LYS	C-N	-6.02	1.26	1.33
2	B	412	GLU	C-N	-6.02	1.26	1.33
2	B	53	VAL	C-N	-6.01	1.25	1.33
8	H	363	ASP	C-N	6.01	1.41	1.34
2	B	464	THR	C-N	-6.01	1.25	1.33
6	F	348	GLU	C-N	-6.01	1.26	1.33
6	F	303	ALA	C-N	6.00	1.42	1.33
4	D	629	PRO	C-N	-6.00	1.27	1.34
1	A	118	ASP	C-N	5.99	1.41	1.33
3	C	173	HIS	C-N	5.99	1.42	1.33
2	B	39	PHE	C-N	-5.98	1.26	1.33
5	E	101	VAL	C-N	-5.98	1.25	1.33
6	F	289	GLU	C-N	5.97	1.42	1.34
1	A	228	SER	C-N	-5.97	1.25	1.33
2	B	13	LYS	C-N	-5.96	1.25	1.33
3	C	133	ASP	C-N	-5.96	1.25	1.34
2	B	438	ASN	C-N	-5.96	1.26	1.33
6	F	201	LYS	C-N	-5.96	1.25	1.33
3	C	287	LEU	C-N	-5.95	1.26	1.33
4	D	384	ALA	C-N	-5.95	1.26	1.33
2	B	507	LEU	C-N	-5.94	1.26	1.33
1	A	146	GLU	C-N	-5.93	1.25	1.33
4	D	418	LEU	C-N	-5.93	1.26	1.33
6	F	109	GLY	C-N	-5.93	1.22	1.33
6	F	254	GLU	C-N	-5.92	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	305	PHE	C-N	-5.92	1.25	1.33
2	B	70	PRO	C-N	-5.91	1.27	1.33
4	D	499	LEU	C-N	-5.91	1.24	1.33
5	E	171	ARG	C-N	-5.91	1.26	1.33
2	B	294	ALA	C-N	5.90	1.42	1.33
6	F	138	MET	C-N	-5.89	1.26	1.33
2	B	499	LYS	C-N	-5.89	1.26	1.33
6	F	168	LEU	C-N	-5.88	1.26	1.33
2	B	81	LEU	C-N	5.88	1.41	1.34
7	G	218	LYS	C-N	-5.87	1.25	1.34
2	B	471	VAL	C-N	-5.87	1.26	1.33
6	F	160	LYS	C-N	5.86	1.40	1.33
8	H	210	LYS	C-N	-5.86	1.26	1.33
5	E	28	LEU	C-N	-5.86	1.25	1.33
2	B	576	ASN	C-N	5.86	1.41	1.33
2	B	92	ILE	C-N	-5.85	1.25	1.33
7	G	9	ALA	C-N	-5.85	1.26	1.33
6	F	90	GLU	C-N	5.85	1.41	1.33
4	D	1	MET	C-N	-5.84	1.26	1.33
4	D	585	SER	C-N	-5.84	1.25	1.33
6	F	53	LYS	C-N	-5.84	1.26	1.33
7	G	179	PRO	N-CD	-5.84	1.39	1.47
2	B	132	CYS	C-N	5.83	1.41	1.33
7	G	202	ASN	C-N	-5.83	1.26	1.33
2	B	290	ALA	C-N	-5.83	1.25	1.34
6	F	238	ARG	C-N	-5.83	1.26	1.33
3	C	62	GLN	C-N	-5.82	1.26	1.33
2	B	133	LEU	C-N	-5.82	1.26	1.33
3	C	330	GLU	C-N	-5.82	1.26	1.33
8	H	326	PHE	C-N	-5.82	1.26	1.33
2	B	328	SER	C-N	-5.81	1.26	1.33
1	A	168	GLU	C-N	-5.81	1.26	1.33
1	A	79	PRO	N-CD	-5.81	1.39	1.47
1	A	251	LYS	C-N	-5.81	1.26	1.33
3	C	80	LEU	C-N	-5.80	1.26	1.33
4	D	469	ARG	C-N	-5.80	1.25	1.33
6	F	57	TYR	C-N	-5.80	1.26	1.33
4	D	267	LYS	C-N	-5.80	1.25	1.34
6	F	171	ASN	C-N	-5.80	1.26	1.33
6	F	178	TYR	C-N	-5.79	1.26	1.33
2	B	251	THR	C-N	-5.78	1.25	1.33
3	C	344	MET	C-N	-5.78	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	280	ILE	C-N	-5.77	1.25	1.33
4	D	217	SER	C-N	5.77	1.41	1.33
5	E	45	HIS	C-N	-5.76	1.26	1.33
7	G	4	GLY	C-N	5.76	1.41	1.33
8	H	173	LEU	C-N	-5.76	1.26	1.33
7	G	123	ASP	C-N	-5.75	1.25	1.33
2	B	359	ALA	C-N	-5.75	1.26	1.33
4	D	628	GLN	C-N	-5.75	1.27	1.34
6	F	87	ARG	C-N	-5.75	1.26	1.33
4	D	586	LEU	C-N	-5.72	1.26	1.33
2	B	261	ARG	C-N	-5.72	1.26	1.33
7	G	59	TYR	C-N	5.72	1.40	1.33
1	A	225	LYS	C-N	-5.72	1.26	1.33
8	H	258	ARG	C-N	-5.72	1.25	1.33
3	C	312	GLN	C-N	5.71	1.41	1.33
4	D	93	ILE	C-N	5.71	1.41	1.33
1	A	214	LEU	C-N	-5.70	1.26	1.33
4	D	175	PHE	C-N	-5.70	1.25	1.33
5	E	159	PRO	C-N	-5.70	1.26	1.33
7	G	101	GLY	C-N	5.70	1.41	1.33
6	F	26	GLU	C-N	-5.69	1.26	1.33
2	B	80	VAL	C-N	-5.68	1.26	1.34
7	G	294	SER	C-N	-5.68	1.26	1.33
4	D	643	THR	C-N	5.68	1.41	1.33
6	F	47	MET	C-N	5.67	1.41	1.33
2	B	467	GLY	C-N	-5.67	1.26	1.33
2	B	354	TYR	C-N	-5.66	1.26	1.33
3	C	29	GLY	C-N	5.66	1.41	1.33
3	C	71	VAL	C-N	-5.66	1.26	1.33
4	D	190	PRO	N-CD	-5.66	1.39	1.47
7	G	69	LEU	C-N	5.66	1.40	1.33
4	D	178	VAL	C-N	5.66	1.45	1.33
3	C	25	ASN	C-N	5.65	1.41	1.33
3	C	143	PRO	N-CD	-5.65	1.39	1.47
5	E	189	TRP	C-N	-5.64	1.26	1.33
8	H	257	THR	C-N	-5.64	1.25	1.33
4	D	27	SER	C-N	-5.63	1.25	1.33
6	F	182	LEU	C-N	-5.63	1.26	1.33
5	E	13	SER	C-N	-5.62	1.26	1.33
4	D	274	ALA	C-N	-5.60	1.26	1.34
6	F	14	GLU	C-N	-5.60	1.26	1.34
2	B	347	MET	C-N	5.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	431	SER	C-N	5.60	1.41	1.33
6	F	212	ALA	C-N	-5.60	1.26	1.34
4	D	578	ASP	C-N	5.59	1.41	1.33
2	B	588	GLU	C-N	5.57	1.41	1.33
7	G	110	SER	C-N	-5.57	1.26	1.33
8	H	214	THR	C-N	-5.57	1.26	1.33
6	F	158	GLN	C-N	5.57	1.41	1.33
2	B	451	GLN	C-N	-5.56	1.26	1.33
3	C	222	GLU	C-N	5.54	1.40	1.33
1	A	238	TYR	C-N	5.54	1.41	1.33
6	F	101	LYS	C-N	5.53	1.40	1.33
7	G	334	LEU	C-N	-5.52	1.26	1.33
2	B	254	ASP	C-N	-5.52	1.26	1.33
2	B	485	GLN	C-N	-5.51	1.26	1.33
2	B	55	ASP	C-N	-5.51	1.26	1.33
3	C	56	ARG	C-N	-5.50	1.26	1.33
7	G	34	GLN	C-N	5.50	1.41	1.33
3	C	317	TYR	C-N	-5.49	1.26	1.33
7	G	84	LEU	C-N	-5.49	1.26	1.33
4	D	397	ALA	C-N	5.47	1.41	1.33
5	E	77	ASP	C-N	-5.46	1.27	1.33
7	G	70	LYS	C-N	-5.46	1.26	1.33
1	A	175	ARG	C-N	-5.46	1.26	1.33
7	G	24	CYS	C-N	-5.45	1.25	1.33
7	G	297	GLN	C-N	-5.44	1.26	1.33
3	C	302	LYS	C-N	-5.44	1.25	1.33
2	B	358	MET	C-N	-5.44	1.26	1.33
3	C	351	SER	C-N	5.43	1.44	1.33
4	D	71	HIS	C-N	-5.43	1.26	1.33
5	E	43	PHE	C-N	-5.43	1.26	1.33
5	E	216	SER	C-N	-5.43	1.28	1.34
4	D	329	GLU	C-N	-5.42	1.27	1.33
7	G	245	PHE	C-N	-5.42	1.26	1.33
8	H	189	GLU	C-N	-5.42	1.26	1.33
8	H	199	LYS	C-N	-5.42	1.26	1.33
2	B	271	HIS	C-N	-5.41	1.26	1.33
4	D	253	ALA	C-N	-5.41	1.26	1.33
7	G	307	ASP	C-N	-5.40	1.27	1.33
6	F	356	ARG	C-N	5.40	1.41	1.33
2	B	84	PHE	C-N	-5.39	1.25	1.33
5	E	56	LYS	C-N	-5.39	1.26	1.33
6	F	165	GLN	C-N	-5.39	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	LYS	C-N	-5.38	1.27	1.33
1	A	80	SER	C-N	5.38	1.41	1.33
2	B	257	LYS	C-N	-5.38	1.26	1.33
6	F	342	HIS	C-N	5.38	1.40	1.33
4	D	136	ALA	C-N	-5.37	1.26	1.33
5	E	155	ILE	C-N	5.36	1.40	1.34
6	F	3	SER	C-N	-5.35	1.25	1.33
2	B	209	SER	C-N	-5.35	1.26	1.33
6	F	376	ASP	C-N	-5.34	1.26	1.33
8	H	211	ARG	C-N	-5.33	1.26	1.33
4	D	517	TYR	C-N	-5.33	1.27	1.33
7	G	116	LEU	C-N	-5.32	1.26	1.33
7	G	215	LYS	C-N	-5.32	1.26	1.33
3	C	177	THR	C-N	5.32	1.41	1.33
1	A	252	ILE	C-N	5.31	1.41	1.33
7	G	169	GLU	C-N	-5.31	1.26	1.33
1	A	60	ALA	C-N	-5.31	1.26	1.33
2	B	581	LYS	C-N	-5.31	1.26	1.33
3	C	73	TYR	C-N	-5.31	1.26	1.33
1	A	139	SER	C-N	-5.30	1.26	1.33
7	G	147	ARG	C-N	-5.30	1.27	1.33
6	F	139	LEU	C-N	5.30	1.41	1.34
2	B	539	LEU	C-N	-5.29	1.26	1.34
5	E	55	ILE	C-N	-5.29	1.27	1.33
4	D	664	SER	C-N	5.28	1.41	1.33
6	F	305	LYS	C-N	-5.27	1.25	1.33
7	G	180	LEU	C-N	-5.26	1.26	1.33
7	G	330	LYS	C-N	-5.26	1.26	1.33
4	D	607	GLN	C-N	-5.26	1.27	1.33
5	E	19	LEU	C-N	-5.26	1.27	1.33
7	G	239	ARG	C-N	-5.26	1.27	1.33
3	C	336	ASP	C-N	5.26	1.41	1.33
4	D	3	ARG	C-N	-5.26	1.27	1.33
4	D	462	GLU	C-N	-5.26	1.27	1.33
2	B	179	SER	C-N	5.22	1.40	1.32
7	G	344	SER	C-N	5.21	1.41	1.33
1	A	210	THR	C-N	5.21	1.40	1.33
1	A	167	PHE	C-N	-5.21	1.26	1.33
7	G	60	PRO	C-N	5.21	1.40	1.33
2	B	268	CYS	C-N	-5.20	1.26	1.33
1	A	127	GLU	C-N	5.20	1.41	1.33
7	G	131	LEU	C-N	-5.20	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	LYS	C-N	-5.20	1.27	1.33
2	B	388	GLY	C-N	-5.19	1.27	1.33
6	F	370	ILE	C-N	-5.19	1.26	1.34
2	B	373	ASP	C-N	-5.18	1.27	1.33
2	B	146	PHE	C-N	5.17	1.41	1.34
8	H	183	ARG	C-N	-5.17	1.26	1.33
3	C	238	ALA	C-N	-5.17	1.26	1.33
4	D	509	ARG	C-N	5.17	1.40	1.33
2	B	202	TYR	C-N	-5.17	1.27	1.33
4	D	146	GLU	C-N	-5.16	1.26	1.33
2	B	307	ASN	C-N	-5.16	1.27	1.33
6	F	204	ARG	C-N	-5.16	1.26	1.33
4	D	92	GLU	C-N	-5.14	1.27	1.33
5	E	41	PRO	C-N	5.14	1.40	1.33
1	A	68	TYR	C-N	-5.14	1.26	1.33
1	A	132	GLU	C-N	-5.14	1.26	1.33
2	B	153	LEU	C-N	5.13	1.40	1.33
2	B	419	GLU	C-N	-5.13	1.26	1.33
4	D	568	GLN	C-N	5.12	1.40	1.33
3	C	210	HIS	C-N	-5.12	1.27	1.33
7	G	128	ASN	C-N	5.12	1.40	1.33
8	H	316	LEU	C-N	-5.11	1.26	1.33
6	F	123	GLY	C-N	-5.11	1.27	1.34
1	A	250	VAL	C-N	5.11	1.41	1.34
2	B	531	GLN	C-N	-5.11	1.27	1.33
5	E	70	ARG	C-N	-5.11	1.26	1.33
2	B	366	SER	C-N	-5.10	1.26	1.33
1	A	233	GLU	C-N	-5.10	1.26	1.33
3	C	256	GLU	C-N	-5.10	1.27	1.33
4	D	505	LEU	C-N	-5.09	1.27	1.34
7	G	212	SER	C-N	-5.08	1.26	1.34
8	H	313	ASN	C-N	-5.08	1.27	1.33
6	F	83	LEU	C-N	5.06	1.40	1.33
8	H	235	PRO	N-CD	-5.06	1.40	1.47
4	D	239	GLU	C-N	-5.05	1.27	1.33
2	B	230	GLU	C-N	5.05	1.40	1.33
8	H	347	ALA	C-N	-5.05	1.27	1.33
6	F	333	GLY	C-N	-5.04	1.27	1.33
7	G	298	PHE	C-N	-5.04	1.27	1.33
7	G	40	LEU	C-N	5.04	1.41	1.33
2	B	38	PRO	C-N	-5.03	1.27	1.33
6	F	115	ALA	C-N	5.03	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	SER	C-N	-5.03	1.25	1.33
2	B	325	HIS	C-N	-5.02	1.27	1.33
6	F	291	GLU	C-N	5.01	1.40	1.34
8	H	188	ALA	C-N	-5.01	1.27	1.33
3	C	26	ALA	C-N	5.01	1.40	1.34
6	F	219	LEU	C-N	5.00	1.41	1.33

