



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 04:14 PM UTC

PDB ID : 8AT4 / pdb_00008at4
EMDB ID : EMD-15633
Title : Structure of the augmin holocomplex in closed 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:

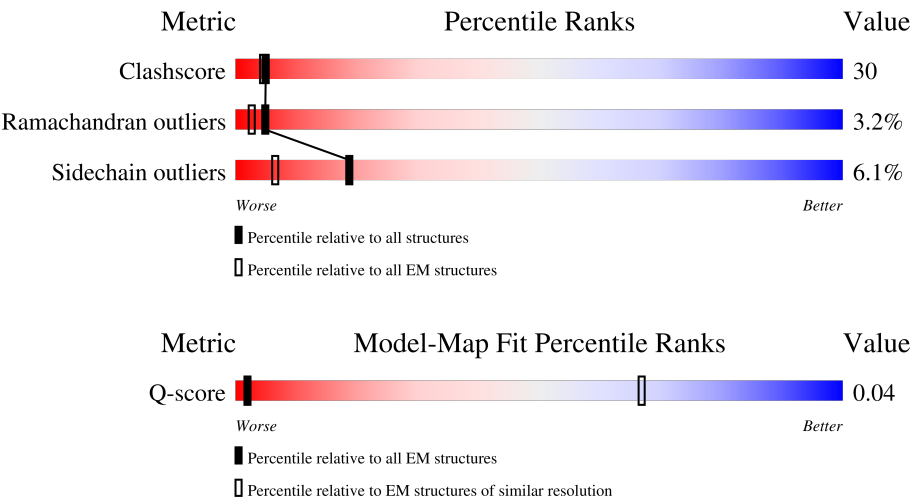
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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	
2	B	597	
3	C	353	
4	D	666	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	222	45% 38% 42% 14%
6	F	978	9% 17% 16% 6% 60%
7	G	348	24% 35% 40% 17% 5%
8	H	367	5% 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		

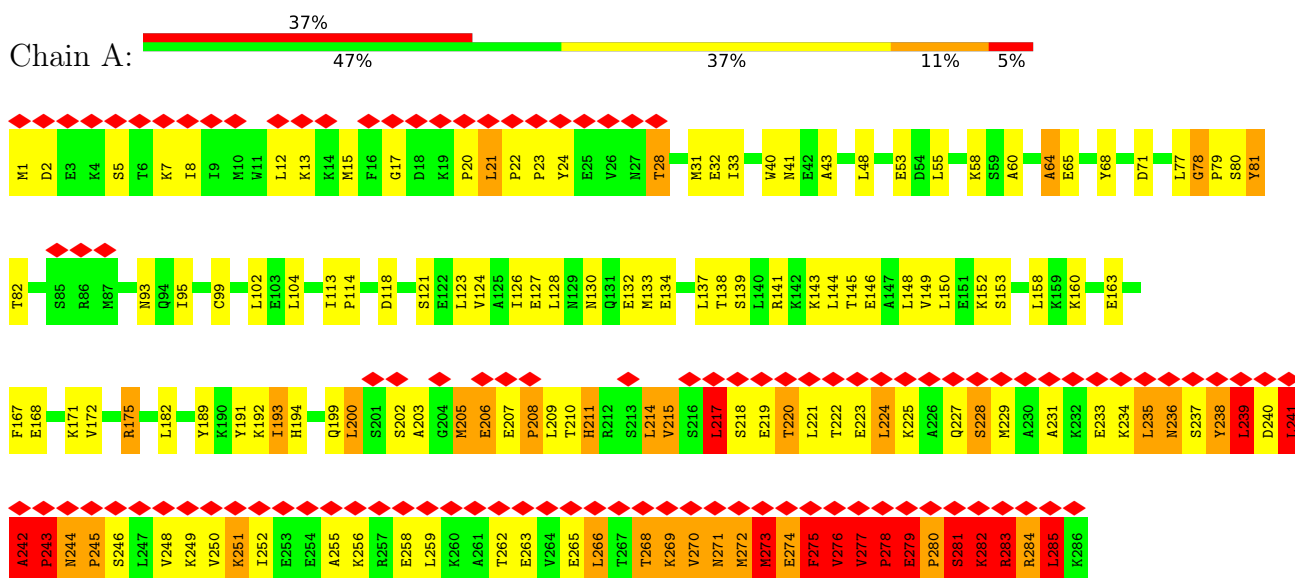
- Molecule 8 is a protein called HAUS augmin-like complex subunit 8.