All (876) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	122	PRO	O-C-N	-34.34	80.94	121.46
2	B	392	GLU	O-C-N	-31.75	88.46	122.12
4	D	304	ASP	O-C-N	-28.48	88.57	121.32
7	G	130	ILE	O-C-N	-27.99	87.58	122.57
3	C	352	LEU	O-C-N	-27.89	89.25	121.32
2	B	392	GLU	CA-C-N	26.13	155.30	120.28
2	B	392	GLU	C-N-CA	26.13	155.30	120.28
4	D	286	GLU	O-C-N	-25.91	88.13	122.59
7	G	228	VAL	O-C-N	-25.90	90.20	122.57
3	C	117	THR	O-C-N	-25.89	88.16	122.59
6	F	1	MET	CA-C-N	24.39	168.13	121.54
6	F	1	MET	C-N-CA	24.39	168.13	121.54
4	D	306	GLN	O-C-N	-22.77	92.30	122.59
4	D	288	SER	O-C-N	-22.76	92.32	122.59
1	A	275	PHE	O-C-N	-22.47	97.76	122.03
1	A	282	LYS	O-C-N	-22.29	92.94	122.59
2	B	591	THR	O-C-N	-22.21	93.54	122.19
7	G	137	SER	O-C-N	-21.73	93.68	122.59
4	D	284	LEU	O-C-N	-21.65	93.80	122.59
4	D	175	PHE	O-C-N	-21.30	98.48	122.55
1	A	283	ARG	O-C-N	-21.00	89.41	123.00
2	B	234	GLU	O-C-N	-20.98	94.69	122.59
1	A	284	ARG	CA-C-N	20.79	158.13	122.79
1	A	284	ARG	C-N-CA	20.79	158.13	122.79
1	A	277	VAL	O-C-N	-20.42	97.83	121.10
5	E	221	HIS	O-C-N	-20.36	100.02	121.60
4	D	301	THR	O-C-N	-19.40	90.49	121.53
2	B	88	LYS	O-C-N	-18.66	97.78	122.59
3	C	119	ASP	O-C-N	-17.89	98.80	122.59
2	B	594	GLY	O-C-N	-17.76	99.61	122.70
2	B	245	SER	O-C-N	-16.78	103.02	122.15
2	B	236	PHE	O-C-N	-16.68	100.40	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	186	THR	O-C-N	-16.66	100.43	122.59
2	B	596	SER	O-C-N	-16.50	100.64	122.59
2	B	231	GLY	O-C-N	-16.44	101.33	122.70
6	F	295	LEU	O-C-N	-16.30	104.13	122.55
7	G	127	SER	O-C-N	-16.24	93.11	122.34
4	D	662	THR	O-C-N	-16.13	101.14	122.59
1	A	280	PRO	CA-C-N	16.09	146.62	122.65
1	A	280	PRO	C-N-CA	16.09	146.62	122.65
2	B	222	PHE	O-C-N	-15.96	101.29	122.83
1	A	283	ARG	CA-C-N	15.79	149.35	122.82
1	A	283	ARG	C-N-CA	15.79	149.35	122.82
2	B	249	ASP	O-C-N	-15.40	102.05	122.38
5	E	39	GLU	O-C-N	-15.36	102.34	122.61
4	D	278	LYS	O-C-N	-15.35	102.18	122.59
1	A	281	SER	O-C-N	15.27	141.06	123.19
1	A	278	PRO	O-C-N	-15.21	102.10	122.64
2	B	84	PHE	O-C-N	-15.21	103.37	122.68
2	B	238	LEU	O-C-N	-15.18	102.39	122.59
2	B	246	PHE	O-C-N	-15.03	102.61	122.59
7	G	123	ASP	O-C-N	-15.00	102.64	122.59
2	B	16	TYR	O-C-N	-14.98	108.28	121.31
2	B	92	ILE	O-C-N	-14.89	103.96	122.57
1	A	278	PRO	CA-C-N	14.88	148.48	121.70
1	A	278	PRO	C-N-CA	14.88	148.48	121.70
3	C	122	PRO	CA-C-N	-14.73	101.43	119.84
3	C	122	PRO	C-N-CA	-14.73	101.43	119.84
2	B	181	PRO	O-C-N	-14.35	103.27	122.64
5	E	220	LEU	O-C-N	-14.32	103.55	122.59
7	G	129	VAL	CA-C-N	14.17	147.47	121.97
7	G	129	VAL	C-N-CA	14.17	147.47	121.97
1	A	277	VAL	CA-C-N	-13.94	102.42	119.84
1	A	277	VAL	C-N-CA	-13.94	102.42	119.84
2	B	95	VAL	O-C-N	-13.83	105.29	122.57
6	F	6	ARG	O-C-N	-13.63	105.64	121.32
2	B	16	TYR	CA-C-N	13.51	135.14	119.47
2	B	16	TYR	C-N-CA	13.51	135.14	119.47
2	B	592	GLY	O-C-N	-13.36	105.33	122.70
1	A	242	ALA	O-C-N	-13.21	110.55	121.38
7	G	133	SER	O-C-N	-12.96	105.35	122.59
4	D	279	GLY	CA-C-N	12.95	136.03	119.84
4	D	279	GLY	C-N-CA	12.95	136.03	119.84
4	D	302	HIS	O-C-N	-12.94	107.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	280	PRO	O-C-N	-12.82	105.33	122.64
2	B	223	GLU	CA-C-N	12.75	142.53	122.51
2	B	223	GLU	C-N-CA	12.75	142.53	122.51
3	C	118	ALA	O-C-N	-12.75	105.63	122.59
4	D	289	GLU	O-C-N	12.71	132.64	121.20
4	D	218	SER	O-C-N	-12.63	107.43	122.46
3	C	351	SER	O-C-N	-12.60	106.13	122.39
2	B	225	MET	O-C-N	-12.59	105.08	122.46
7	G	196	LYS	CA-C-N	12.57	146.05	121.41
7	G	196	LYS	C-N-CA	12.57	146.05	121.41
7	G	124	THR	CA-C-N	12.57	144.59	121.97
7	G	124	THR	C-N-CA	12.57	144.59	121.97
1	A	282	LYS	CA-C-N	12.42	144.06	121.70
1	A	282	LYS	C-N-CA	12.42	144.06	121.70
4	D	219	VAL	O-C-N	-12.29	107.21	122.57
4	D	216	SER	O-C-N	-12.26	102.68	122.42
2	B	23	ASP	CA-C-N	12.18	135.48	120.13
2	B	23	ASP	C-N-CA	12.18	135.48	120.13
2	B	432	ALA	CA-C-N	-12.17	101.91	121.26
2	B	432	ALA	C-N-CA	-12.17	101.91	121.26
2	B	593	GLY	O-C-N	-12.08	106.99	122.70
1	A	276	VAL	CA-C-N	12.01	144.35	122.13
1	A	276	VAL	C-N-CA	12.01	144.35	122.13
3	C	123	PRO	O-C-N	-11.99	106.45	122.64
4	D	184	SER	O-C-N	-11.94	108.54	122.15
6	F	224	ASP	O-C-N	-11.90	107.47	122.34
7	G	130	ILE	CA-C-N	11.87	137.15	120.29
7	G	130	ILE	C-N-CA	11.87	137.15	120.29
4	D	177	ALA	O-C-N	-11.80	106.89	122.59
4	D	663	GLY	CA-C-N	-11.62	103.66	122.26
4	D	663	GLY	C-N-CA	-11.62	103.66	122.26
4	D	287	PHE	CA-C-N	11.61	143.71	121.54
4	D	287	PHE	C-N-CA	11.61	143.71	121.54
6	F	3	SER	O-C-N	-11.57	110.38	122.64
1	A	244	ASN	CA-C-N	11.55	132.49	119.32
1	A	244	ASN	C-N-CA	11.55	132.49	119.32
2	B	242	ASN	O-C-N	-11.48	107.32	122.59
1	A	281	SER	CA-C-N	-11.46	99.65	121.54
1	A	281	SER	C-N-CA	-11.46	99.65	121.54
7	G	183	ALA	CA-C-N	11.45	137.42	121.05
7	G	183	ALA	C-N-CA	11.45	137.42	121.05
4	D	280	PRO	CA-C-N	-11.37	102.42	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	280	PRO	C-N-CA	-11.37	102.42	120.60
3	C	344	MET	O-C-N	-11.28	109.91	122.09
7	G	230	ASP	O-C-N	-11.26	107.61	122.59
6	F	223	VAL	O-C-N	-11.21	111.24	122.23
3	C	320	LEU	CA-C-N	11.19	139.44	121.87
3	C	320	LEU	C-N-CA	11.19	139.44	121.87
6	F	146	ALA	O-C-N	-11.18	108.87	122.96
1	A	284	ARG	O-C-N	-11.18	107.62	122.94
5	E	43	PHE	CA-C-N	11.16	135.24	120.28
5	E	43	PHE	C-N-CA	11.16	135.24	120.28
4	D	182	LEU	O-C-N	-11.16	107.94	122.56
2	B	93	GLU	O-C-N	-11.15	107.77	122.59
6	F	225	ARG	O-C-N	-11.09	110.36	122.12
2	B	96	ALA	O-C-N	-11.06	107.89	122.59
1	A	236	ASN	O-C-N	-10.95	109.41	122.22
3	C	320	LEU	O-C-N	-10.90	104.87	122.42
8	H	156	PRO	O-C-N	-10.90	107.93	122.64
7	G	272	SER	O-C-N	-10.88	110.40	121.28
2	B	242	ASN	CA-C-N	10.82	141.45	121.97
2	B	242	ASN	C-N-CA	10.82	141.45	121.97
2	B	237	GLN	CA-C-N	10.78	142.13	121.54
2	B	237	GLN	C-N-CA	10.78	142.13	121.54
5	E	2	MET	O-C-N	-10.71	108.34	122.59
4	D	178	VAL	O-C-N	-10.66	109.24	122.57
2	B	2	SER	O-C-N	-10.60	108.91	123.01
2	B	223	GLU	O-C-N	-10.58	110.37	123.06
6	F	159	SER	O-C-N	-10.57	108.40	122.57
3	C	344	MET	CA-C-N	10.40	134.22	120.28
3	C	344	MET	C-N-CA	10.40	134.22	120.28
2	B	456	ASP	O-C-N	-10.37	108.68	122.57
2	B	229	VAL	O-C-N	-10.32	108.53	122.05
6	F	8	HIS	O-C-N	-10.21	108.37	122.46
7	G	128	ASN	O-C-N	-10.20	109.02	122.59
3	C	119	ASP	CA-C-N	-10.18	103.66	120.87
3	C	119	ASP	C-N-CA	-10.18	103.66	120.87
6	F	6	ARG	CA-C-N	10.18	132.57	119.84
6	F	6	ARG	C-N-CA	10.18	132.57	119.84
6	F	227	ILE	O-C-N	-10.15	108.76	122.05
7	G	132	GLU	O-C-N	-10.04	109.24	122.59
6	F	228	SER	O-C-N	-9.96	109.35	122.59
7	G	137	SER	CA-C-N	9.95	140.54	121.54
7	G	137	SER	C-N-CA	9.95	140.54	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LYS	O-C-N	-9.94	109.11	122.43
4	D	188	LEU	O-C-N	-9.94	108.96	122.48
2	B	88	LYS	CA-C-N	-9.91	103.79	122.13
2	B	88	LYS	C-N-CA	-9.91	103.79	122.13
3	C	348	LEU	O-C-N	-9.90	110.87	122.15
3	C	342	ARG	O-C-N	9.89	133.43	122.15
6	F	108	ALA	O-C-N	-9.89	109.28	122.43
2	B	595	SER	O-C-N	-9.83	109.52	122.59
6	F	2	GLN	CA-C-N	9.83	138.06	123.12
6	F	2	GLN	C-N-CA	9.83	138.06	123.12
2	B	230	GLU	O-C-N	-9.81	109.55	122.59
2	B	240	GLN	O-C-N	-9.80	109.55	122.59
4	D	216	SER	CA-C-N	9.73	140.12	121.54
4	D	216	SER	C-N-CA	9.73	140.12	121.54
3	C	280	CYS	O-C-N	-9.71	109.60	122.23
4	D	221	PRO	O-C-N	-9.71	109.53	122.64
2	B	241	LEU	O-C-N	-9.66	109.74	122.59
4	D	386	MET	O-C-N	9.66	132.36	122.12
1	A	238	TYR	O-C-N	-9.66	110.80	122.48
2	B	591	THR	CA-C-N	9.61	140.25	121.41
2	B	591	THR	C-N-CA	9.61	140.25	121.41
4	D	576	ASN	O-C-N	9.59	130.53	120.85
1	A	215	VAL	O-C-N	9.57	131.15	121.87
7	G	226	SER	CA-C-N	9.53	135.12	121.02
7	G	226	SER	C-N-CA	9.53	135.12	121.02
3	C	321	GLY	CA-C-N	9.53	129.76	119.28
3	C	321	GLY	C-N-CA	9.53	129.76	119.28
2	B	23	ASP	O-C-N	-9.45	112.27	123.13
7	G	272	SER	CA-C-N	9.37	131.55	119.84
7	G	272	SER	C-N-CA	9.37	131.55	119.84
4	D	665	ARG	CA-C-N	-9.28	104.99	121.70
4	D	665	ARG	C-N-CA	-9.28	104.99	121.70
1	A	241	LEU	O-C-N	-9.28	111.43	123.13
4	D	628	GLN	CA-C-N	9.27	129.51	119.87
4	D	628	GLN	C-N-CA	9.27	129.51	119.87
7	G	197	GLY	O-C-N	-9.27	110.65	122.70
2	B	556	MET	O-C-N	-9.25	112.32	122.12
7	G	199	ASP	O-C-N	-9.23	109.82	122.46
4	D	404	LYS	O-C-N	9.22	131.89	122.12
1	A	228	SER	O-C-N	-9.20	111.67	122.15
8	H	255	ASP	O-C-N	-9.19	111.47	122.22
2	B	458	THR	O-C-N	-9.13	110.44	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	LEU	CA-C-N	9.13	132.51	120.28
1	A	217	LEU	C-N-CA	9.13	132.51	120.28
1	A	242	ALA	CA-C-N	9.12	131.24	119.84
1	A	242	ALA	C-N-CA	9.12	131.24	119.84
5	E	43	PHE	O-C-N	-9.11	110.45	122.47
5	E	42	CYS	O-C-N	-9.10	111.65	123.21
7	G	28	VAL	O-C-N	-9.10	109.88	122.62
5	E	42	CYS	CA-C-N	9.10	135.63	122.35
5	E	42	CYS	C-N-CA	9.10	135.63	122.35
3	C	347	GLU	O-C-N	-8.99	111.21	122.27
4	D	308	THR	O-C-N	-8.95	110.68	122.59
2	B	459	GLN	O-C-N	-8.94	110.70	122.59
1	A	279	GLU	O-C-N	-8.93	108.71	123.00
5	E	4	ALA	O-C-N	-8.93	110.71	122.59
2	B	82	LYS	O-C-N	8.86	132.59	122.22
2	B	188	SER	CA-C-N	-8.86	109.66	122.77
2	B	188	SER	C-N-CA	-8.86	109.66	122.77
1	A	191	TYR	O-C-N	-8.85	112.07	122.15
1	A	221	LEU	O-C-N	-8.85	112.74	122.12
2	B	250	GLY	CA-C-N	8.83	133.35	120.90
2	B	250	GLY	C-N-CA	8.83	133.35	120.90
6	F	3	SER	CA-C-N	8.72	138.51	121.41
6	F	3	SER	C-N-CA	8.72	138.51	121.41
1	A	274	GLU	O-C-N	-8.67	111.88	122.11
6	F	216	GLN	CA-C-N	8.65	132.58	120.29
6	F	216	GLN	C-N-CA	8.65	132.58	120.29
4	D	665	ARG	O-C-N	-8.62	111.13	122.59
4	D	279	GLY	O-C-N	-8.61	113.16	121.77
1	A	228	SER	CA-C-N	8.59	132.49	120.29
1	A	228	SER	C-N-CA	8.59	132.49	120.29
7	G	70	LYS	CA-C-N	8.59	132.15	120.38
7	G	70	LYS	C-N-CA	8.59	132.15	120.38
6	F	76	PHE	CA-C-N	8.58	132.13	120.38
6	F	76	PHE	C-N-CA	8.58	132.13	120.38
3	C	316	SER	CA-C-N	8.55	132.43	120.29
3	C	316	SER	C-N-CA	8.55	132.43	120.29
1	A	221	LEU	CA-C-N	8.54	131.73	120.28
1	A	221	LEU	C-N-CA	8.54	131.73	120.28
1	A	191	TYR	CA-C-N	8.52	133.26	120.31
1	A	191	TYR	C-N-CA	8.52	133.26	120.31
2	B	240	GLN	CA-C-N	8.48	137.75	121.54
2	B	240	GLN	C-N-CA	8.48	137.75	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	359	SER	O-C-N	-8.48	113.12	123.04
6	F	220	ALA	O-C-N	-8.47	111.22	122.23
6	F	5	SER	O-C-N	-8.44	111.37	122.59
8	H	258	ARG	O-C-N	-8.41	110.47	122.41
6	F	216	GLN	O-C-N	-8.39	112.58	122.15
4	D	458	PRO	O-C-N	-8.35	110.92	122.37
7	G	275	GLY	CA-C-N	8.35	128.04	119.19
7	G	275	GLY	C-N-CA	8.35	128.04	119.19
1	A	234	LYS	CA-C-N	8.34	134.84	120.58
1	A	234	LYS	C-N-CA	8.34	134.84	120.58
1	A	285	LEU	O-C-N	-8.34	110.69	122.03
2	B	228	PHE	O-C-N	-8.30	110.92	122.37
3	C	348	LEU	CA-C-N	8.25	131.16	120.44
3	C	348	LEU	C-N-CA	8.25	131.16	120.44
5	E	5	ASN	O-C-N	-8.23	111.85	121.32
1	A	217	LEU	O-C-N	-8.23	112.77	122.15
6	F	209	GLU	CA-C-N	8.23	131.30	120.28
6	F	209	GLU	C-N-CA	8.23	131.30	120.28
2	B	186	GLU	O-C-N	-8.21	111.67	122.59
2	B	47	ALA	O-C-N	-8.19	113.10	122.93
6	F	220	ALA	CA-C-N	8.18	132.74	120.31
6	F	220	ALA	C-N-CA	8.18	132.74	120.31
3	C	316	SER	O-C-N	-8.16	112.85	122.15
1	A	224	LEU	O-C-N	-8.15	112.86	122.15
4	D	455	LYS	O-C-N	-8.08	111.53	122.36
5	E	3	ALA	O-C-N	-8.08	111.84	122.59
1	A	224	LEU	CA-C-N	8.08	131.10	120.28
1	A	224	LEU	C-N-CA	8.08	131.10	120.28
1	A	202	SER	O-C-N	-8.07	112.35	122.27
2	B	235	ASN	CA-C-N	8.04	136.89	121.54
2	B	235	ASN	C-N-CA	8.04	136.89	121.54
4	D	575	THR	O-C-N	-8.04	112.02	122.39
2	B	185	CYS	CA-C-N	-8.02	106.22	121.54
2	B	185	CYS	C-N-CA	-8.02	106.22	121.54
7	G	274	MET	O-C-N	-8.02	111.48	122.46
3	C	293	ARG	O-C-N	7.96	131.23	122.15
4	D	285	LYS	CA-C-N	7.93	136.69	121.54
4	D	285	LYS	C-N-CA	7.93	136.69	121.54
1	A	271	ASN	O-C-N	-7.92	113.53	122.09
6	F	146	ALA	CA-C-N	7.92	132.46	120.82
6	F	146	ALA	C-N-CA	7.92	132.46	120.82
7	G	275	GLY	O-C-N	-7.91	113.86	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	91	ALA	O-C-N	-7.90	112.08	122.59
1	A	274	GLU	CA-C-N	7.88	131.35	120.63
1	A	274	GLU	C-N-CA	7.88	131.35	120.63
2	B	86	ILE	CA-C-N	-7.85	109.40	121.02
2	B	86	ILE	C-N-CA	-7.85	109.40	121.02
1	A	237	SER	O-C-N	-7.83	111.65	122.46
3	C	181	GLY	CA-C-N	7.79	131.49	120.28
3	C	181	GLY	C-N-CA	7.79	131.49	120.28
4	D	535	ALA	CA-C-N	7.79	127.50	119.56
4	D	535	ALA	C-N-CA	7.79	127.50	119.56
5	E	38	LEU	CA-C-N	-7.76	110.72	122.21
5	E	38	LEU	C-N-CA	-7.76	110.72	122.21
4	D	576	ASN	C-N-CD	-7.75	103.55	120.60
2	B	432	ALA	O-C-N	-7.72	112.32	122.59
4	D	515	ALA	CA-C-N	7.71	127.76	119.28
4	D	515	ALA	C-N-CA	7.71	127.76	119.28
7	G	196	LYS	O-C-N	-7.68	112.28	122.57
6	F	163	ASP	CA-C-N	7.67	127.57	119.05
6	F	163	ASP	C-N-CA	7.67	127.57	119.05
4	D	5	SER	O-C-N	-7.66	114.18	122.07
4	D	282	CYS	CA-C-N	7.64	131.97	121.05
4	D	282	CYS	C-N-CA	7.64	131.97	121.05
5	E	217	ILE	O-C-N	-7.63	113.36	122.06
4	D	181	ASP	CA-C-N	-7.62	110.50	122.23
4	D	181	ASP	C-N-CA	-7.62	110.50	122.23
2	B	182	GLU	O-C-N	-7.60	112.48	122.59
8	H	305	PHE	O-C-N	-7.59	114.19	122.09
3	C	120	SER	CA-C-N	7.57	136.14	122.13
3	C	120	SER	C-N-CA	7.57	136.14	122.13
2	B	304	LYS	O-C-N	-7.55	112.97	123.01
4	D	281	SER	O-C-N	-7.54	112.59	122.39
7	G	59	TYR	CA-C-N	7.51	128.12	120.38
7	G	59	TYR	C-N-CA	7.51	128.12	120.38
7	G	146	ILE	O-C-N	7.47	129.24	121.91
6	F	276	ALA	O-C-N	-7.47	113.57	122.46
1	A	231	ALA	CA-C-N	7.46	130.89	120.29
1	A	231	ALA	C-N-CA	7.46	130.89	120.29
7	G	135	SER	CA-C-N	-7.46	110.31	120.82
7	G	135	SER	C-N-CA	-7.46	110.31	120.82
4	D	17	GLU	O-C-N	-7.45	113.15	122.17
7	G	131	LEU	CA-C-N	-7.45	107.31	121.54
7	G	131	LEU	C-N-CA	-7.45	107.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	133	SER	CA-C-N	7.42	135.72	121.54
7	G	133	SER	C-N-CA	7.42	135.72	121.54
8	H	232	VAL	O-C-N	-7.41	114.96	122.23
4	D	38	GLN	CA-C-N	7.41	131.57	120.31
4	D	38	GLN	C-N-CA	7.41	131.57	120.31
5	E	41	PRO	O-C-N	7.41	131.53	123.01
7	G	70	LYS	O-C-N	-7.40	114.13	122.86
4	D	5	SER	CA-C-N	7.39	130.18	120.28
4	D	5	SER	C-N-CA	7.39	130.18	120.28
2	B	549	ASP	CA-C-N	7.35	130.72	120.29
2	B	549	ASP	C-N-CA	7.35	130.72	120.29
7	G	126	SER	CA-C-N	-7.32	107.69	122.55
7	G	126	SER	C-N-CA	-7.32	107.69	122.55
4	D	119	LEU	CA-C-N	-7.31	111.67	122.41
4	D	119	LEU	C-N-CA	-7.31	111.67	122.41
1	A	243	PRO	O-C-N	-7.29	112.79	122.64
2	B	184	ALA	CA-C-N	-7.29	110.51	120.28
2	B	184	ALA	C-N-CA	-7.29	110.51	120.28
7	G	273	PRO	O-C-N	-7.28	112.82	122.64
3	C	338	ILE	O-C-N	7.25	128.90	121.87
7	G	167	SER	O-C-N	7.21	127.30	121.17
7	G	127	SER	CA-C-N	-7.20	107.78	121.54
7	G	127	SER	C-N-CA	-7.20	107.78	121.54
7	G	178	LYS	O-C-N	7.18	127.46	120.71
4	D	288	SER	CA-C-N	7.17	137.20	121.63
4	D	288	SER	C-N-CA	7.17	137.20	121.63
2	B	556	MET	CA-C-N	7.14	132.82	120.68
2	B	556	MET	C-N-CA	7.14	132.82	120.68
6	F	84	ASP	CA-C-N	7.14	129.85	120.28
6	F	84	ASP	C-N-CA	7.14	129.85	120.28
6	F	229	ASP	O-C-N	-7.12	112.65	122.19
4	D	386	MET	CA-C-N	-7.11	111.19	120.44
4	D	386	MET	C-N-CA	-7.11	111.19	120.44
2	B	244	ASN	O-C-N	-7.04	113.61	122.27
1	A	194	HIS	O-C-N	7.04	131.38	122.23
2	B	250	GLY	O-C-N	-7.03	113.56	122.70
1	A	78	GLY	CA-C-N	7.00	127.14	119.87
1	A	78	GLY	C-N-CA	7.00	127.14	119.87
2	B	222	PHE	CA-C-N	6.99	131.04	121.05
2	B	222	PHE	C-N-CA	6.99	131.04	121.05
2	B	431	SER	CA-C-N	6.98	134.87	121.54
2	B	431	SER	C-N-CA	6.98	134.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	101	GLY	O-C-N	-6.95	114.76	122.55
4	D	277	SER	O-C-N	-6.94	114.24	122.15
2	B	521	THR	O-C-N	6.93	131.07	123.10
4	D	217	SER	O-C-N	-6.92	113.38	122.59
4	D	278	LYS	CA-C-N	-6.92	111.01	121.87
4	D	278	LYS	C-N-CA	-6.92	111.01	121.87
1	A	236	ASN	CA-C-N	6.90	134.84	121.18
1	A	236	ASN	C-N-CA	6.90	134.84	121.18
6	F	366	ASP	O-C-N	-6.90	114.64	122.09
2	B	256	CYS	O-C-N	6.89	129.42	122.12
3	C	347	GLU	CA-C-N	6.88	130.06	120.29
3	C	347	GLU	C-N-CA	6.88	130.06	120.29
7	G	20	LEU	O-C-N	-6.87	113.58	122.37
4	D	303	LEU	CA-C-N	-6.84	105.11	121.80
4	D	303	LEU	C-N-CA	-6.84	105.11	121.80
7	G	74	THR	O-C-N	-6.84	114.87	122.12
4	D	221	PRO	CA-C-N	6.83	134.81	121.41
4	D	221	PRO	C-N-CA	6.83	134.81	121.41
3	C	268	LYS	O-C-N	6.82	129.45	122.09
1	A	211	HIS	O-C-N	6.82	129.34	122.12
1	A	244	ASN	O-C-N	-6.81	113.35	121.12
7	G	20	LEU	CA-C-N	6.81	132.06	122.46
7	G	20	LEU	C-N-CA	6.81	132.06	122.46
8	H	324	ARG	O-C-N	6.81	129.08	122.07
7	G	184	GLU	O-C-N	-6.80	114.90	123.06
6	F	333	GLY	CA-C-N	6.79	130.21	120.98
6	F	333	GLY	C-N-CA	6.79	130.21	120.98
2	B	552	LEU	CA-C-N	6.78	129.91	120.29
2	B	552	LEU	C-N-CA	6.78	129.91	120.29
2	B	433	SER	O-C-N	-6.75	113.82	123.07
4	D	631	GLN	O-C-N	-6.75	113.38	122.43
8	H	363	ASP	CA-C-N	6.73	131.45	123.44
8	H	363	ASP	C-N-CA	6.73	131.45	123.44
8	H	200	ASP	O-C-N	-6.73	114.99	122.12
4	D	82	GLN	CA-C-N	6.72	129.58	120.44
4	D	82	GLN	C-N-CA	6.72	129.58	120.44
1	A	231	ALA	O-C-N	-6.69	113.53	122.23
4	D	397	ALA	O-C-N	6.66	129.74	122.15
6	F	209	GLU	O-C-N	-6.66	114.56	122.15
1	A	199	GLN	CA-C-N	6.65	129.73	120.29
1	A	199	GLN	C-N-CA	6.65	129.73	120.29
2	B	126	SER	O-C-N	6.64	129.73	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	311	ARG	O-C-N	-6.64	115.23	122.07
2	B	547	LEU	O-C-N	6.61	129.69	122.15
4	D	379	ARG	O-C-N	6.61	129.12	122.12
6	F	1	MET	O-C-N	-6.60	112.45	123.00
6	F	392	CYS	CA-C-N	6.59	126.53	119.28
6	F	392	CYS	C-N-CA	6.59	126.53	119.28
3	C	342	ARG	CA-C-N	-6.58	111.46	120.28
3	C	342	ARG	C-N-CA	-6.58	111.46	120.28
2	B	304	LYS	CA-C-N	6.56	134.07	121.54
2	B	304	LYS	C-N-CA	6.56	134.07	121.54
6	F	106	VAL	O-C-N	-6.55	114.40	121.80
8	H	214	THR	O-C-N	-6.52	114.72	122.15
2	B	299	ASP	O-C-N	-6.52	113.46	122.46
2	B	457	ASN	CA-C-N	-6.52	109.09	121.54
2	B	457	ASN	C-N-CA	-6.52	109.09	121.54
2	B	295	SER	CA-C-N	6.51	131.32	120.64
2	B	295	SER	C-N-CA	6.51	131.32	120.64
5	E	5	ASN	CA-C-N	6.51	127.98	119.84
5	E	5	ASN	C-N-CA	6.51	127.98	119.84
2	B	90	PRO	O-C-N	-6.51	113.85	122.64
7	G	129	VAL	O-C-N	-6.50	114.44	122.57
4	D	21	PRO	CA-C-N	6.50	129.87	120.38
4	D	21	PRO	C-N-CA	6.50	129.87	120.38
4	D	275	ASP	O-C-N	-6.50	114.28	122.27
5	E	213	SER	CA-C-N	-6.49	110.45	120.31
5	E	213	SER	C-N-CA	-6.49	110.45	120.31
3	C	125	ASP	CA-C-N	-6.48	113.55	122.30
3	C	125	ASP	C-N-CA	-6.48	113.55	122.30
2	B	544	VAL	O-C-N	6.47	128.49	121.83
8	H	305	PHE	CA-C-N	6.47	129.47	120.29
8	H	305	PHE	C-N-CA	6.47	129.47	120.29
3	C	340	ASP	O-C-N	-6.46	115.41	122.07
6	F	321	LEU	O-C-N	6.46	128.97	122.12
8	H	271	ASN	CA-C-N	6.46	129.23	120.38
8	H	271	ASN	C-N-CA	6.46	129.23	120.38
4	D	62	ASN	O-C-N	6.46	128.97	122.12
2	B	65	LYS	O-C-N	6.44	128.94	122.12
4	D	186	THR	CA-C-N	-6.44	111.97	121.24
4	D	186	THR	C-N-CA	-6.44	111.97	121.24
7	G	228	VAL	CA-C-N	-6.42	111.84	120.90
7	G	228	VAL	C-N-CA	-6.42	111.84	120.90
2	B	48	SER	CA-C-N	6.41	129.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	SER	C-N-CA	6.41	129.52	120.28
2	B	185	CYS	O-C-N	-6.41	115.32	122.12
2	B	85	SER	O-C-N	-6.41	114.48	123.01
6	F	77	ARG	CA-C-N	-6.40	112.41	122.65
6	F	77	ARG	C-N-CA	-6.40	112.41	122.65
7	G	274	MET	CA-C-N	6.40	131.92	121.87
7	G	274	MET	C-N-CA	6.40	131.92	121.87
7	G	339	GLU	O-C-N	6.39	129.44	122.15
8	H	304	SER	CA-C-N	6.38	129.16	120.54
8	H	304	SER	C-N-CA	6.38	129.16	120.54
5	E	41	PRO	CA-C-N	-6.37	113.69	122.93
5	E	41	PRO	C-N-CA	-6.37	113.69	122.93
2	B	593	GLY	CA-C-N	6.37	133.90	121.41
2	B	593	GLY	C-N-CA	6.37	133.90	121.41
2	B	299	ASP	CA-C-N	6.34	132.24	121.14
2	B	299	ASP	C-N-CA	6.34	132.24	121.14
5	E	58	GLU	CA-C-N	6.34	129.15	120.46
5	E	58	GLU	C-N-CA	6.34	129.15	120.46
2	B	539	LEU	CA-C-N	6.33	129.40	120.28
2	B	539	LEU	C-N-CA	6.33	129.40	120.28
8	H	238	THR	O-C-N	-6.33	114.49	122.27
4	D	300	SER	O-C-N	-6.32	114.18	122.59
7	G	122	PRO	O-C-N	-6.32	114.11	122.64
6	F	213	LEU	CA-C-N	6.31	128.73	120.28
6	F	213	LEU	C-N-CA	6.31	128.73	120.28
7	G	3	GLY	O-C-N	-6.31	114.50	122.70
1	A	280	PRO	O-C-N	6.30	130.82	123.01
5	E	124	GLU	CA-C-N	6.30	129.35	120.28
5	E	124	GLU	C-N-CA	6.30	129.35	120.28
6	F	58	VAL	CA-C-N	6.29	129.08	120.46
6	F	58	VAL	C-N-CA	6.29	129.08	120.46
5	E	103	ARG	O-C-N	-6.29	114.86	122.22
1	A	238	TYR	CA-C-N	6.25	131.27	120.58
1	A	238	TYR	C-N-CA	6.25	131.27	120.58
7	G	184	GLU	CA-C-N	6.25	133.48	121.54
7	G	184	GLU	C-N-CA	6.25	133.48	121.54
5	E	58	GLU	O-C-N	-6.24	115.50	122.12
6	F	163	ASP	O-C-N	-6.23	116.19	121.23
4	D	38	GLN	O-C-N	-6.22	114.09	122.43
4	D	404	LYS	CA-C-N	-6.22	111.94	120.28
4	D	404	LYS	C-N-CA	-6.22	111.94	120.28
4	D	185	SER	O-C-N	-6.21	114.03	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	588	GLU	CA-C-N	6.20	128.59	120.28
2	B	588	GLU	C-N-CA	6.20	128.59	120.28
2	B	549	ASP	O-C-N	-6.20	115.55	122.12
6	F	304	GLY	O-C-N	-6.20	114.47	122.34
6	F	224	ASP	CA-C-N	-6.19	111.98	120.28
6	F	224	ASP	C-N-CA	-6.19	111.98	120.28
6	F	64	PHE	O-C-N	6.18	128.67	122.12
2	B	539	LEU	O-C-N	-6.17	115.58	122.12
4	D	35	PHE	O-C-N	6.17	129.85	122.26
4	D	151	SER	CA-C-N	6.16	128.54	120.28
4	D	151	SER	C-N-CA	6.16	128.54	120.28
6	F	76	PHE	O-C-N	-6.14	114.94	122.25
6	F	282	ASN	O-C-N	6.13	128.62	122.12
2	B	101	GLU	O-C-N	6.13	128.62	122.12
3	C	313	ILE	CA-C-N	6.13	129.11	120.28
3	C	313	ILE	C-N-CA	6.13	129.11	120.28
4	D	189	GLU	CA-C-N	-6.13	113.44	119.76
4	D	189	GLU	C-N-CA	-6.13	113.44	119.76
7	G	74	THR	CA-C-N	6.12	128.49	120.28
7	G	74	THR	C-N-CA	6.12	128.49	120.28
8	H	285	ILE	O-C-N	6.12	128.14	121.83
4	D	25	ALA	CA-C-N	6.10	126.11	119.89
4	D	25	ALA	C-N-CA	6.10	126.11	119.89
3	C	269	LEU	CA-C-N	6.10	128.95	120.29
3	C	269	LEU	C-N-CA	6.10	128.95	120.29
2	B	491	GLN	O-C-N	6.10	129.10	122.15
4	D	358	GLY	O-C-N	-6.06	115.02	122.23
7	G	198	LYS	O-C-N	-6.05	114.54	122.59
4	D	286	GLU	CA-C-N	-6.05	112.12	120.71
4	D	286	GLU	C-N-CA	-6.05	112.12	120.71
4	D	648	ARG	O-C-N	6.05	128.53	122.12
4	D	593	GLU	O-C-N	-6.05	115.26	122.15
6	F	296	GLN	O-C-N	-6.04	114.56	122.59
3	C	340	ASP	CA-C-N	6.03	128.36	120.28
3	C	340	ASP	C-N-CA	6.03	128.36	120.28
7	G	242	LEU	O-C-N	6.03	129.02	122.15
4	D	25	ALA	O-C-N	-6.02	116.19	121.31
4	D	236	SER	O-C-N	6.02	128.50	122.12
5	E	216	SER	O-C-N	-6.00	114.58	122.39
5	E	220	LEU	CA-C-N	-6.00	111.43	121.03
5	E	220	LEU	C-N-CA	-6.00	111.43	121.03
2	B	311	ARG	CA-C-N	6.00	128.34	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	311	ARG	C-N-CA	6.00	128.34	120.60
2	B	251	THR	O-C-N	-6.00	115.65	122.97
7	G	243	THR	CA-C-N	6.00	128.24	120.44
7	G	243	THR	C-N-CA	6.00	128.24	120.44
6	F	114	VAL	O-C-N	-6.00	117.03	123.14
2	B	541	HIS	O-C-N	5.99	128.98	122.15
2	B	552	LEU	O-C-N	-5.99	115.63	122.09
4	D	411	GLN	O-C-N	5.98	128.46	122.12
4	D	664	SER	O-C-N	-5.98	114.48	122.38
3	C	319	PHE	O-C-N	-5.97	114.44	122.43
2	B	295	SER	O-C-N	-5.96	114.23	122.46
3	C	312	GLN	CA-C-N	5.96	128.89	120.42
3	C	312	GLN	C-N-CA	5.96	128.89	120.42
7	G	30	LEU	O-C-N	-5.96	116.43	123.22
6	F	77	ARG	O-C-N	5.96	128.43	122.12
6	F	389	LEU	O-C-N	-5.96	114.51	122.49
1	A	163	GLU	O-C-N	5.95	128.94	122.15
3	C	298	ALA	CA-C-N	5.95	126.55	120.00
3	C	298	ALA	C-N-CA	5.95	126.55	120.00
4	D	63	LEU	O-C-N	5.95	128.20	122.07
1	A	259	LEU	CA-C-N	5.92	128.70	120.29
1	A	259	LEU	C-N-CA	5.92	128.70	120.29
6	F	11	TRP	O-C-N	-5.92	115.29	122.22
2	B	235	ASN	O-C-N	-5.92	114.72	122.59
1	A	203	ALA	CA-C-N	5.91	131.45	120.87
1	A	203	ALA	C-N-CA	5.91	131.45	120.87
2	B	123	MET	O-C-N	5.91	128.47	122.09
4	D	87	LYS	O-C-N	5.90	128.38	122.12
4	D	147	ALA	O-C-N	-5.90	115.43	122.15
3	C	301	LYS	CA-C-N	5.89	128.17	120.28
3	C	301	LYS	C-N-CA	5.89	128.17	120.28
2	B	244	ASN	CA-C-N	-5.87	111.95	120.29
2	B	244	ASN	C-N-CA	-5.87	111.95	120.29
2	B	91	ALA	CA-C-N	-5.87	111.40	121.97
2	B	91	ALA	C-N-CA	-5.87	111.40	121.97
3	C	308	SER	CA-C-N	5.87	128.42	120.44
3	C	308	SER	C-N-CA	5.87	128.42	120.44
8	H	214	THR	CA-C-N	5.87	128.62	120.29
8	H	214	THR	C-N-CA	5.87	128.62	120.29
4	D	70	GLN	O-C-N	5.86	128.19	122.09
7	G	199	ASP	CA-C-N	5.84	130.47	120.71
7	G	199	ASP	C-N-CA	5.84	130.47	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	546	ILE	CA-C-N	5.84	128.58	120.29
2	B	546	ILE	C-N-CA	5.84	128.58	120.29
1	A	259	LEU	O-C-N	-5.83	115.50	122.15
6	F	37	THR	CA-C-N	5.83	129.93	120.60