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

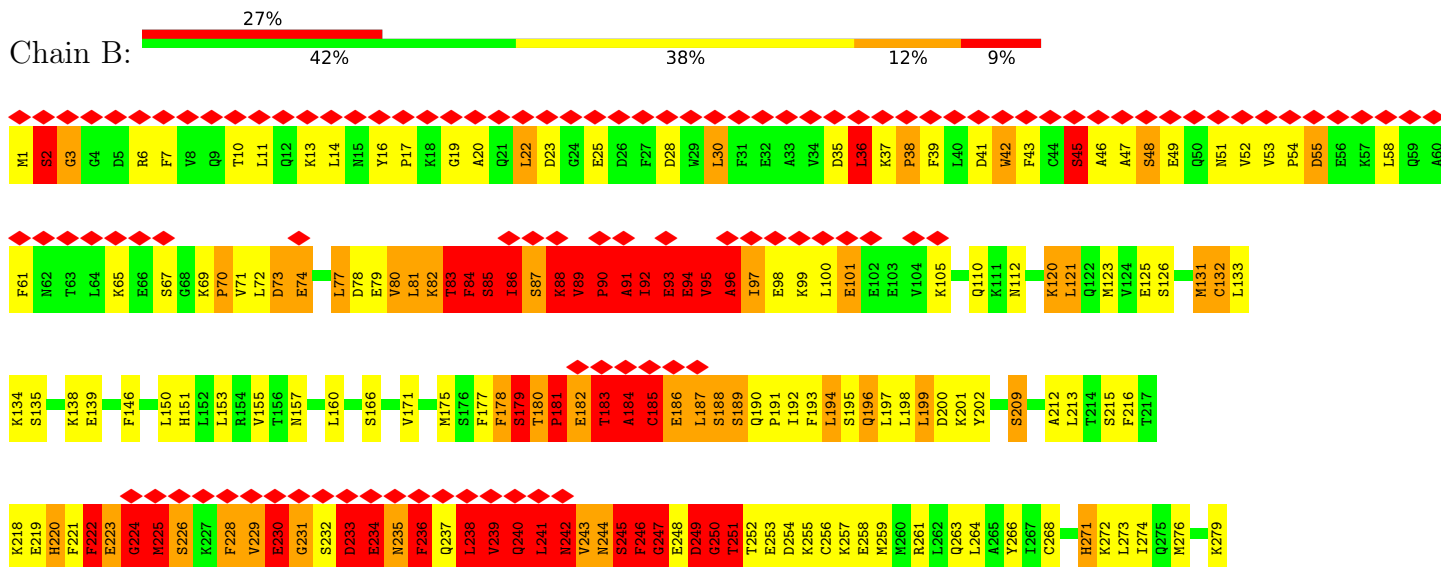
3 Residue-property plots

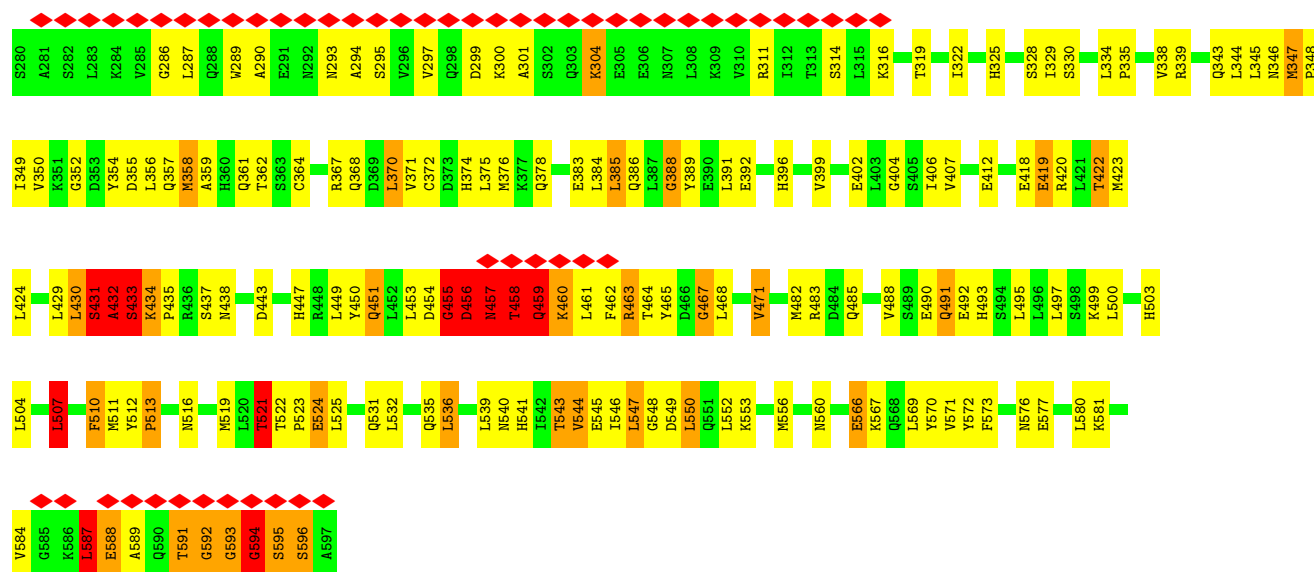
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