6	F	37	THR	C-N-CA	5.83	129.93	120.60
6	F	79	CYS	O-C-N	-5.83	115.88	122.23
3	C	305	GLN	CA-C-N	5.81	128.07	120.28
3	C	305	GLN	C-N-CA	5.81	128.07	120.28
1	A	203	ALA	O-C-N	-5.81	113.80	122.39
3	C	180	GLU	CA-C-N	5.79	127.07	120.53
3	C	180	GLU	C-N-CA	5.79	127.07	120.53
4	D	630	VAL	O-C-N	-5.79	114.46	122.05
4	D	394	GLU	O-C-N	5.76	128.23	122.12
6	F	333	GLY	O-C-N	-5.74	115.23	122.70
6	F	6	ARG	C-N-CD	-5.74	101.49	125.00
7	G	124	THR	O-C-N	-5.73	114.97	122.59
5	E	158	ILE	O-C-N	-5.72	116.01	120.07
4	D	184	SER	CA-C-N	-5.71	112.36	122.07
4	D	184	SER	C-N-CA	-5.71	112.36	122.07
4	D	189	GLU	O-C-N	5.71	127.89	121.32
2	B	581	LYS	O-C-N	5.71	128.17	122.12
6	F	191	GLU	CA-C-N	5.70	127.92	120.28
6	F	191	GLU	C-N-CA	5.70	127.92	120.28
4	D	486	LEU	CA-C-N	-5.70	113.75	119.56
4	D	486	LEU	C-N-CA	-5.70	113.75	119.56
4	D	630	VAL	CA-C-N	5.70	130.24	120.72
4	D	630	VAL	C-N-CA	5.70	130.24	120.72
1	A	202	SER	CA-C-N	5.70	133.33	121.94
1	A	202	SER	C-N-CA	5.70	133.33	121.94
3	C	293	ARG	CA-C-N	-5.68	112.67	120.28
3	C	293	ARG	C-N-CA	-5.68	112.67	120.28
6	F	114	VAL	CA-C-N	5.68	128.46	120.28
6	F	114	VAL	C-N-CA	5.68	128.46	120.28
3	C	280	CYS	CA-C-N	5.68	132.68	123.37
3	C	280	CYS	C-N-CA	5.68	132.68	123.37
2	B	112	ASN	O-C-N	5.67	128.13	122.12
4	D	147	ALA	CA-C-N	5.67	128.33	120.29
4	D	147	ALA	C-N-CA	5.67	128.33	120.29
4	D	35	PHE	CA-C-N	-5.66	115.07	122.37
4	D	35	PHE	C-N-CA	-5.66	115.07	122.37
2	B	247	GLY	O-C-N	-5.65	115.35	122.70
2	B	431	SER	O-C-N	5.65	130.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	19	GLY	O-C-N	-5.65	115.72	122.33
4	D	266	LYS	O-C-N	5.65	128.59	122.15
7	G	282	HIS	O-C-N	-5.65	116.15	122.03
4	D	538	SER	CA-C-N	5.65	127.68	120.56
4	D	538	SER	C-N-CA	5.65	127.68	120.56
2	B	358	MET	O-C-N	5.65	128.11	122.12
3	C	331	TYR	O-C-N	5.64	128.10	122.12
2	B	234	GLU	CA-C-N	5.64	132.31	121.54
2	B	234	GLU	C-N-CA	5.64	132.31	121.54
2	B	572	TYR	CA-C-N	5.64	127.84	120.28
2	B	572	TYR	C-N-CA	5.64	127.84	120.28
3	C	223	ILE	CA-C-N	5.64	127.82	120.26
3	C	223	ILE	C-N-CA	5.64	127.82	120.26
4	D	158	ARG	CA-C-N	5.64	127.83	120.28
4	D	158	ARG	C-N-CA	5.64	127.83	120.28
4	D	260	ASN	O-C-N	5.62	128.08	122.12
8	H	255	ASP	CA-C-N	5.62	132.31	121.18
8	H	255	ASP	C-N-CA	5.62	132.31	121.18
6	F	36	LYS	O-C-N	-5.61	116.63	123.19
2	B	52	VAL	O-C-N	-5.61	116.10	122.94
5	E	76	ALA	O-C-N	-5.61	115.76	122.15
3	C	39	LEU	O-C-N	-5.59	116.67	123.27
1	A	270	VAL	O-C-N	-5.59	114.46	121.84
8	H	176	LYS	CA-C-N	5.59	127.70	120.44
8	H	176	LYS	C-N-CA	5.59	127.70	120.44
4	D	593	GLU	CA-C-N	5.58	128.80	120.31
4	D	593	GLU	C-N-CA	5.58	128.80	120.31
8	H	273	HIS	O-C-N	5.58	128.51	122.15
7	G	3	GLY	CA-C-N	5.58	132.34	121.41
7	G	3	GLY	C-N-CA	5.58	132.34	121.41
3	C	15	LEU	CA-C-N	-5.58	113.42	122.34
3	C	15	LEU	C-N-CA	-5.58	113.42	122.34
5	E	150	LYS	O-C-N	5.58	128.03	122.12
1	A	270	VAL	CA-C-N	5.57	128.02	120.44
1	A	270	VAL	C-N-CA	5.57	128.02	120.44
2	B	155	VAL	O-C-N	5.57	127.69	121.90
8	H	333	SER	CA-C-N	5.55	127.65	120.44
8	H	333	SER	C-N-CA	5.55	127.65	120.44
4	D	329	GLU	CA-C-N	5.54	127.65	120.44
4	D	329	GLU	C-N-CA	5.54	127.65	120.44
7	G	172	PRO	O-C-N	-5.54	113.65	122.52
1	A	235	LEU	CA-C-N	5.54	128.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	LEU	C-N-CA	5.54	128.26	120.28
1	A	279	GLU	CA-C-N	-5.54	114.08	119.78
1	A	279	GLU	C-N-CA	-5.54	114.08	119.78
2	B	178	PHE	O-C-N	-5.54	115.17	122.42
4	D	473	SER	CA-C-N	5.54	127.65	120.56
4	D	473	SER	C-N-CA	5.54	127.65	120.56
1	A	237	SER	CA-C-N	5.53	131.18	122.11
1	A	237	SER	C-N-CA	5.53	131.18	122.11
4	D	627	GLU	O-C-N	-5.53	114.51	122.36
3	C	313	ILE	O-C-N	-5.53	116.14	121.83
4	D	48	ARG	O-C-N	-5.53	114.16	122.28
7	G	106	PHE	O-C-N	5.53	127.98	122.12
4	D	201	LYS	O-C-N	5.53	127.98	122.12
6	F	226	LYS	O-C-N	-5.53	112.39	122.34
2	B	233	ASP	O-C-N	-5.52	115.24	122.59
6	F	58	VAL	O-C-N	-5.52	116.16	121.90
8	H	304	SER	O-C-N	-5.52	114.84	122.46
6	F	110	PHE	CA-C-N	5.51	125.45	119.78
6	F	110	PHE	C-N-CA	5.51	125.45	119.78
6	F	207	ARG	O-C-N	5.51	128.43	122.15
4	D	71	HIS	O-C-N	5.50	127.95	122.12
3	C	244	LEU	CA-C-N	-5.50	115.89	122.44
3	C	244	LEU	C-N-CA	-5.50	115.89	122.44
6	F	123	GLY	CA-C-N	5.50	125.15	119.05
6	F	123	GLY	C-N-CA	5.50	125.15	119.05
1	A	199	GLN	O-C-N	-5.49	115.52	122.27
1	A	160	LYS	O-C-N	5.48	127.93	122.12
2	B	459	GLN	CA-C-N	-5.48	112.91	121.02
2	B	459	GLN	C-N-CA	-5.48	112.91	121.02
4	D	631	GLN	CA-C-N	5.48	131.15	122.60
4	D	631	GLN	C-N-CA	5.48	131.15	122.60
8	H	344	SER	CA-C-N	5.48	127.57	120.44
8	H	344	SER	C-N-CA	5.48	127.57	120.44
4	D	623	MET	CA-C-N	5.47	127.62	120.28
4	D	623	MET	C-N-CA	5.47	127.62	120.28
5	E	76	ALA	CA-C-N	5.47	129.36	120.60
5	E	76	ALA	C-N-CA	5.47	129.36	120.60
6	F	10	ALA	O-C-N	-5.46	116.19	122.09
6	F	250	GLU	O-C-N	-5.46	115.11	122.43
2	B	105	LYS	O-C-N	5.46	128.37	122.15
4	D	626	TRP	O-C-N	-5.46	115.13	122.23
8	H	200	ASP	CA-C-N	5.46	128.04	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	200	ASP	C-N-CA	5.46	128.04	120.29
1	A	215	VAL	CA-C-N	-5.45	112.97	120.28
1	A	215	VAL	C-N-CA	-5.45	112.97	120.28
6	F	52	ASN	CA-C-N	5.45	128.03	120.29
6	F	52	ASN	C-N-CA	5.45	128.03	120.29
6	F	137	VAL	O-C-N	-5.43	116.60	121.87
7	G	28	VAL	CA-C-N	5.43	131.18	123.14
7	G	28	VAL	C-N-CA	5.43	131.18	123.14
7	G	273	PRO	CA-C-N	5.42	131.20	121.66
7	G	273	PRO	C-N-CA	5.42	131.20	121.66
2	B	584	VAL	CA-C-N	5.41	125.99	119.98
2	B	584	VAL	C-N-CA	5.41	125.99	119.98
4	D	283	GLN	CA-C-N	5.41	131.88	121.54
4	D	283	GLN	C-N-CA	5.41	131.88	121.54
4	D	423	LYS	O-C-N	5.40	127.85	122.12
7	G	282	HIS	CA-C-N	5.40	127.52	120.28
7	G	282	HIS	C-N-CA	5.40	127.52	120.28
2	B	548	GLY	O-C-N	5.40	127.38	122.19
7	G	60	PRO	O-C-N	-5.40	115.09	121.46
1	A	255	ALA	CA-C-N	5.40	127.96	120.29
1	A	255	ALA	C-N-CA	5.40	127.96	120.29
1	A	206	GLU	CA-C-N	5.40	126.84	120.09
1	A	206	GLU	C-N-CA	5.40	126.84	120.09
7	G	178	LYS	CA-C-N	-5.39	113.35	119.28
7	G	178	LYS	C-N-CA	-5.39	113.35	119.28
4	D	473	SER	O-C-N	-5.38	116.42	122.12
6	F	34	ALA	O-C-N	-5.38	115.46	122.39
2	B	546	ILE	O-C-N	-5.37	116.30	121.83
4	D	515	ALA	O-C-N	-5.37	115.77	121.30
2	B	553	LYS	CA-C-N	5.37	127.91	120.29
2	B	553	LYS	C-N-CA	5.37	127.91	120.29
2	B	239	VAL	CA-C-N	5.37	131.79	121.54
2	B	239	VAL	C-N-CA	5.37	131.79	121.54
2	B	355	ASP	O-C-N	5.37	127.81	122.12
5	E	95	ASN	O-C-N	5.37	127.59	122.07
6	F	11	TRP	CA-C-N	5.37	127.47	120.28
6	F	11	TRP	C-N-CA	5.37	127.47	120.28
6	F	137	VAL	CA-C-N	5.36	127.41	120.44
6	F	137	VAL	C-N-CA	5.36	127.41	120.44
5	E	39	GLU	CA-C-N	-5.36	114.16	121.61
5	E	39	GLU	C-N-CA	-5.36	114.16	121.61
5	E	219	ASN	O-C-N	-5.35	104.72	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	309	THR	CA-C-N	5.35	127.45	120.28
3	C	309	THR	C-N-CA	5.35	127.45	120.28
4	D	29	GLU	O-C-N	5.35	128.25	122.15
7	G	22	CYS	CA-C-N	5.35	125.01	119.56
7	G	22	CYS	C-N-CA	5.35	125.01	119.56
2	B	92	ILE	CA-C-N	-5.34	111.34	121.54
2	B	92	ILE	C-N-CA	-5.34	111.34	121.54
2	B	180	THR	O-C-N	-5.34	116.40	121.20
6	F	38	LEU	O-C-N	-5.34	115.45	122.39
4	D	390	ARG	O-C-N	5.34	127.78	122.12
7	G	174	PRO	CA-C-N	5.33	127.86	120.29
7	G	174	PRO	C-N-CA	5.33	127.86	120.29
5	E	31	ASN	O-C-N	5.33	127.77	122.12
8	H	257	THR	O-C-N	-5.33	115.44	122.42
4	D	203	ARG	CA-C-N	5.32	127.72	120.54
4	D	203	ARG	C-N-CA	5.32	127.72	120.54
5	E	78	ILE	CA-C-N	-5.32	111.38	121.54
5	E	78	ILE	C-N-CA	-5.32	111.38	121.54
4	D	187	PHE	CA-C-N	5.32	131.11	122.07
4	D	187	PHE	C-N-CA	5.32	131.11	122.07
2	B	545	GLU	CA-C-N	5.31	127.96	120.42
2	B	545	GLU	C-N-CA	5.31	127.96	120.42
3	C	276	VAL	CA-C-N	5.31	127.83	120.29
3	C	276	VAL	C-N-CA	5.31	127.83	120.29
2	B	532	LEU	CA-C-N	5.31	125.87	119.98
2	B	532	LEU	C-N-CA	5.31	125.87	119.98
3	C	308	SER	O-C-N	-5.31	116.10	122.15
4	D	306	GLN	CA-C-N	-5.30	111.42	121.54
4	D	306	GLN	C-N-CA	-5.30	111.42	121.54
7	G	132	GLU	CA-C-N	5.30	131.66	121.54
7	G	132	GLU	C-N-CA	5.30	131.66	121.54
7	G	135	SER	O-C-N	-5.30	113.93	122.41
3	C	180	GLU	O-C-N	-5.30	117.01	123.10
6	F	37	THR	O-C-N	-5.29	117.02	123.16
4	D	418	LEU	O-C-N	5.29	128.18	122.15
6	F	211	VAL	O-C-N	5.29	127.27	121.83
1	A	193	ILE	O-C-N	-5.28	115.83	121.80
1	A	250	VAL	O-C-N	5.28	127.26	121.83
5	E	20	GLU	O-C-N	5.28	127.71	122.12
4	D	570	ALA	CA-C-N	5.27	127.78	120.29
4	D	570	ALA	C-N-CA	5.27	127.78	120.29
3	C	287	LEU	CA-C-N	5.27	127.20	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	287	LEU	C-N-CA	5.27	127.20	120.56
2	B	49	GLU	O-C-N	-5.26	116.06	122.22
4	D	151	SER	O-C-N	-5.26	116.54	122.12
2	B	17	PRO	O-C-N	-5.25	115.82	122.17
3	C	15	LEU	O-C-N	5.25	129.48	123.02
2	B	488	VAL	O-C-N	5.25	127.05	121.91
6	F	191	GLU	O-C-N	-5.25	116.56	122.12
7	G	26	GLU	O-C-N	-5.25	116.03	123.01
4	D	156	GLN	O-C-N	5.24	127.68	122.12
6	F	84	ASP	O-C-N	-5.24	115.44	122.94
6	F	366	ASP	CA-C-N	5.23	128.26	120.31
6	F	366	ASP	C-N-CA	5.23	128.26	120.31
4	D	6	LEU	O-C-N	5.22	127.66	122.12
4	D	30	MET	CA-C-N	5.22	129.44	120.72
4	D	30	MET	C-N-CA	5.22	129.44	120.72
2	B	126	SER	CA-C-N	-5.22	114.26	120.00
2	B	126	SER	C-N-CA	-5.22	114.26	120.00
2	B	350	VAL	O-C-N	5.22	127.32	121.90
5	E	72	GLU	CA-C-N	5.21	127.69	120.29
5	E	72	GLU	C-N-CA	5.21	127.69	120.29
4	D	200	CYS	CA-C-N	5.21	127.26	120.28
4	D	200	CYS	C-N-CA	5.21	127.26	120.28
3	C	312	GLN	O-C-N	-5.20	116.22	122.15
4	D	646	GLN	O-C-N	5.20	128.08	122.15
4	D	399	LYS	CA-C-N	5.20	127.24	120.28
4	D	399	LYS	C-N-CA	5.20	127.24	120.28
7	G	177	PHE	CA-C-N	5.19	126.58	120.09
7	G	177	PHE	C-N-CA	5.19	126.58	120.09
4	D	397	ALA	CA-C-N	-5.19	113.66	120.14
4	D	397	ALA	C-N-CA	-5.19	113.66	120.14
3	C	68	ARG	O-C-N	5.18	127.41	122.07
4	D	58	LYS	O-C-N	5.18	127.41	122.07
3	C	243	ARG	O-C-N	-5.18	115.91	122.17
8	H	158	ASP	CA-C-N	5.16	127.45	120.44
8	H	158	ASP	C-N-CA	5.16	127.45	120.44
3	C	57	ARG	O-C-N	5.15	128.03	122.15
3	C	198	ASP	O-C-N	5.15	127.58	122.12
4	D	305	PRO	O-C-N	-5.15	115.69	122.64
6	F	213	LEU	O-C-N	-5.15	115.94	122.27
2	B	179	SER	O-C-N	-5.12	116.72	123.02
2	B	513	PRO	O-C-N	-5.12	116.09	122.23
2	B	588	GLU	O-C-N	-5.12	115.98	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	181	GLY	O-C-N	-5.12	115.11	122.69
4	D	188	LEU	CA-C-N	5.11	134.28	121.80
4	D	188	LEU	C-N-CA	5.11	134.28	121.80
2	B	354	TYR	O-C-N	5.11	127.33	122.07
8	H	296	SER	O-C-N	-5.11	116.25	122.22
7	G	26	GLU	CA-C-N	5.10	131.82	121.93
7	G	26	GLU	C-N-CA	5.10	131.82	121.93
2	B	249	ASP	CA-C-N	5.09	131.39	121.41
2	B	249	ASP	C-N-CA	5.09	131.39	121.41
2	B	535	GLN	CA-C-N	5.09	128.04	120.31
2	B	535	GLN	C-N-CA	5.09	128.04	120.31
2	B	566	GLU	O-C-N	5.08	127.51	122.12
2	B	22	LEU	O-C-N	-5.07	117.44	123.22
8	H	225	LEU	CA-C-N	5.07	127.62	120.42
8	H	225	LEU	C-N-CA	5.07	127.62	120.42
4	D	135	ARG	O-C-N	5.07	127.29	122.07
1	A	43	ALA	CA-C-N	5.06	127.48	120.29
1	A	43	ALA	C-N-CA	5.06	127.48	120.29
3	C	336	ASP	CA-C-N	5.06	127.47	120.29
3	C	336	ASP	C-N-CA	5.06	127.47	120.29
8	H	326	PHE	O-C-N	-5.06	116.39	122.15
8	H	258	ARG	CA-C-N	5.05	130.80	121.70
8	H	258	ARG	C-N-CA	5.05	130.80	121.70
3	C	343	TRP	CA-C-N	5.05	127.31	120.44
3	C	343	TRP	C-N-CA	5.05	127.31	120.44
1	A	24	TYR	O-C-N	-5.04	116.59	123.15
2	B	553	LYS	O-C-N	-5.04	116.41	122.15
6	F	246	GLN	CA-C-N	5.04	127.03	120.28
6	F	246	GLN	C-N-CA	5.04	127.03	120.28
4	D	30	MET	O-C-N	-5.04	116.41	122.15
2	B	186	GLU	CA-C-N	5.03	131.15	121.54
2	B	186	GLU	C-N-CA	5.03	131.15	121.54
5	E	107	SER	O-C-N	5.03	127.45	122.12
1	A	194	HIS	CA-C-N	-5.02	113.55	120.28
1	A	194	HIS	C-N-CA	-5.02	113.55	120.28
4	D	275	ASP	CA-C-N	5.02	129.17	120.58
4	D	275	ASP	C-N-CA	5.02	129.17	120.58
1	A	214	LEU	CA-C-N	5.02	127.34	120.46
1	A	214	LEU	C-N-CA	5.02	127.34	120.46
6	F	46	ASN	CA-C-N	5.02	127.51	120.28
6	F	46	ASN	C-N-CA	5.02	127.51	120.28
2	B	1	MET	O-C-N	-5.01	114.99	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	211	HIS	CA-C-N	5.00	126.98	120.28
4	D	211	HIS	C-N-CA	5.00	126.98	120.28
6	F	202	GLN	CA-C-N	5.00	127.52	120.42
6	F	202	GLN	C-N-CA	5.00	127.52	120.42