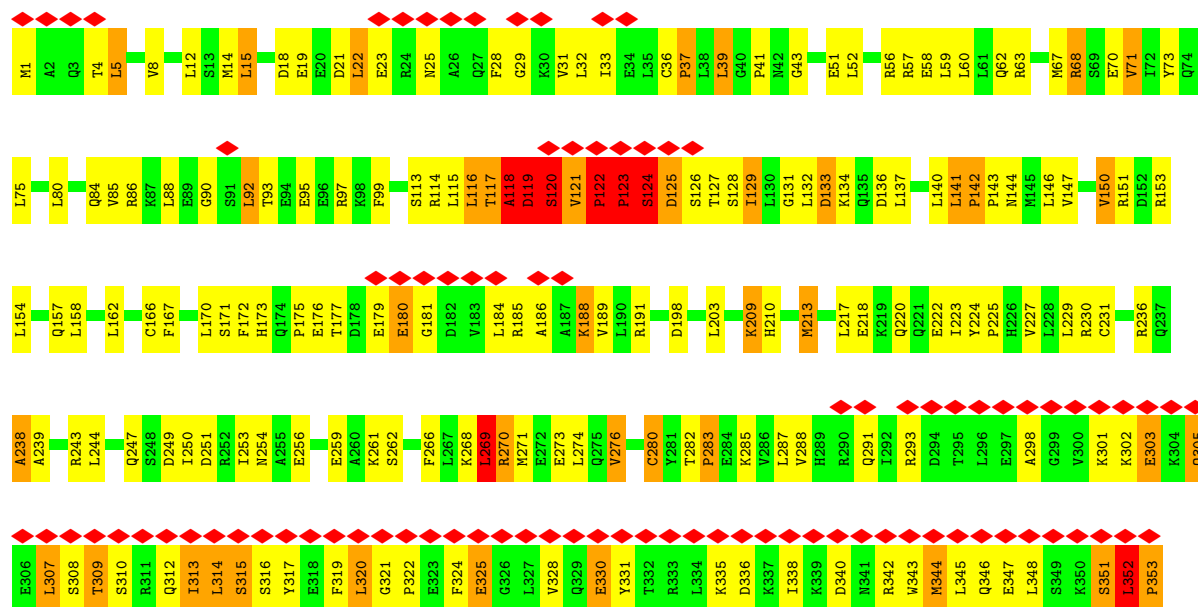


• Molecule 2: HAUS augmin-like complex subunit 3

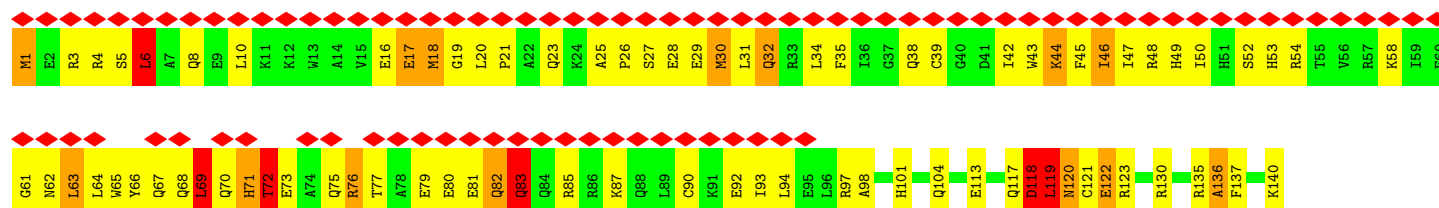
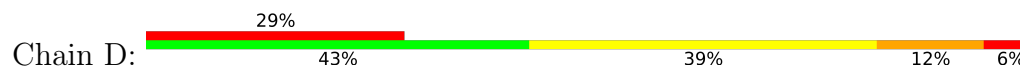