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	Peptide,Mainchain
1	A	275	PHE	Peptide,Mainchain
1	A	276	VAL	Peptide
1	A	278	PRO	Peptide,Mainchain
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	Peptide,Mainchain
2	B	231	GLY	Peptide,Mainchain
2	B	232	SER	Mainchain
2	B	233	ASP	Peptide,Mainchain
2	B	234	GLU	Mainchain
2	B	235	ASN	Mainchain
2	B	236	PHE	Mainchain
2	B	238	LEU	Mainchain

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Mol	Chain	Res	Type	Group
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	Peptide,Mainchain
2	B	247	GLY	Mainchain
2	B	249	ASP	Mainchain
2	B	250	GLY	Mainchain
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	Peptide,Mainchain
2	B	596	SER	Peptide,Mainchain
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

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Mol	Chain	Res	Type	Group
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	Peptide,Mainchain
4	D	118	ASP	Mainchain
4	D	119	LEU	Mainchain
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	Peptide,Mainchain
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	Peptide,Mainchain
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

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Mol	Chain	Res	Type	Group
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	Peptide,Mainchain
5	E	221	HIS	Peptide,Mainchain
5	E	3	ALA	Mainchain
5	E	38	LEU	Mainchain
5	E	39	GLU	Mainchain
5	E	4	ALA	Mainchain
5	E	5	ASN	Mainchain
6	F	1	MET	Peptide,Mainchain
6	F	122	GLY	Mainchain
6	F	146	ALA	Mainchain
6	F	159	SER	Mainchain
6	F	2	GLN	Peptide,Mainchain
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	Peptide,Mainchain
7	G	132	GLU	Mainchain
7	G	133	SER	Peptide,Mainchain
7	G	134	LEU	Mainchain

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Mol	Chain	Res	Type	Group
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
7	G	28	VAL	Mainchain
7	G	3	GLY	Mainchain
8	H	156	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2360	224	0
2	B	4771	0	4788	446	0
3	C	2885	0	2956	245	0
4	D	5415	0	5447	551	0
5	E	1717	0	1723	200	0
6	F	3171	0	3250	267	0
7	G	2687	0	2656	266	0
8	H	1671	0	1682	218	0
All	All	24599	0	24862	1557	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 (1557) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:114:GLN:CD	7:G:277:PHE:CZ	1.86	1.46
1:A:283:ARG:C	1:A:284:ARG:N	1.70	1.46
1:A:284:ARG:C	1:A:285:LEU:N	1.69	1.46
1:A:280:PRO:C	1:A:281:SER:N	1.75	1.45
6:F:247:MET:HB2	8:H:240:LYS:NZ	1.23	1.44
8:H:294:MET:HE1	8:H:298:ALA:CB	1.46	1.44
4:D:288:SER:C	4:D:289:GLU:N	1.78	1.42
1:A:189:TYR:CD1	3:C:271:MET:HE1	1.54	1.41
1:A:71:ASP:HB3	3:C:114:ARG:NH2	1.18	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
2:B:223:GLU:C	2:B:224:GLY:N	1.81	1.39
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
1:A:277:VAL:C	1:A:278:PRO:N	1.79	1.38
2:B:138:LYS:CD	3:C:84:GLN:NE2	1.86	1.38
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: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
4:D:307:GLU:CD	7:G:324:ILE:HD11	1.50	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
2:B:138:LYS:HD2	3:C:84:GLN:CD	1.56	1.30
1:A:277:VAL:O	1:A:278:PRO:C	1.74	1.30
1:A:145:THR:HG21	4:D:69:LEU:CD1	1.61	1.30
3:C:118:ALA:C	3:C:120:SER:H	1.40	1.30
8:H:259:HIS:C	8:H:291:GLU:HG2	1.54	1.30
3:C:63:ARG:NH2	4:D:535:ALA:HB2	1.43	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
4:D:662:THR:C	4:D:664:SER:H	1.32	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:307:GLU:CD	7:G:324:ILE:CD1	2.08	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
6:F:263:ARG:C	7:G:279:GLN:NE2	1.93	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
5:E:106:ARG:HH11	7:G:271:MET:CA	1.49	1.26
2:B:97:ILE:HD12	4:D:82:GLN:CD	1.61	1.25
2:B:120:LYS:NZ	3:C:171:SER:O	1.70	1.25
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
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:OE2	7:G:324:ILE:HD12	1.39	1.21
2:B:138:LYS:HE3	3:C:84:GLN:NE2	1.52	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
8:H:259:HIS:C	8:H:291:GLU:CG	2.15	1.19
2:B:138:LYS:CD	3:C:84:GLN:HE22	1.48	1.19
1:A:148:LEU:HD13	2:B:80:VAL:CG2	1.72	1.19
6:F:260:ALA:HB1	8:H:258:ARG:NH1	1.55	1.19
6:F:260:ALA:CB	8:H:258:ARG:HH12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:E:106:ARG:HH11	7:G:271:MET:C	1.45	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
1:A:278:PRO:HB3	1:A:279:GLU:HG3	1.29	1.15
7:G:143:VAL:CG2	8:H:159:MET:HE1	1.76	1.14
6:F:377:ARG:HH12	8:H:343:GLN:CA	1.60	1.14
4:D:307:GLU:OE2	7:G:324:ILE:CD1	1.92	1.14
6:F:377:ARG:NH1	8:H:343:GLN:HA	1.62	1.14
2:B:55:ASP:CG	4:D:49:HIS:HE1	1.56	1.13
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
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
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
1:A:152:LYS:NZ	2:B:73:ASP:CG	2.09	1.11
5:E:106:ARG:NH1	7:G:271:MET:C	1.95	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
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
6:F:44:GLY:H	6:F:47:MET:HE2	1.03	1.10
8:H:359:GLN:CG	8:H:363:ASP:OD2	2.00	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:CD1	3:C:271:MET:CE	2.34	1.09
2:B:138:LYS:CD	3:C:84:GLN:CD	2.20	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
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
6:F:206:MET:HE1	8:H:199:LYS:CG	1.83	1.08
7:G:312:ARG:HH12	8:H:323:ALA:HB2	1.07	1.08
2:B:175:MET:HG3	4:D:460:PRO:HG3	1.27	1.08
5:E:60:ASN:HB3	8:H:207:HIS:NE2	1.68	1.08
4:D:662:THR:C	4:D:664:SER:N	1.95	1.07
2:B:97:ILE:HD11	4:D:82:GLN:CB	1.84	1.07
8:H:294:MET:CE	8:H:298:ALA:CB	2.29	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
5:E:104:GLU:OE2	5:E:124:GLU:OE2	1.71	1.06
5:E:104:GLU:CD	5:E:124:GLU:CD	2.23	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
6:F:206:MET:CE	8:H:199:LYS:HG3	1.84	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
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
6:F:247:MET:CB	8:H:240:LYS:NZ	2.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:138:LYS:CE	3:C:84:GLN:CD	2.31	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:55:ASP:CG	4:D:49:HIS:CE1	2.36	1.02
2:B:138:LYS:HG3	3:C:84:GLN:NE2	1.73	1.02
2:B:131:MET:HE3	3:C:85:VAL:HG21	1.40	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
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
7:G:143:VAL:HG22	8:H:159:MET:HE1	1.04	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:236:ARG:HH12	4:D:575:THR:HA	1.22	0.99
7:G:274:MET:HE1	8:H:280:GLN:N	1.78	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
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
1:A:189:TYR:HD1	3:C:271:MET:HE1	0.86	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
4:D:175:PHE:CD1	4:D:193:LEU:HD21	1.98	0.98
6:F:263:ARG:C	7:G:279:GLN:HE22	1.71	0.97
5:E:49:LEU:HD23	8:H:196:ASN:HD22	1.24	0.97
2:B:443:ASP:CG	4:D:509:ARG:HH22	1.72	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:H:259:HIS:C	8:H:291:GLU:CD	2.35	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
3:C:118:ALA:C	3:C:120:SER:N	2.07	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
5:E:114:GLN:CD	7:G:277:PHE:HZ	1.38	0.94
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
1:A:1:MET:HE1	1:A:28:THR:HG22	1.50	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
6:F:206:MET:HE1	8:H:199:LYS:HG3	0.95	0.94
2:B:91:ALA:O	2:B:93:GLU:N	2.01	0.94
2:B:443:ASP:CG	4:D:509:ARG:NH2	2.26	0.94
6:F:326:ARG:NH1	8:H:295:PRO:CD	2.12	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:E:104:GLU:CD	5:E:124:GLU:OE2	2.12	0.92
5:E:181:GLU:CD	7:G:335:ARG:HH12	1.78	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
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
1:A:189:TYR:HA	3:C:271:MET:HE2	1.51	0.92
2:B:131:MET:HE1	3:C:85:VAL:HG21	1.49	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
7:G:274:MET:HE1	8:H:280:GLN:HB2	1.51	0.92
2:B:134:LYS:CD	3:C:85:VAL:HG13	2.00	0.92
6:F:247:MET:CB	8:H:240:LYS:HZ1	1.80	0.91
7:G:131:LEU:O	7:G:132:GLU:C	2.04	0.91
4:D:197:ARG:HG2	4:D:201:LYS:HE3	1.49	0.91
2:B:347:MET:HE2	4:D:403:MET:SD	2.11	0.91
2:B:407:VAL:CG2	4:D:459:TRP:CZ3	2.53	0.91
2:B:97:ILE:CD1	4:D:82:GLN:CD	2.44	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
6:F:260:ALA:HB3	8:H:258:ARG:NH1	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:376:MET:HE1	4:D:211:HIS:HB2	1.51	0.89
3:C:18:ASP:OD1	3:C:21:ASP:CG	2.15	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
1:A:145:THR:HG23	4:D:65:TRP:CZ2	2.07	0.89
1:A:189:TYR:HD1	3:C:271:MET:CE	1.77	0.89
2:B:55:ASP:OD1	4:D:49:HIS:HE1	1.39	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
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
6:F:44:GLY:N	6:F:47:MET:HE2	1.89	0.88
2:B:74:GLU:OE1	4:D:54:ARG:HG3	1.73	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
8:H:359:GLN:HG2	8:H:363:ASP:CG	1.98	0.87
2:B:507:LEU:HD12	4:D:579:THR:HG22	1.55	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
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:134:LYS:HD3	3:C:85:VAL:HG13	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:263:ARG:C	7:G:279:GLN:CD	2.42	0.86
6:F:326:ARG:NH2	7:G:291:GLU:OE2	2.07	0.86
6:F:377:ARG:HH22	8:H:343:GLN:CD	1.83	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
4:D:304:ASP:C	4:D:306:GLN:H	1.83	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
1:A:99:CYS:HB3	3:C:67:MET:HE2	1.58	0.85
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
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
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
5:E:104:GLU:OE1	5:E:124:GLU:CD	2.19	0.84
5:E:104:GLU:CD	5:E:127:TYR:CE2	2.56	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
7:G:274:MET:HE1	8:H:280:GLN:CB	2.08	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:247:MET:HB2	8:H:240:LYS:HZ1	1.03	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