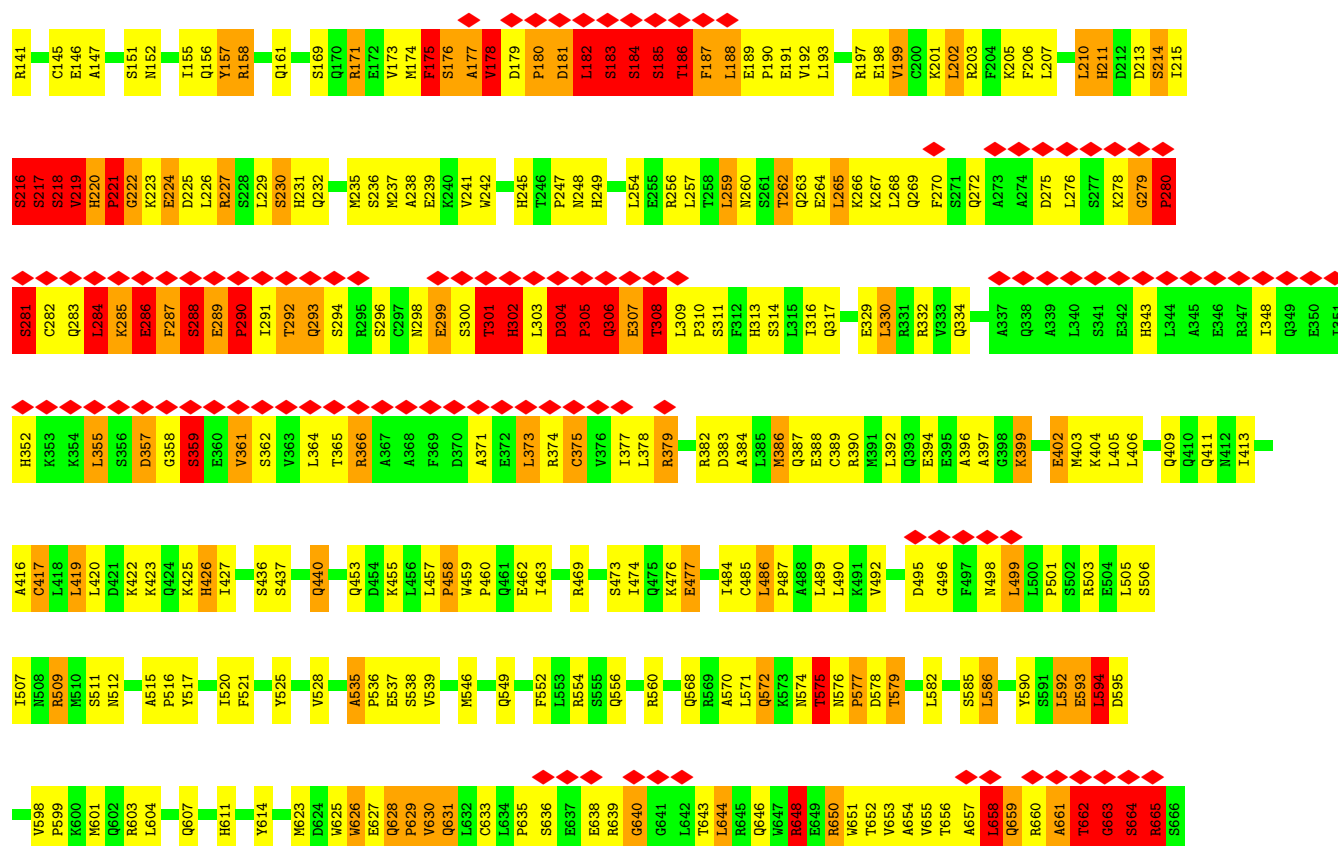


• Molecule 3: HAUS augmin like complex subunit 4 L homeolog



• Molecule 4: HAUS augmin-like complex subunit 5



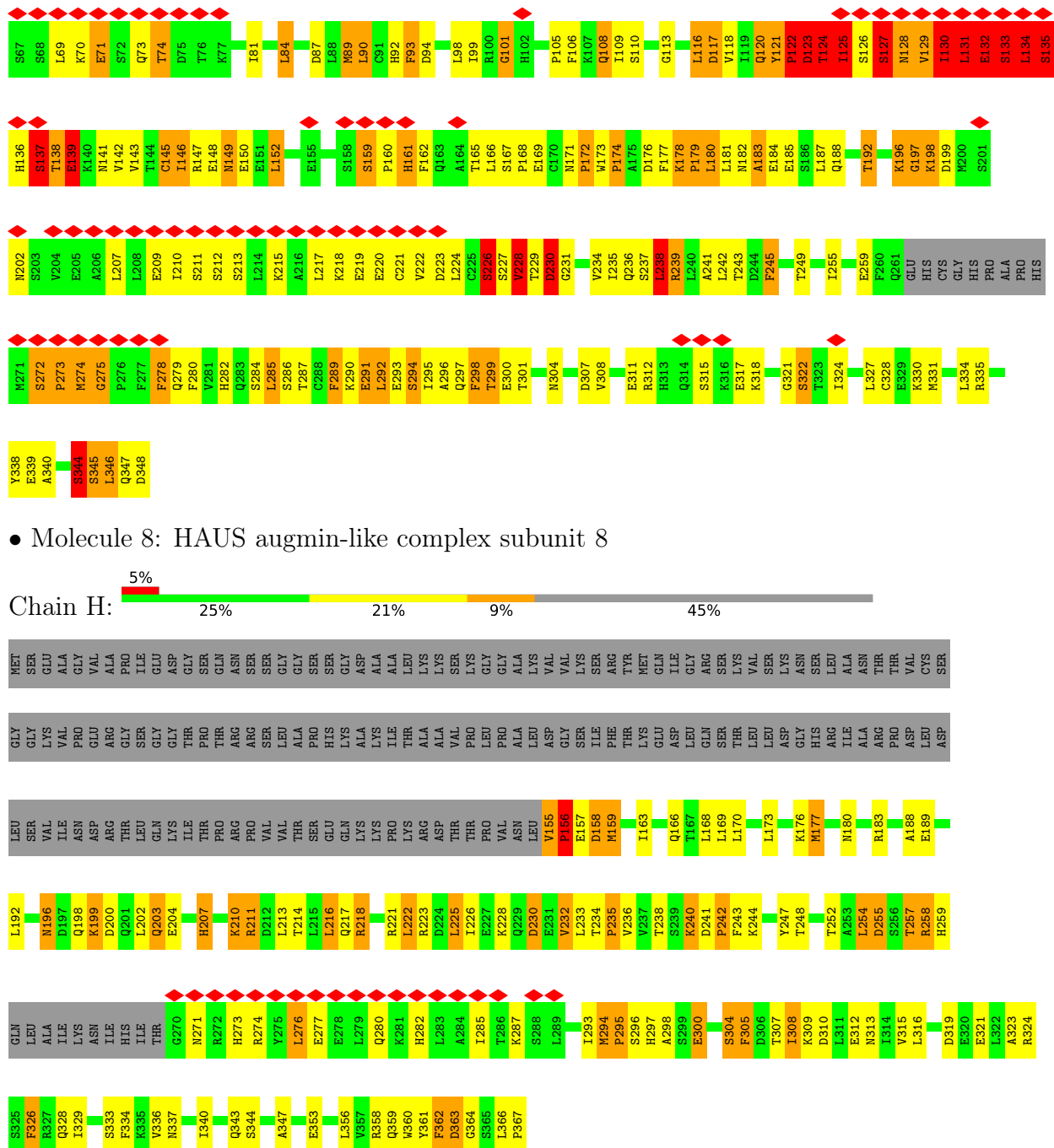


• Molecule 5: HAUS augmin like complex subunit 2 L homeolog



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10658	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	0.138	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0245	Depositor
Map size (Å)	601.6, 601.6, 601.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.35, 2.35, 2.35	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.23	77/2309 (3.3%)	2.16	106/3102 (3.4%)
2	B	1.66	150/4836 (3.1%)	1.89	185/6496 (2.8%)
3	C	1.45	68/2920 (2.3%)	1.82	95/3925 (2.4%)
4	D	1.56	145/5503 (2.6%)	1.91	193/7400 (2.6%)
5	E	2.05	84/1743 (4.8%)	1.58	47/2359 (2.0%)
6	F	1.86	130/3229 (4.0%)	1.73	109/4333 (2.5%)
7	G	1.86	117/2736 (4.3%)	1.91	105/3698 (2.8%)
8	H	1.70	62/1692 (3.7%)	1.46	40/2278 (1.8%)
All	All	1.76	833/24968 (3.3%)	1.85	880/33591 (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	15
2	B	0	68
3	C	0	11
4	D	0	41
5	E	0	11
6	F	0	19
7	G	0	27
8	H	0	1
All	All	0	193