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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	0.83
5:E:181:GLU:CD	7:G:335:ARG:NH1	2.37	0.83
7:G:41:CYS:HA	7:G:47:ARG:HH12	1.40	0.83
1:A:152:LYS:HZ1	2:B:73:ASP:CG	1.78	0.83
2:B:131:MET:HE2	3:C:85:VAL:HG21	1.61	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:HE1	8:H:243:PHE:HD1	1.41	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
2:B:96:ALA:C	2:B:98:GLU:N	2.34	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
5:E:106:ARG:NH1	7:G:271:MET:CA	2.32	0.82
7:G:274:MET:HE1	8:H:280:GLN:H	1.43	0.82
2:B:96:ALA:C	2:B:98:GLU:H	1.86	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
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
7:G:280:PHE:CD1	8:H:287:LYS:HG3	2.15	0.81
7:G:274:MET:CE	8:H:280:GLN:CB	2.58	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
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
2:B:94:GLU:CD	4:D:79:GLU:OE2	2.17	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
2:B:222:PHE:CD1	2:B:241:LEU:CD1	2.58	0.81
2:B:456:ASP:C	2:B:458:THR:H	1.88	0.81
6:F:247:MET:HB2	8:H:240:LYS:HZ2	1.01	0.81
1:A:235:LEU:HD11	3:C:313:ILE:CG2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:152:LYS:HZ2	2:B:73:ASP:CG	1.79	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
1:A:1:MET:HE1	1:A:28:THR:CG2	2.11	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
4:D:4:ARG:HG3	4:D:32:GLN:HE21	1.43	0.79
1:A:277:VAL:C	1:A:278:PRO:CA	2.55	0.79
2:B:276:MET:HE3	4:D:334:GLN:HG2	1.65	0.79
2:B:407:VAL:HG21	4:D:459:TRP:CE3	2.17	0.79
6:F:359:ARG:HG3	8:H:328:GLN:CD	2.07	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
7:G:274:MET:HE1	8:H:280:GLN:CA	2.12	0.78
4:D:211:HIS:CE1	4:D:215:ILE:CD1	2.65	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
5:E:106:ARG:O	7:G:273:PRO:HB3	1.84	0.78
6:F:377:ARG:HH22	8:H:343:GLN:HG3	1.46	0.78
5:E:111:ARG:HH22	7:G:280:PHE:HB2	1.48	0.78
6:F:247:MET:CB	8:H:240:LYS:HZ2	1.85	0.78
6:F:325:GLU:OE2	6:F:325:GLU:CA	2.26	0.78
2:B:376:MET:HE1	4:D:211:HIS:CB	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:305:PRO:C	4:D:307:GLU:H	1.91	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
1:A:211:HIS:HA	4:D:630:VAL:HG23	1.65	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
3:C:5:LEU:CD1	3:C:22:LEU:HD12	2.15	0.77
4:D:185:SER:OG	4:D:187:PHE:CE2	2.37	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
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
4:D:528:VAL:CG1	4:D:546:MET:SD	2.73	0.76
2:B:87:SER:C	2:B:89:VAL:H	1.93	0.76
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:5:SER:HA	1:A:31:MET:HE1	1.67	0.76
1:A:189:TYR:HA	3:C:271:MET:CE	2.15	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
4:D:280:PRO:O	4:D:281:SER:C	2.09	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
3:C:133:ASP:OD1	3:C:136:ASP:CG	2.28	0.76
4:D:211:HIS:CE1	4:D:215:ILE:HD11	2.21	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
8:H:294:MET:HE1	8:H:298:ALA:HB3	0.77	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:68:GLN:O	4:D:72:THR:OG1	2.04	0.75
2:B:490:GLU:HG2	4:D:560:ARG:NH1	2.01	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:131:MET:HE1	3:C:85:VAL:CG2	2.13	0.75
2:B:424:LEU:CD2	4:D:484:ILE:HD11	2.15	0.75
3:C:123:PRO:C	3:C:125:ASP:H	1.93	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
2:B:120:LYS:NZ	3:C:171:SER:C	2.45	0.74
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
4:D:189:GLU:CD	4:D:197:ARG:HH12	1.95	0.74
1:A:33:ILE:HG23	3:C:15:LEU:HD22	1.68	0.74
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
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
6:F:224:ASP:CG	6:F:227:ILE:HD11	2.12	0.73
2:B:166:SER:CB	4:D:152:ASN:ND2	2.50	0.73
1:A:99:CYS:CB	3:C:67:MET:HE2	2.18	0.73
2:B:42:TRP:CD2	4:D:20:LEU:HD13	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:130:ILE:CG2	7:G:131:LEU:N	2.49	0.73
6:F:297:MET:HE1	6:F:314:LEU:HG	1.69	0.72
2:B:132:CYS:SG	4:D:119:LEU:CD1	2.76	0.72
5:E:107:SER:CB	7:G:276:PRO:CD	2.57	0.72
1:A:228:SER:HA	3:C:307:LEU:HD12	1.71	0.72
2:B:456:ASP:C	2:B:458:THR:N	2.48	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
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
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: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
2:B:87:SER:C	2:B:89:VAL:N	2.48	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
4:D:189:GLU:CD	4:D:197:ARG:NH1	2.48	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
1:A:64:ALA:HB1	4:D:492:VAL:CG1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:289:GLU:C	4:D:291:ILE:H	1.98	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
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
3:C:123:PRO:C	3:C:125:ASP:N	2.50	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: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
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
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
2:B:513:PRO:HG2	2:B:519:MET:HE2	1.75	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:138:THR:HG1	2:B:92:ILE:CD1	2.01	0.69
1:A:172:VAL:CG1	3:C:253:ILE:HG21	2.22	0.69
2:B:205:LEU:HD22	4:D:259:LEU:HD21	1.75	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
2:B:195:SER:O	2:B:196:GLN:C	2.33	0.68
4:D:177:ALA:CB	4:D:256:ARG:NH2	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:ASN:HB3	4:D:299:GLU:HB3	1.73	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
1:A:275:PHE:O	1:A:276:VAL:C	2.32	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
5:E:114:GLN:CD	7:G:277:PHE:CE1	2.60	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
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
2:B:35:ASP:HB3	4:D:30:MET:HE1	1.76	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
6:F:44:GLY:O	6:F:47:MET:HE3	1.95	0.67
2:B:138:LYS:HE3	3:C:84:GLN:CD	2.09	0.67
2:B:216:PHE:CE2	4:D:272:GLN:OE1	2.47	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
1:A:270:VAL:HA	1:A:273:MET:HE3	1.76	0.67
3:C:129:ILE:HD11	4:D:489:LEU:HD22	1.76	0.67
4:D:185:SER:C	4:D:187:PHE:H	2.03	0.67
5:E:47:GLU:HG3	6:F:195:LYS:HZ3	1.59	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
7:G:274:MET:HE2	8:H:280:GLN:HB2	1.73	0.67
4:D:195:ASP:O	4:D:199:VAL:HG23	1.95	0.67
6:F:9:LEU:HD21	6:F:124:PRO:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:GLU:CD	4:D:54:ARG:HG3	2.21	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
5:E:97:HIS:CD2	8:H:247:TYR:HH	2.12	0.66
6:F:224:ASP:O	6:F:225:ARG:C	2.25	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
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
2:B:2:SER:OG	2:B:28:ASP:CG	2.39	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
2:B:272:LYS:HE3	2:B:276:MET:HE2	1.79	0.65
6:F:176:GLN:CD	7:G:117:ASP:HB3	2.22	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
2:B:77:LEU:HD21	4:D:61:GLY:C	2.21	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:120:LYS:NZ	3:C:175:PRO:HA	2.11	0.65
5:E:221:HIS:HB3	5:E:222:PRO:C	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:192:TYR:OH	7:G:173:TRP:NE1	2.27	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
2:B:482:MET:HE3	4:D:554:ARG:HG2	1.79	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
2:B:91:ALA:C	2:B:93:GLU:N	2.56	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:245:SER:O	2:B:246:PHE:C	2.32	0.64
4:D:304:ASP:C	4:D:306:GLN:N	2.45	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
2:B:81:LEU:O	2:B:84:PHE:HB2	1.98	0.64
2:B:513:PRO:HG2	2:B:519:MET:HE3	1.77	0.64
3:C:133:ASP:OD1	3:C:136:ASP:OD2	2.16	0.64
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
6:F:44:GLY:H	6:F:47:MET:CE	1.95	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:247:MET:HE1	8:H:243:PHE:CD1	2.27	0.63
6:F:295:LEU:HD21	6:F:317:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:130:ASN:HB3	3:C:213:MET:HE1	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
4:D:601:MET:HE2	4:D:604:LEU:HD12	1.79	0.62
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
6:F:170:ARG:CG	7:G:89:MET:HE2	2.29	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
4:D:306:GLN:C	4:D:307:GLU:O	2.43	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:114:GLN:NE2	7:G:277:PHE:CZ	2.63	0.62
3:C:128:SER:OG	3:C:132:LEU:O	2.12	0.61
5:E:179:MET:CG	8:H:329:ILE:CD1	2.77	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:LEU:HD21	3:C:261:LYS:CG	2.30	0.61
6:F:92:ARG:HH12	6:F:119:LEU:C	2.08	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
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
1:A:130:ASN:CB	3:C:213:MET:HE1	2.31	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
1:A:78:GLY:O	1:A:81:TYR:HD1	1.84	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
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
2:B:35:ASP:CB	4:D:30:MET:HE3	2.31	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
4:D:307:GLU:CD	7:G:324:ILE:HD12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:F:359:ARG:CG	8:H:328:GLN:CD	2.70	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: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
6:F:173:LEU:CD2	7:G:90:LEU:HD21	2.33	0.59
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
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
7:G:123:ASP:O	7:G:124:THR:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:LEU:HB3	5:E:136:PRO:CD	2.29	0.58
8:H:294:MET:CE	8:H:298:ALA:HB2	2.28	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
2:B:199:LEU:O	2:B:200:ASP:C	2.47	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:195:SER:O	2:B:197:LEU:N	2.36	0.58
2:B:344:LEU:HD22	2:B:347:MET:CE	2.34	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:99:CYS:HB3	3:C:67:MET:CE	2.32	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:195:SER:C	2:B:197:LEU:N	2.61	0.57
2:B:588:GLU:CD	4:D:650:ARG:HH21	2.11	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
5:E:178:GLU:OE2	7:G:331:MET:HE3	2.04	0.57
7:G:131:LEU:C	7:G:132:GLU:O	2.46	0.57
2:B:97:ILE:HD12	4:D:82:GLN:NE2	2.17	0.57
7:G:280:PHE:CE2	8:H:258:ARG:C	2.83	0.57
7:G:142:VAL:HG13	8:H:163:ILE:HD11	1.86	0.57
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:6:ARG:C	6:F:8:HIS:H	2.12	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:120:LYS:HZ3	3:C:171:SER:C	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:418:GLU:O	2:B:422:THR:HG23	2.05	0.56
4:D:601:MET:HE2	4:D:601:MET:HA	1.85	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
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
2:B:490:GLU:C	4:D:560:ARG:NH2	2.59	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
1:A:228:SER:CA	3:C:307:LEU:HD12	2.36	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
4:D:661:ALA:C	4:D:663:GLY:H	2.14	0.56
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
4:D:189:GLU:OE2	4:D:197:ARG:NH1	2.38	0.56
5:E:104:GLU:CD	5:E:124:GLU:OE1	2.48	0.56
6:F:170:ARG:HG2	7:G:89:MET:HE2	1.88	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
6:F:377:ARG:NH2	8:H:343:GLN:CD	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:180:GLU:CD	3:C:188:LYS:HZ2	2.14	0.55
4:D:185:SER:C	4:D:187:PHE:N	2.61	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
7:G:93:PHE:CE2	7:G:94:ASP:CG	2.85	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
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
2:B:402:GLU:CD	4:D:158:ARG:NH2	2.66	0.54
2:B:511:MET:C	2:B:513:PRO:HD3	2.33	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
4:D:575:THR:O	4:D:577:PRO:C	2.51	0.54
6:F:157:LEU:CA	6:F:170:ARG:HH22	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:601:MET:HE1	4:D:604:LEU:HD12	1.90	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
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
3:C:351:SER:C	3:C:353:PRO:HD2	2.32	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
3:C:63:ARG:NH1	4:D:537:GLU:CD	2.67	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
2:B:80:VAL:O	2:B:83:THR:OG1	2.21	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
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
2:B:94:GLU:O	2:B:95:VAL:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:507:LEU:HD11	4:D:579:THR:CG2	2.33	0.53
7:G:2:THR:HG21	7:G:37:TYR:CZ	2.44	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
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
5:E:107:SER:HA	7:G:273:PRO:C	2.34	0.52
6:F:326:ARG:NH1	8:H:295:PRO:HG3	2.24	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
1:A:205:MET:HE1	1:A:209:LEU:C	2.34	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
1:A:152:LYS:CE	2:B:73:ASP:CG	2.83	0.52
2:B:220:HIS:O	2:B:367:ARG:NH1	2.43	0.52
2:B:251:THR:C	2:B:253:GLU:N	2.63	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
5:E:154:THR:HG21	7:G:299:THR:HG21	1.92	0.52
6:F:44:GLY:O	6:F:47:MET:CE	2.57	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: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
2:B:344:LEU:HD22	2:B:347:MET:HE1	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
4:D:210:LEU:CD2	4:D:227:ARG:NH1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:197:ARG:HD2	4:D:201:LYS:HZ1	1.75	0.52
1:A:171:LYS:HE2	1:A:175:ARG:CZ	2.40	0.51
2:B:89:VAL:O	2:B:90:PRO:C	2.50	0.51
2:B:454:ASP:C	2:B:456:ASP:H	2.17	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
6:F:240:MET:HE1	8:H:230:ASP:OD1	2.10	0.51
1:A:24:TYR:HB3	3:C:31:VAL:HG21	1.92	0.51
6:F:156:ALA:C	6:F:170:ARG:HH22	2.19	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
6:F:182:LEU:CD1	8:H:177:MET:HE1	2.40	0.51
8:H:259:HIS:O	8:H:291:GLU:HB3	2.10	0.51
1:A:189:TYR:CA	3:C:271:MET:HE2	2.30	0.51
1:A:280:PRO:CA	1:A:281:SER:N	2.67	0.51
2:B:386:GLN:NE2	4:D:440:GLN:CD	2.69	0.51
3:C:285:LYS:HZ1	4:D:628:GLN:HE22	1.57	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:242:ALA:C	1:A:244:ASN:H	2.19	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
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
2:B:482:MET:HE3	4:D:554:ARG:CG	2.41	0.51
6:F:297:MET:HE3	6:F:313:GLN:HB2	1.91	0.51
7:G:143:VAL:HG23	8:H:159:MET:HE1	1.85	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
4:D:117:GLN:O	4:D:118:ASP:C	2.54	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
4:D:661:ALA:C	4:D:663:GLY:N	2.69	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
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
2:B:93:GLU:O	2:B:94:GLU:C	2.50	0.50
2:B:259:MET:CE	2:B:346:ASN:HB3	2.41	0.50
6:F:251:MET:HE3	8:H:247:TYR:CD1	2.46	0.50
4:D:185:SER:HG	4:D:187:PHE:HD2	0.63	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
7:G:123:ASP:C	7:G:124:THR:O	2.53	0.50
2:B:361:GLN:HE22	4:D:413:ILE:HG23	1.77	0.50
1:A:152:LYS:HE3	2:B:73:ASP:OD1	2.11	0.50
2:B:482:MET:HE3	4:D:554:ARG:HE	1.77	0.50
5:E:79:THR:HG21	8:H:222:LEU:CD1	2.42	0.50
2:B:458:THR:C	2:B:460:LYS:N	2.69	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
2:B:125:GLU:CD	4:D:113:GLU:OE2	2.46	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
3:C:1:MET:HE1	3:C:23:GLU:HA	1.94	0.49
2:B:37:LYS:N	2:B:38:PRO:CD	2.75	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
8:H:156:PRO:C	8:H:158:ASP:N	2.70	0.49
2:B:225:MET:O	2:B:226:SER:C	2.50	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
3:C:303:GLU:OE2	3:C:303:GLU:CA	2.58	0.49
5:E:104:GLU:CD	5:E:126:SER:OG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:H:156:PRO:C	8:H:158:ASP:H	2.20	0.49
2:B:374:HIS:CE1	4:D:265:LEU:HD11	2.48	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
3:C:36:CYS:N	3:C:37:PRO:HD2	2.28	0.48
1:A:40:TRP:CH2	3:C:43:GLY:HA3	2.48	0.48
2:B:243:VAL:HG12	2:B:243:VAL:O	2.12	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: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
3:C:209:LYS:HG2	3:C:213:MET:HE2	1.95	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
2:B:500:LEU:CD2	4:D:571:LEU:HD11	2.43	0.48
1:A:99:CYS:CB	3:C:67:MET:CE	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:LEU:HD13	6:F:381:TRP:CZ2	2.45	0.48
3:C:63:ARG:CZ	4:D:535:ALA:HB1	2.37	0.48
6:F:138:MET:HE1	8:H:169:LEU:HA	1.95	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
5:E:94:MET:HE1	6:F:251:MET:HE2	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
6:F:182:LEU:HD12	8:H:177:MET:HE1	1.95	0.48
5:E:111:ARG:NH2	7:G:280:PHE:HB2	2.24	0.47
6:F:138:MET:HE1	8:H:169:LEU:HD23	1.96	0.47
7:G:137:SER:C	7:G:139:GLU:H	2.22	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:190:GLN:CD	4:D:170:GLN:HA	2.39	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
1:A:271:ASN:C	1:A:273:MET:N	2.69	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: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
2:B:51:ASN:HD22	4:D:18:MET:HE1	1.79	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)
1:A:123:LEU:O	1:A:126:ILE:HG22	2.15	0.47
2:B:89:VAL:C	2:B:90:PRO:O	2.58	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
3:C:180:GLU:CD	3:C:184:LEU:HD23	2.40	0.47
6:F:288:ILE:CD1	6:F:314:LEU:CD2	2.93	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:251:MET:HE1	8:H:243:PHE:CE1	2.50	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
4:D:289:GLU:C	4:D:291:ILE:N	2.58	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
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
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
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
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: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
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
2:B:430:LEU:C	2:B:431:SER:O	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:135:SER:O	7:G:136:HIS:C	2.52	0.46
8:H:259:HIS:C	8:H:291:GLU:CB	2.87	0.46
2:B:86:ILE:HG22	2:B:86:ILE:O	2.14	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:93:GLU:C	2:B:94:GLU:O	2.58	0.45
2:B:330:SER:O	2:B:335:PRO:HD3	2.16	0.45
2:B:432:ALA:C	2:B:433:SER:O	2.57	0.45
4:D:46:ILE:HA	4:D:50:ILE:HD12	1.99	0.45
5:E:207:CYS:O	5:E:208:ILE:C	2.58	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:162:PHE:O	7:G:165:THR:OG1	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:180:GLU:CD	3:C:188:LYS:NZ	2.75	0.45
4:D:172:GLU:C	4:D:173:VAL:HG23	2.41	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
4:D:120:ASN:C	4:D:122:GLU:H	2.25	0.45
6:F:64:PHE:CD1	6:F:98:TRP:CE3	3.05	0.45
7:G:127:SER:C	7:G:129:VAL:N	2.75	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
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
6:F:224:ASP:CG	8:H:216:LEU:HD21	2.39	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
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
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
7:G:188:GLN:O	7:G:192:THR:OG1	2.35	0.44
8:H:358:ARG:HH21	8:H:366:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:84:ASP:OD1	6:F:87:ARG:HD2	2.16	0.44
7:G:340:ALA:O	7:G:344:SER:OG	2.34	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
4:D:172:GLU:HB2	4:D:249:HIS:HE2	1.82	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
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:206:GLU:C	1:A:208:PRO:HD2	2.43	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
5:E:111:ARG:NH1	7:G:276:PRO:C	2.75	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
6:F:247:MET:HE2	8:H:243:PHE:CD1	2.51	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:190:GLN:OE1	4:D:169:SER:C	2.61	0.43
2:B:407:VAL:HG23	4:D:459:TRP:CZ3	2.50	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:GLN:NE2	7:G:277:PHE:CE1	2.85	0.43
7:G:176:ASP:OD1	7:G:176:ASP:N	2.50	0.43
1:A:277:VAL:C	1:A:278:PRO:CD	2.79	0.43
2:B:35:ASP:HB2	4:D:30:MET:HE3	2.00	0.43
2:B:85:SER:C	2:B:87:SER:N	2.73	0.43
2:B:588:GLU:OE1	4:D:650:ARG:NE	2.48	0.43
3:C:118:ALA:O	3:C:119:ASP:C	2.48	0.43
4:D:293:GLN:HE21	4:D:295:ARG:HB2	1.84	0.43
4:D:305:PRO:C	4:D:307:GLU:N	2.52	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:90:PRO:O	2:B:91:ALA:C	2.61	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
2:B:96:ALA:O	2:B:97:ILE:C	2.62	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:183:THR:C	2:B:185:CYS:N	2.77	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: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
4:D:663:GLY:C	4:D:665:ARG:N	2.76	0.43
7:G:280:PHE:CE2	8:H:258:ARG:HA	2.54	0.43
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
5:E:103:ARG:O	5:E:124:GLU:OE1	2.36	0.42
2:B:229:VAL:O	2:B:230:GLU:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:ARG:NH1	7:G:272:SER:N	2.61	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:104:GLU:HA	5:E:124:GLU:CD	2.44	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
1:A:284:ARG:O	1:A:285:LEU:N	2.38	0.42
4:D:352:HIS:CB	4:D:366:ARG:NH2	2.37	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
2:B:456:ASP:O	2:B:458:THR:N	2.51	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
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:454:ASP:C	2:B:456:ASP:N	2.78	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)
1:A:281:SER:O	1:A:282:LYS:C	2.22	0.41
2:B:247:GLY:C	2:B:249:ASP:N	2.77	0.41
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: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
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
2:B:200:ASP:O	2:B:201:LYS:C	2.63	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: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
6:F:297:MET:HE1	6:F:314:LEU:CG	2.45	0.41
1:A:3:GLU:O	1:A:6:THR:OG1	2.37	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:51:ASN:ND2	4:D:18:MET:HE1	2.36	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

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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: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
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
4:D:601:MET:HE1	4:D:604:LEU:CD1	2.50	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
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
7:G:280:PHE:HE2	8:H:258:ARG:C	2.14	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
1:A:270:VAL:CA	1:A:273:MET:HE3	2.47	0.40
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: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
5:E:9:PRO:HB3	6:F:197:GLN:CD	2.44	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
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
1:A:4:LYS:HG2	1:A:35:TYR:CE2	2.56	0.40
1:A:189:TYR:CD1	3:C:271:MET:HE3	2.45	0.40
2:B:78:ASP:O	2:B:82:LYS:HG3	2.22	0.40
2:B:199:LEU:O	2:B:201:LYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	4	26
2	B	595/597 (100%)	542 (91%)	18 (3%)	35 (6%)	1	13
3	C	351/353 (99%)	338 (96%)	7 (2%)	6 (2%)	7	36
4	D	662/666 (99%)	622 (94%)	19 (3%)	21 (3%)	3	21
5	E	213/222 (96%)	203 (95%)	5 (2%)	5 (2%)	5	28
6	F	383/978 (39%)	365 (95%)	9 (2%)	9 (2%)	5	28
7	G	335/348 (96%)	311 (93%)	9 (3%)	15 (4%)	2	17
8	H	199/367 (54%)	197 (99%)	1 (0%)	1 (0%)	24	63
All	All	3022/3817 (79%)	2851 (94%)	72 (2%)	99 (3%)	5	21

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	244 (94%)	16 (6%)	16	38
2	B	541/541 (100%)	505 (93%)	36 (7%)	15	36
3	C	326/326 (100%)	310 (95%)	16 (5%)	22	43
4	D	605/605 (100%)	566 (94%)	39 (6%)	16	37
5	E	190/195 (97%)	179 (94%)	11 (6%)	18	40
6	F	343/882 (39%)	328 (96%)	15 (4%)	25	47
7	G	313/320 (98%)	292 (93%)	21 (7%)	15	36
8	H	192/328 (58%)	186 (97%)	6 (3%)	35	56
All	All	2770/3457 (80%)	2610 (94%)	160 (6%)	20	40

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	28	THR
1	A	32	GLU
1	A	153	SER
1	A	200	LEU
1	A	217	LEU
1	A	218	SER
1	A	220	THR
1	A	223	GLU
1	A	224	LEU
1	A	239	LEU
1	A	246	SER
1	A	262	THR
1	A	266	LEU
1	A	268	THR
1	A	285	LEU
2	B	30	LEU
2	B	36	LEU
2	B	45	SER

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Mol	Chain	Res	Type
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	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	521	THR
2	B	536	LEU
2	B	547	LEU
2	B	550	LEU
2	B	587	LEU
2	B	591	THR
3	C	5	LEU
3	C	60	LEU
3	C	92	LEU
3	C	120	SER
3	C	141	LEU
3	C	158	LEU
3	C	176	GLU
3	C	269	LEU
3	C	303	GLU

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Mol	Chain	Res	Type
3	C	305	GLN
3	C	307	LEU
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	6	LEU
4	D	64	LEU
4	D	69	LEU
4	D	72	THR
4	D	73	GLU
4	D	77	THR
4	D	83	GLN
4	D	122	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	355	LEU
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
4	D	594	LEU
4	D	636	SER
4	D	648	ARG

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Mol	Chain	Res	Type
4	D	656	THR
4	D	658	LEU
4	D	662	THR
4	D	664	SER
5	E	18	LEU
5	E	28	LEU
5	E	38	LEU
5	E	69	LEU
5	E	121	LEU
5	E	206	SER
5	E	207	CYS
5	E	209	THR
5	E	212	THR
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	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	71	GLU
7	G	74	THR
7	G	124	THR
7	G	127	SER
7	G	134	LEU
7	G	135	SER
7	G	138	THR

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Mol	Chain	Res	Type
7	G	139	GLU
7	G	180	LEU
7	G	192	THR
7	G	226	SER
7	G	229	THR
7	G	238	LEU
7	G	322	SER
7	G	344	SER
7	G	346	LEU
8	H	202	LEU
8	H	204	GLU
8	H	213	LEU
8	H	216	LEU
8	H	254	LEU
8	H	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
2	B	114	HIS
2	B	190	GLN
2	B	263	GLN
2	B	271	HIS
2	B	346	ASN
2	B	361	GLN
2	B	374	HIS
2	B	386	GLN
2	B	493	HIS
2	B	579	GLN
3	C	174	GLN
3	C	220	GLN
3	C	247	GLN
4	D	32	GLN
4	D	49	HIS
4	D	51	HIS
4	D	68	GLN
4	D	70	GLN
4	D	71	HIS
4	D	102	HIS
4	D	104	GLN
4	D	117	GLN

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Mol	Chain	Res	Type
4	D	152	ASN
4	D	161	GLN
4	D	211	HIS
4	D	248	ASN
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	30	GLN
5	E	45	HIS
5	E	114	GLN
6	F	21	GLN
6	F	40	HIS
6	F	61	HIS
6	F	183	GLN
6	F	313	GLN
7	G	18	GLN
7	G	46	HIS
7	G	92	HIS
7	G	102	HIS
7	G	161	HIS
7	G	279	GLN
8	H	166	GLN
8	H	196	ASN
8	H	207	HIS
8	H	282	HIS
8	H	297	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

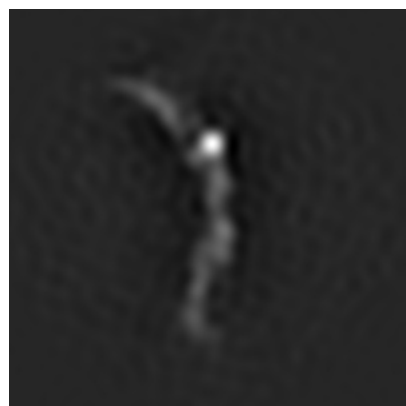
6 Map visualisation [i](#)

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.

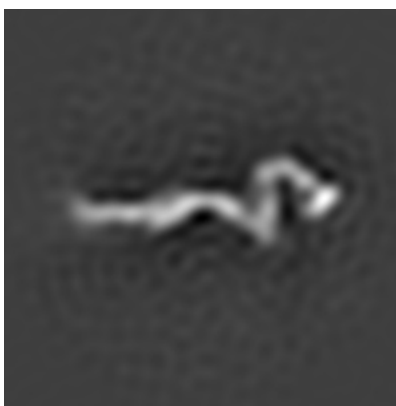
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

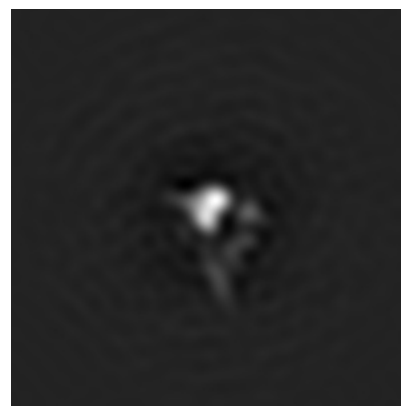
6.1.1 Primary map



X

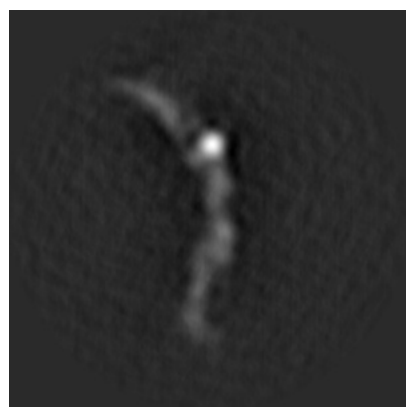


Y

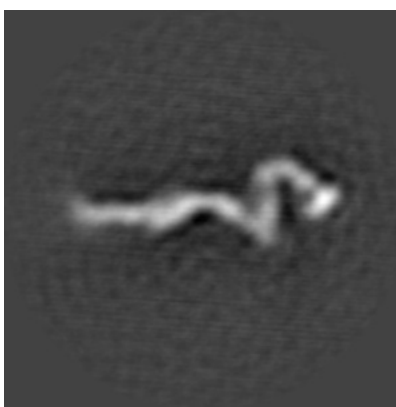


Z

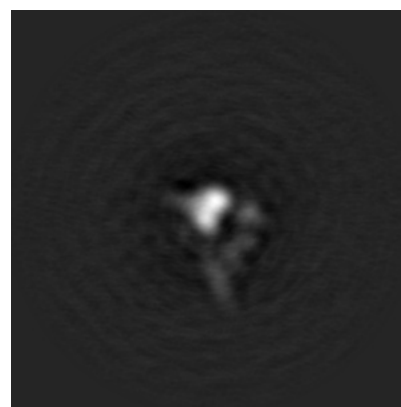
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

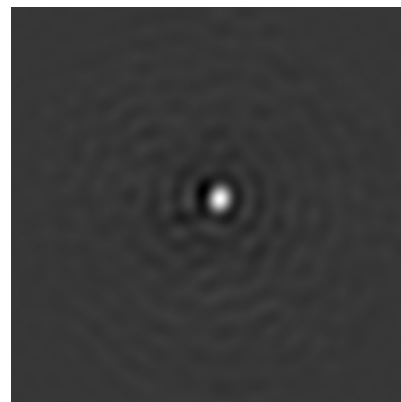
6.2.1 Primary map



X Index: 128

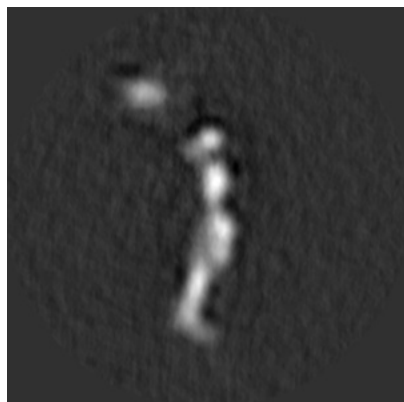


Y Index: 128

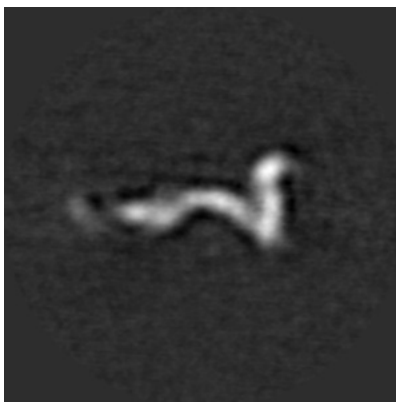


Z Index: 128

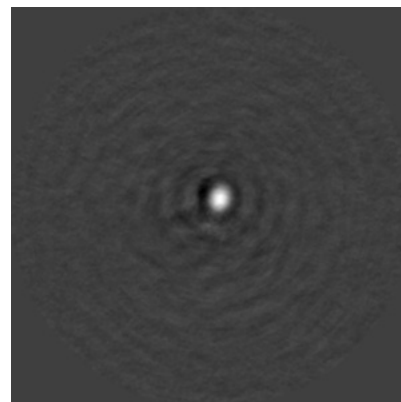
6.2.2 Raw map



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

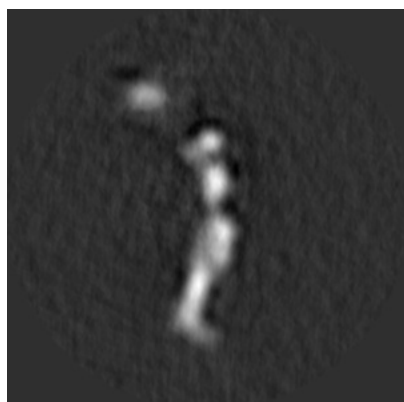


Y Index: 132

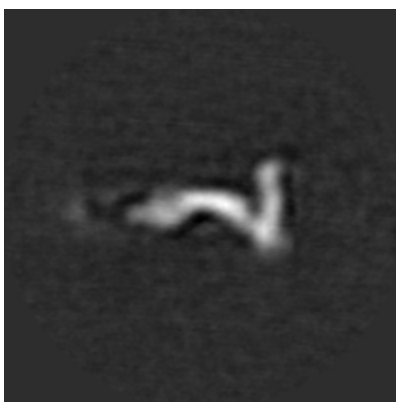


Z Index: 169

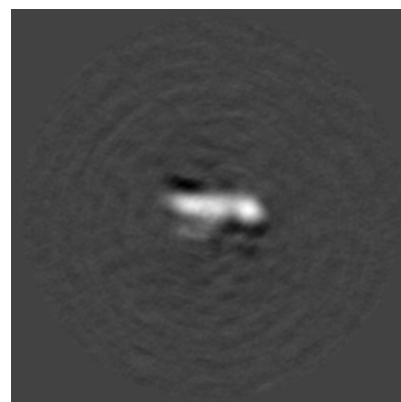
6.3.2 Raw map



X Index: 127



Y Index: 132

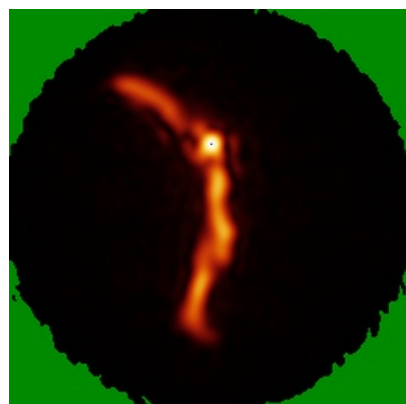


Z Index: 169

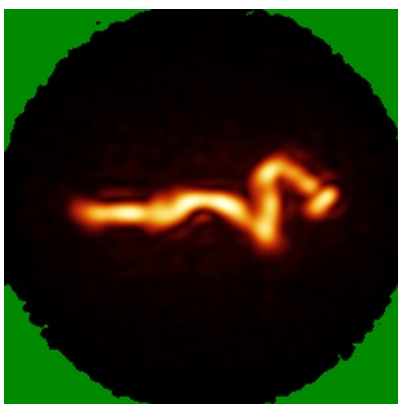
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

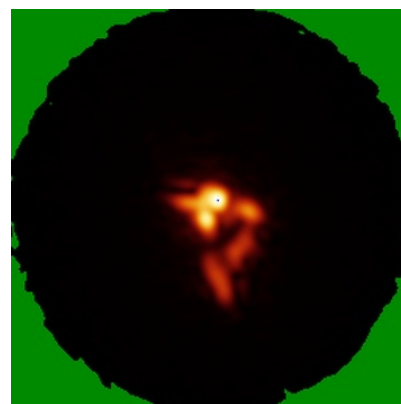
6.4.1 Primary map



X



Y



Z

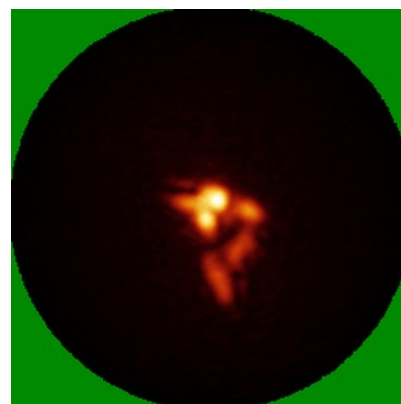
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 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.

6.5.2 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.

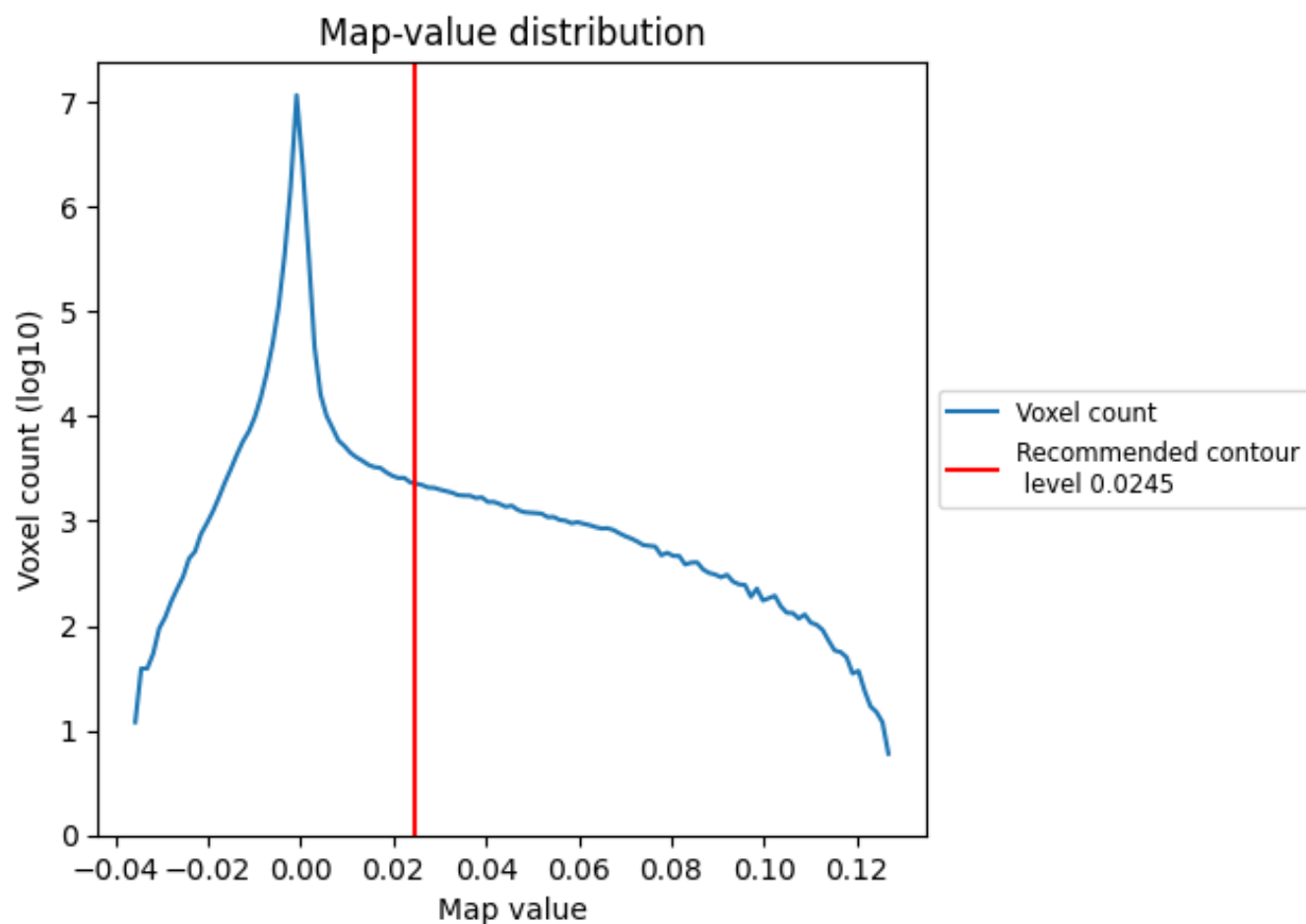
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

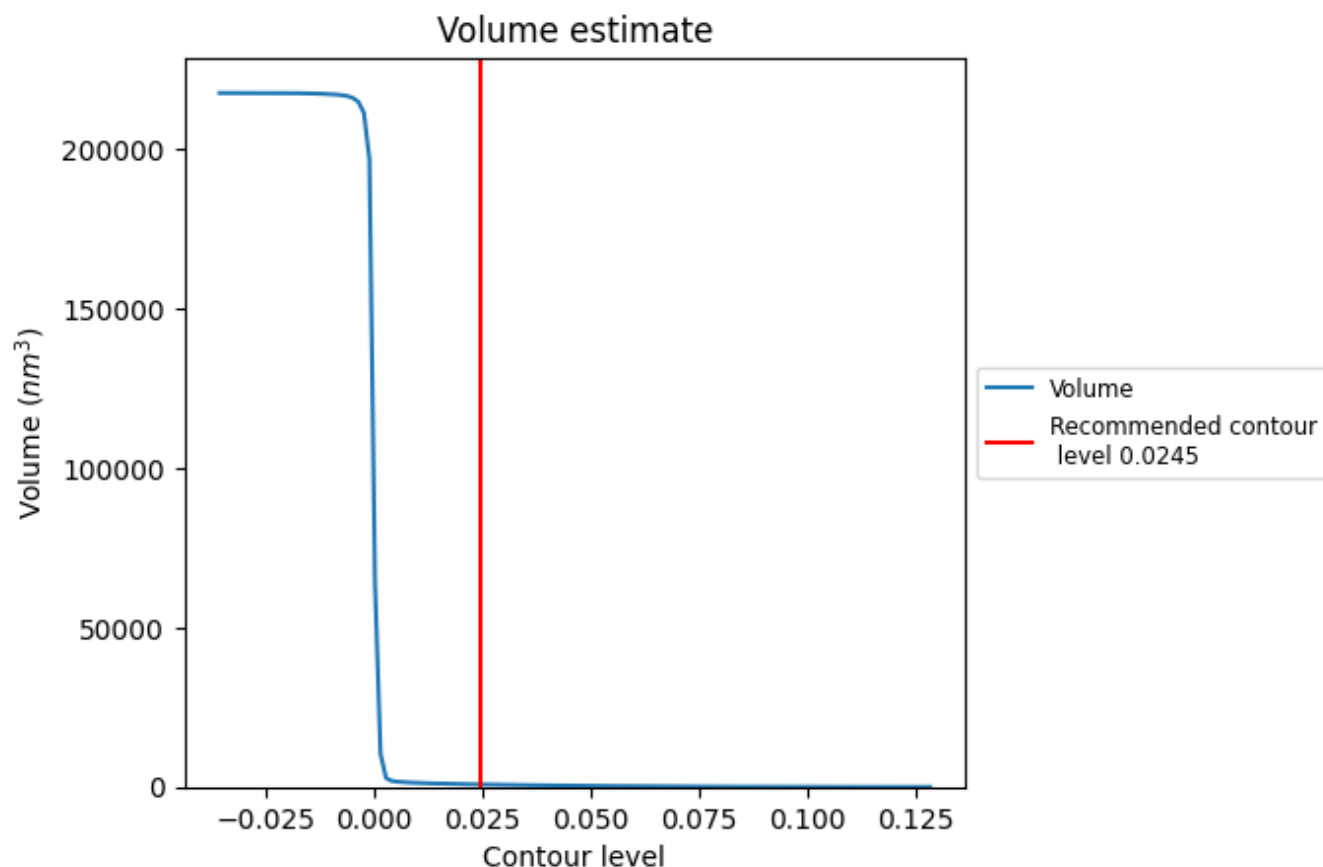
This section contains the results of statistical analysis of the map.