All (833) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	PRO	C-N	29.15	1.75	1.33
2	B	223	GLU	C-N	28.76	1.81	1.33
1	A	276	VAL	C-N	28.18	1.65	1.33
1	A	284	ARG	C-N	27.99	1.69	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ARG	C-N	26.67	1.70	1.33
1	A	272	MET	C-N	-25.20	0.96	1.33
2	B	591	THR	C-N	22.68	1.66	1.33
6	F	34	ALA	C-N	20.44	1.59	1.33
3	C	319	PHE	C-N	20.00	1.66	1.33
1	A	277	VAL	C-N	19.68	1.79	1.33
1	A	274	GLU	C-N	19.08	1.58	1.33
1	A	273	MET	C-N	19.03	1.57	1.33
1	A	282	LYS	C-N	18.56	1.59	1.33
2	B	560	ASN	C-N	16.68	1.56	1.34
1	A	269	LYS	C-N	-16.04	1.12	1.33
2	B	593	GLY	C-N	15.97	1.56	1.33
4	D	227	ARG	C-N	-15.74	1.14	1.33
6	F	1	MET	C-N	-15.59	1.11	1.33
4	D	659	GLN	C-N	15.05	1.54	1.33
2	B	592	GLY	C-N	-14.88	1.11	1.33
4	D	72	THR	C-N	14.85	1.52	1.33
4	D	69	LEU	C-N	14.35	1.51	1.33
4	D	402	GLU	C-N	-14.24	1.14	1.33
7	G	315	SER	C-N	14.06	1.52	1.33
1	A	229	MET	C-N	-14.03	1.15	1.34
6	F	213	LEU	C-N	-13.95	1.15	1.33
2	B	455	GLY	C-N	13.91	1.52	1.33
2	B	587	LEU	C-N	13.84	1.53	1.33
5	E	86	GLN	C-N	-13.78	1.15	1.34
5	E	133	GLU	C-N	-13.60	1.15	1.34
1	A	265	GLU	C-N	-13.57	1.15	1.33
6	F	146	ALA	C-N	-13.56	1.15	1.33
4	D	180	PRO	C-N	13.55	1.51	1.33
6	F	262	VAL	C-N	-13.54	1.14	1.33
4	D	495	ASP	C-N	13.53	1.52	1.33
7	G	234	VAL	C-N	-13.52	1.16	1.33
1	A	206	GLU	C-N	-13.35	1.15	1.33
2	B	73	ASP	C-N	-13.24	1.16	1.33
5	E	69	LEU	C-N	-13.16	1.16	1.33
6	F	44	GLY	C-N	-13.14	1.18	1.33
6	F	258	VAL	C-N	-13.05	1.16	1.33
4	D	224	GLU	C-N	12.97	1.50	1.33
7	G	345	SER	C-N	12.95	1.51	1.34
1	A	268	THR	C-N	-12.92	1.16	1.33
1	A	2	ASP	C-N	12.85	1.50	1.33
2	B	215	SER	C-N	-12.80	1.18	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	289	PHE	C-N	-12.78	1.16	1.33
7	G	226	SER	C-N	12.65	1.51	1.33
1	A	239	LEU	C-N	12.63	1.53	1.33
7	G	275	GLY	C-N	-12.61	1.18	1.34
6	F	222	LYS	C-N	12.60	1.49	1.33
5	E	73	LYS	C-N	-12.52	1.16	1.33
7	G	27	GLY	C-N	12.51	1.52	1.33
2	B	6	ARG	C-N	-12.48	1.18	1.33
3	C	291	GLN	C-N	-12.36	1.19	1.34
8	H	333	SER	C-N	-12.25	1.18	1.33
2	B	589	ALA	C-N	-12.25	1.17	1.33
6	F	106	VAL	C-N	12.24	1.51	1.33
6	F	209	GLU	C-N	-12.22	1.18	1.33
2	B	150	LEU	C-N	12.10	1.49	1.33
8	H	300	GLU	C-N	-11.96	1.18	1.33
2	B	17	PRO	N-CD	-11.95	1.31	1.47
7	G	141	ASN	C-N	-11.95	1.18	1.33
5	E	6	PRO	N-CD	-11.88	1.31	1.47
2	B	513	PRO	N-CD	-11.84	1.31	1.47
8	H	196	ASN	C-N	-11.84	1.18	1.33
5	E	58	GLU	C-N	-11.83	1.19	1.33
7	G	122	PRO	C-N	-11.82	1.17	1.33
7	G	122	PRO	N-CD	-11.80	1.31	1.47
7	G	161	HIS	C-N	-11.80	1.18	1.33
4	D	576	ASN	C-N	11.78	1.56	1.34
1	A	82	THR	C-N	11.76	1.46	1.33
1	A	270	VAL	C-N	11.75	1.49	1.33
5	E	9	PRO	N-CD	-11.75	1.31	1.47
1	A	245	PRO	N-CD	-11.74	1.31	1.47
5	E	82	LEU	C-N	-11.74	1.17	1.34
8	H	367	PRO	N-CD	-11.74	1.31	1.47
4	D	21	PRO	N-CD	-11.68	1.31	1.47
1	A	22	PRO	N-CD	-11.67	1.31	1.47
6	F	253	LYS	C-N	-11.67	1.18	1.33
4	D	313	HIS	C-N	-11.63	1.18	1.34
4	D	221	PRO	N-CD	-11.62	1.31	1.47
4	D	652	THR	C-N	11.58	1.48	1.33
7	G	196	LYS	C-N	11.58	1.50	1.33
6	F	202	GLN	C-N	-11.52	1.19	1.33
4	D	26	PRO	N-CD	-11.51	1.31	1.47
2	B	594	GLY	C-N	-11.48	1.17	1.33
7	G	71	GLU	C-N	11.47	1.49	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	314	LEU	C-N	-11.45	1.18	1.34
4	D	180	PRO	N-CD	-11.42	1.31	1.47
1	A	208	PRO	N-CD	-11.40	1.31	1.47
2	B	90	PRO	N-CD	-11.38	1.31	1.47
2	B	222	PHE	C-N	-11.36	1.18	1.33
2	B	54	PRO	N-CD	-11.35	1.31	1.47
7	G	130	ILE	C-N	11.33	1.49	1.33
5	E	222	PRO	N-CD	-11.33	1.31	1.47
5	E	15	ALA	C-N	-11.31	1.19	1.33
5	E	93	ALA	C-N	-11.30	1.18	1.34
6	F	260	ALA	C-N	-11.27	1.19	1.33
1	A	17	GLY	C-N	11.23	1.50	1.33
3	C	113	SER	C-N	-11.20	1.17	1.33
4	D	280	PRO	N-CD	-11.19	1.32	1.47
3	C	124	SER	C-N	11.18	1.48	1.33
3	C	283	PRO	N-CD	-11.15	1.32	1.47
4	D	176	SER	C-N	11.14	1.49	1.33
3	C	22	LEU	C-N	11.09	1.49	1.33
3	C	313	ILE	C-N	-11.07	1.19	1.34
6	F	329	TYR	C-N	11.03	1.47	1.33
3	C	353	PRO	N-CD	-10.98	1.32	1.47
6	F	292	MET	C-N	10.96	1.49	1.34
5	E	41	PRO	N-CD	-10.96	1.32	1.47
4	D	290	PRO	N-CD	-10.95	1.32	1.47
6	F	7	PRO	N-CD	-10.94	1.32	1.47
4	D	190	PRO	N-CD	-10.93	1.32	1.47
3	C	122	PRO	N-CD	-10.90	1.32	1.47
3	C	322	PRO	N-CD	-10.89	1.32	1.47
5	E	95	ASN	C-N	-10.85	1.20	1.33
6	F	121	PRO	C-N	-10.84	1.17	1.33
4	D	650	ARG	C-N	-10.84	1.20	1.33
6	F	175	ARG	C-N	-10.84	1.20	1.33
4	D	501	PRO	C-N	-10.83	1.19	1.34
6	F	195	LYS	C-N	-10.80	1.19	1.33
5	E	61	GLN	C-N	-10.79	1.19	1.33
2	B	181	PRO	N-CD	-10.79	1.32	1.47
8	H	361	TYR	C-N	10.79	1.50	1.33
4	D	496	GLY	C-N	10.79	1.48	1.33
6	F	380	GLU	C-N	-10.77	1.19	1.33
5	E	22	CYS	C-N	-10.75	1.19	1.33
1	A	222	THR	C-N	-10.72	1.19	1.33
5	E	51	ARG	C-N	-10.70	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	191	PRO	N-CD	-10.68	1.32	1.47
2	B	233	ASP	C-N	10.68	1.48	1.33
5	E	88	HIS	C-N	-10.67	1.19	1.33
5	E	78	ILE	C-N	-10.66	1.18	1.33
7	G	299	THR	C-N	-10.64	1.20	1.33
6	F	256	ASP	C-N	-10.63	1.20	1.33
4	D	18	MET	C-N	10.61	1.47	1.33
8	H	218	ARG	C-N	-10.61	1.19	1.34
6	F	51	PRO	C-N	-10.58	1.17	1.33
5	E	136	PRO	C-N	-10.54	1.20	1.33
8	H	319	ASP	C-N	-10.53	1.20	1.33
7	G	287	THR	C-N	-10.51	1.20	1.33
7	G	129	VAL	C-N	10.50	1.48	1.33
8	H	297	HIS	C-N	-10.46	1.20	1.33
2	B	516	ASN	C-N	-10.45	1.19	1.33
4	D	311	SER	C-N	-10.42	1.19	1.33
6	F	173	LEU	C-N	-10.39	1.20	1.33
4	D	83	GLN	C-N	10.38	1.47	1.33
3	C	213	MET	C-N	-10.37	1.20	1.33
7	G	290	LYS	C-N	-10.37	1.20	1.33
5	E	25	ALA	C-N	10.35	1.47	1.33
4	D	305	PRO	N-CD	-10.29	1.33	1.47
6	F	390	GLY	C-N	10.28	1.47	1.33
6	F	148	ALA	C-N	10.25	1.50	1.33
7	G	278	PHE	C-N	-10.25	1.20	1.33
5	E	128	HIS	C-N	-10.24	1.20	1.33
6	F	82	PRO	N-CD	-10.18	1.33	1.47
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	117	ASP	C-N	-10.09	1.21	1.33
7	G	23	PRO	N-CD	-10.08	1.33	1.47
6	F	27	SER	C-N	10.08	1.46	1.33
7	G	159	SER	C-N	10.02	1.45	1.34
4	D	221	PRO	C-N	-10.00	1.18	1.33