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.

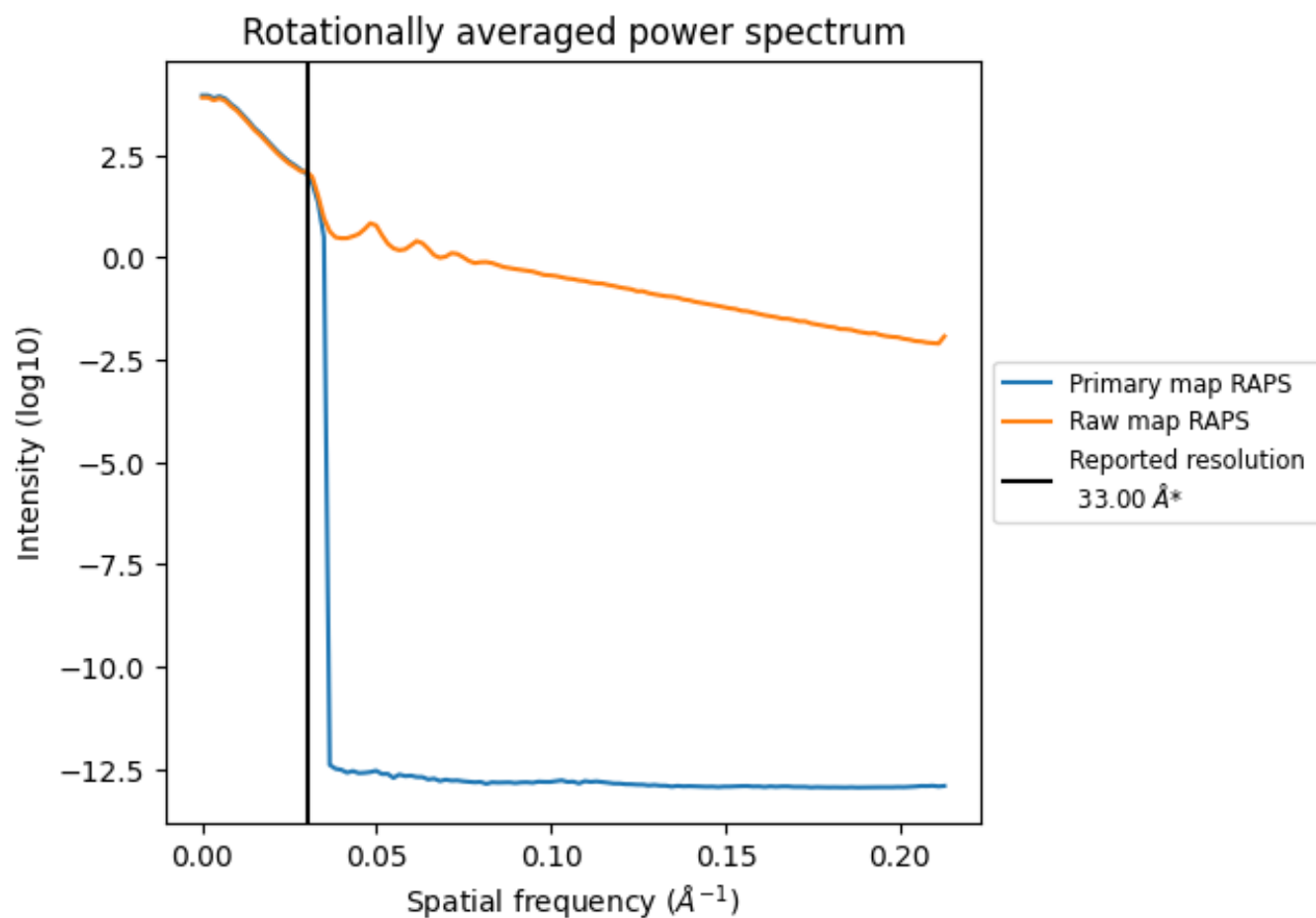
7.2 Volume estimate [i](#)



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 ⓘ

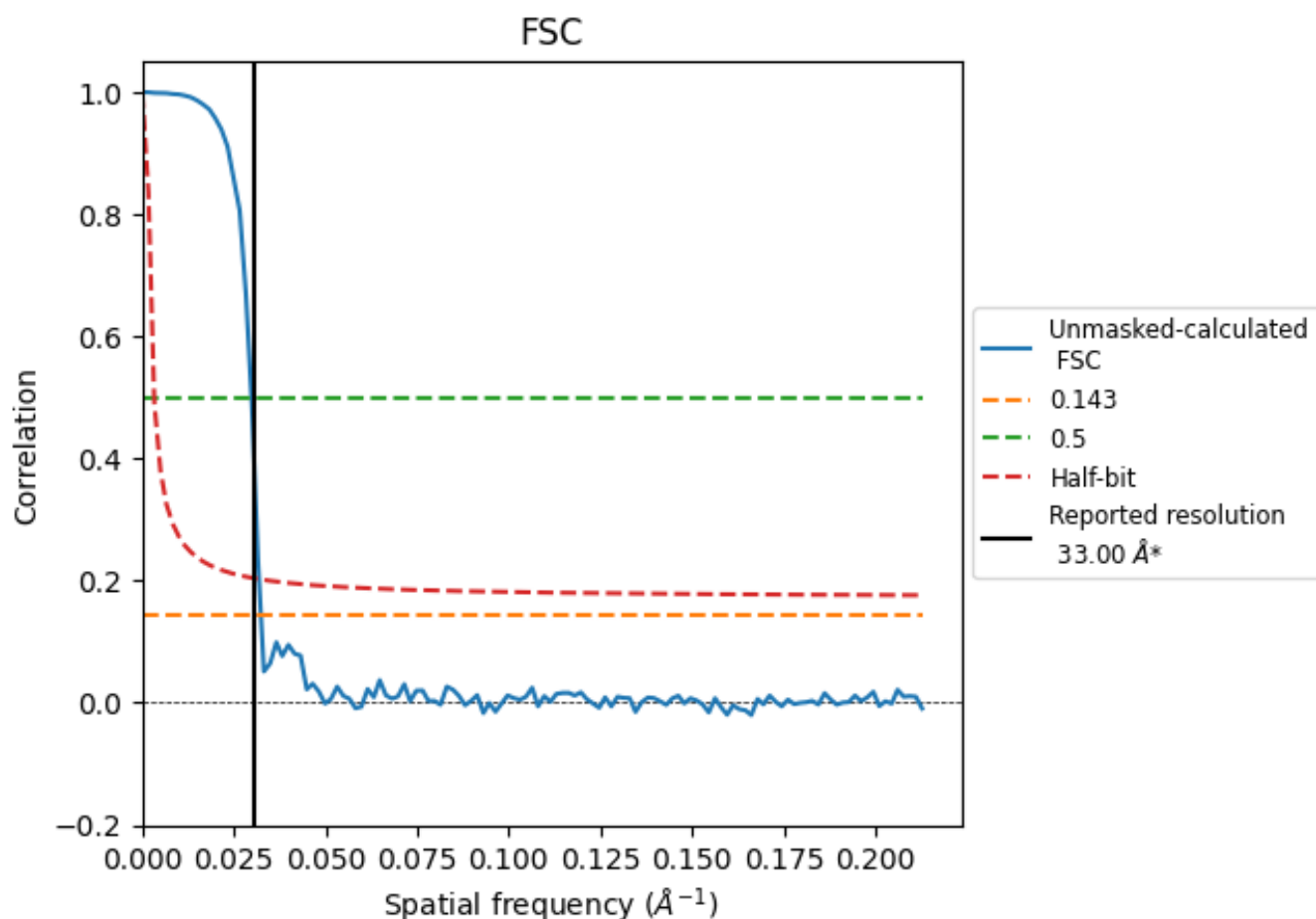


*Reported resolution corresponds to spatial frequency of 0.030 $\text{\AA}^{-1}$

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 Å⁻¹

8.2 Resolution estimates [i](#)

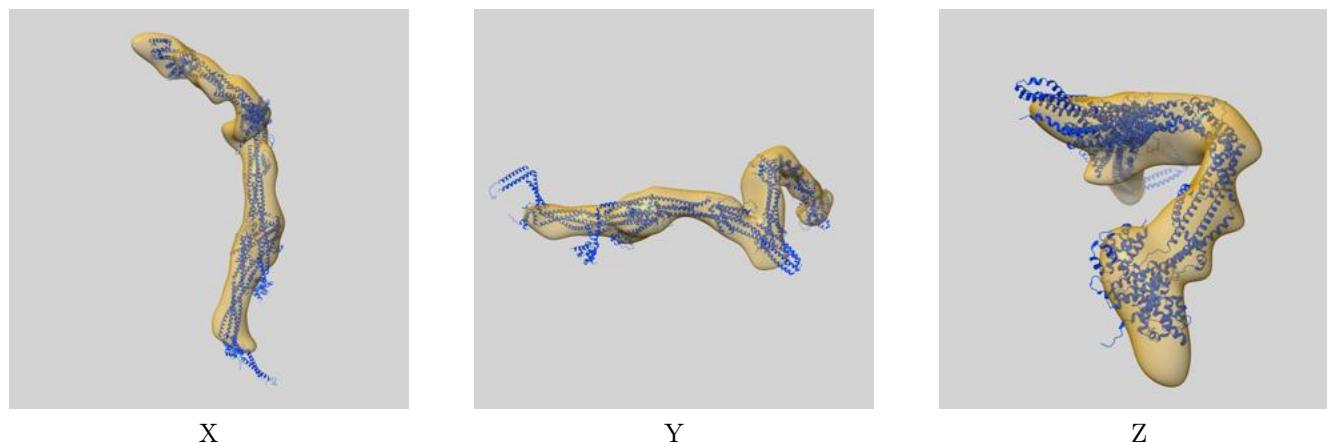
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	33.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	30.86	33.56	31.35

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

9 Map-model fit [i](#)

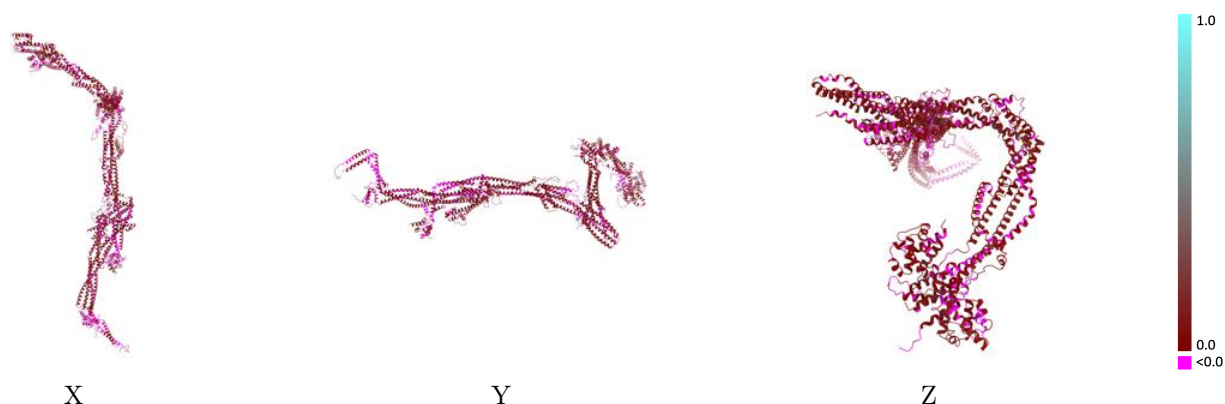
This section contains information regarding the fit between EMDB map EMD-15632 and PDB model 8AT3. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



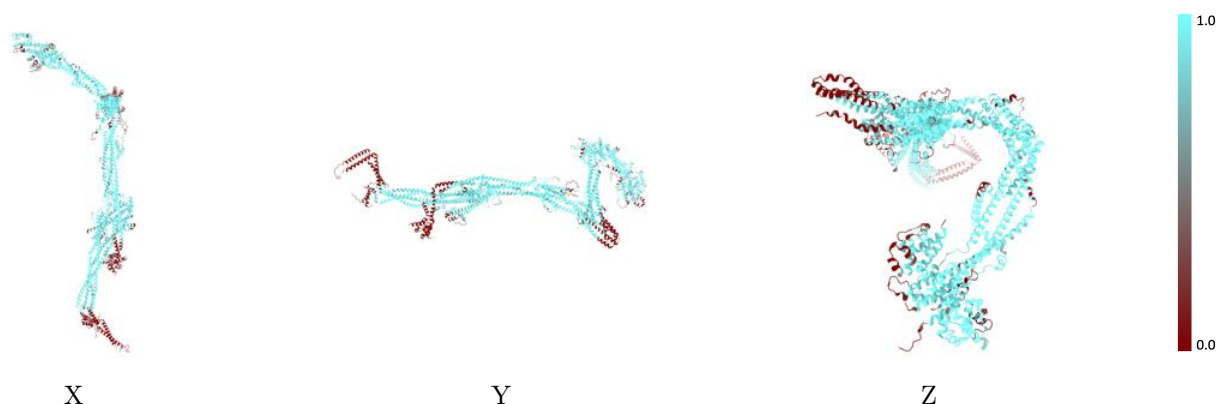
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



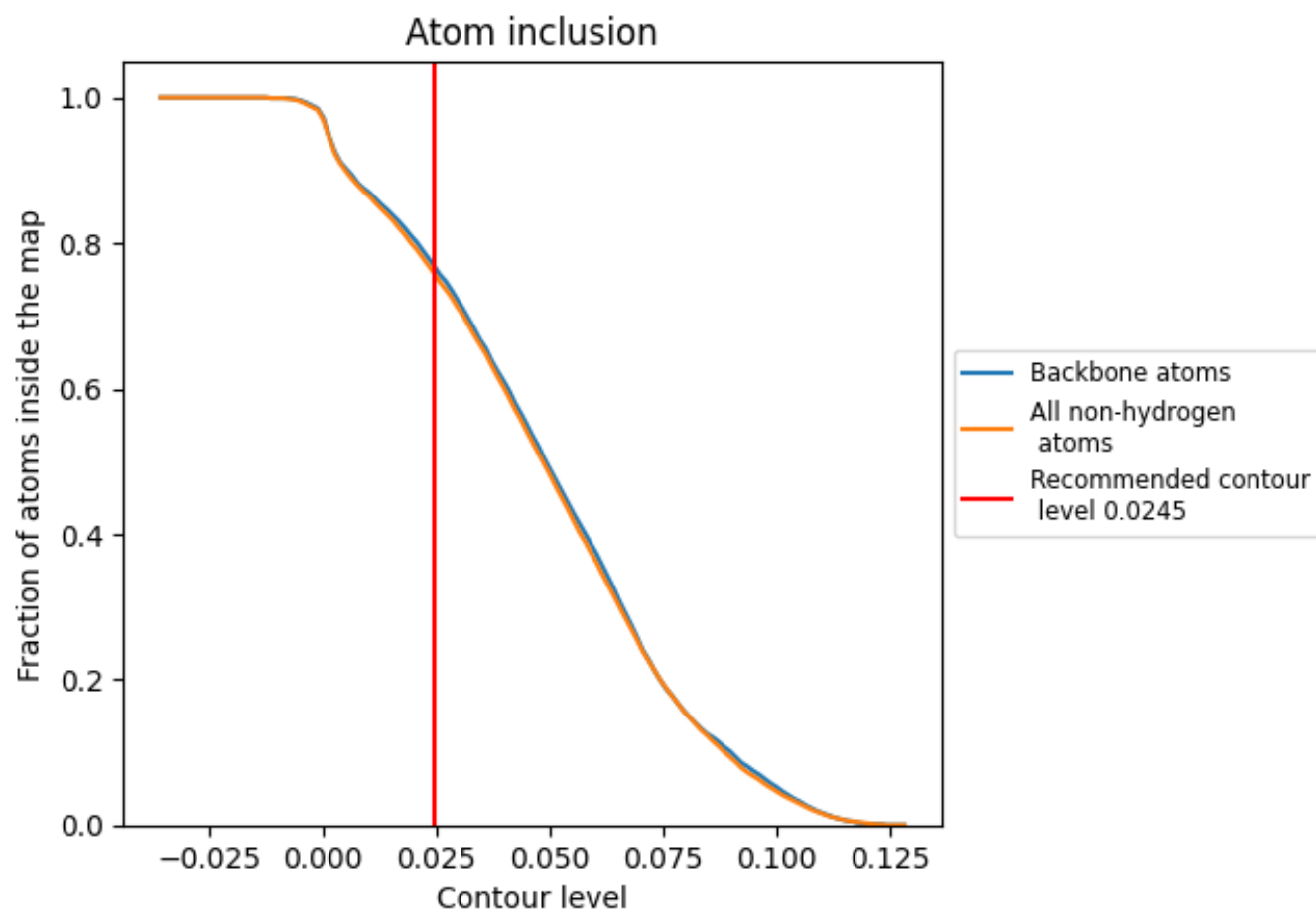
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.7590	0.0470
A	0.6830	0.0420
B	0.7180	0.0420
C	0.7320	0.0500
D	0.6880	0.0430
E	0.7950	0.0480
F	0.8470	0.0400
G	0.8080	0.0510
H	0.9680	0.0890

1.0

0.0

<0.0