1	A	81	TYR	C-N	10.00	1.49	1.33
5	E	11	GLN	C-N	-10.00	1.20	1.33
7	G	90	LEU	C-N	9.99	1.46	1.33
7	G	237	SER	C-N	-9.99	1.20	1.33
4	D	635	PRO	N-CD	-9.89	1.33	1.47
6	F	121	PRO	N-CD	-9.86	1.33	1.47
3	C	123	PRO	N-CD	-9.85	1.33	1.47
5	E	137	LEU	C-N	-9.85	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	251	MET	C-N	-9.80	1.21	1.33
4	D	53	HIS	C-N	-9.79	1.21	1.33
2	B	70	PRO	N-CD	-9.78	1.34	1.47
4	D	357	ASP	C-N	9.78	1.47	1.33
8	H	156	PRO	N-CD	-9.78	1.34	1.47
8	H	364	GLY	C-N	9.77	1.48	1.33
4	D	653	VAL	C-N	-9.75	1.20	1.33
6	F	205	ASP	C-N	-9.65	1.20	1.33
7	G	311	GLU	C-N	-9.62	1.20	1.34
5	E	81	PRO	C-N	-9.55	1.21	1.33
4	D	638	GLU	C-N	-9.54	1.20	1.33
4	D	90	CYS	C-N	9.53	1.46	1.33
7	G	98	LEU	C-N	-9.52	1.22	1.33
6	F	206	MET	C-N	-9.51	1.21	1.33
6	F	279	ASN	C-N	-9.50	1.24	1.33
5	E	9	PRO	C-N	-9.49	1.20	1.33
7	G	279	GLN	C-N	-9.45	1.21	1.33
7	G	89	MET	C-N	-9.44	1.20	1.33
1	A	278	PRO	N-CD	-9.43	1.34	1.47
3	C	144	ASN	C-N	9.41	1.47	1.34
2	B	3	GLY	C-N	-9.41	1.22	1.33
6	F	197	GLN	C-N	-9.38	1.22	1.33
6	F	223	VAL	C-N	9.38	1.47	1.33
8	H	222	LEU	C-N	-9.34	1.21	1.33
7	G	113	GLY	C-N	-9.34	1.21	1.33
4	D	646	GLN	C-N	-9.33	1.21	1.33
7	G	145	CYS	C-N	-9.32	1.22	1.33
4	D	191	GLU	C-N	9.27	1.45	1.33
7	G	63	GLN	C-N	9.23	1.46	1.34
6	F	246	GLN	C-N	-9.22	1.21	1.33
4	D	572	GLN	C-N	9.22	1.46	1.34
6	F	393	PRO	N-CD	-9.21	1.34	1.47
2	B	250	GLY	C-N	-9.21	1.21	1.33
1	A	245	PRO	C-N	9.20	1.46	1.33
8	H	295	PRO	N-CD	-9.20	1.34	1.47
7	G	317	GLU	C-N	9.18	1.46	1.33
6	F	257	VAL	C-N	-9.17	1.22	1.33
7	G	286	SER	C-N	-9.16	1.22	1.33
6	F	68	ASP	C-N	-9.16	1.22	1.33
7	G	282	HIS	C-N	-9.16	1.22	1.33
4	D	644	LEU	C-N	-9.16	1.22	1.33
6	F	237	THR	C-N	-9.16	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	191	GLU	C-N	-9.14	1.22	1.33
5	E	62	LYS	C-N	-9.13	1.22	1.33
4	D	662	THR	C-N	9.13	1.46	1.33
4	D	396	ALA	C-N	9.09	1.46	1.33
7	G	209	GLU	C-N	-9.08	1.22	1.33
8	H	344	SER	C-N	-9.05	1.22	1.33
4	D	511	SER	C-N	9.05	1.47	1.33
5	E	47	GLU	C-N	-9.03	1.22	1.33
4	D	158	ARG	C-N	-9.02	1.22	1.33
6	F	276	ALA	C-N	9.01	1.46	1.33
6	F	306	VAL	C-N	-8.98	1.21	1.33
7	G	213	SER	C-N	-8.98	1.21	1.33
4	D	175	PHE	C-N	8.98	1.45	1.33
8	H	242	PRO	C-N	-8.97	1.22	1.33
5	E	140	ASN	C-N	-8.97	1.21	1.33
6	F	103	SER	C-N	8.96	1.46	1.33
5	E	94	MET	C-N	-8.94	1.22	1.33
2	B	422	THR	C-N	-8.93	1.21	1.33
1	A	20	PRO	N-CD	-8.91	1.35	1.47
5	E	65	GLU	C-N	-8.91	1.22	1.33
3	C	88	LEU	C-N	8.90	1.47	1.33
4	D	171	ARG	C-N	8.90	1.46	1.33
5	E	85	GLY	C-N	-8.89	1.22	1.33
7	G	124	THR	C-N	8.87	1.45	1.33
2	B	219	GLU	C-N	-8.85	1.21	1.33
8	H	207	HIS	C-N	-8.85	1.22	1.33
5	E	23	LEU	C-N	8.84	1.46	1.34
5	E	98	LEU	C-N	-8.82	1.22	1.33
6	F	108	ALA	C-N	-8.82	1.20	1.33
3	C	331	TYR	C-N	-8.81	1.22	1.33
3	C	118	ALA	C-N	8.77	1.46	1.33
1	A	78	GLY	C-N	-8.76	1.24	1.34
6	F	224	ASP	C-N	-8.76	1.22	1.33
1	A	285	LEU	C-N	8.74	1.45	1.33
6	F	194	ARG	C-N	-8.74	1.22	1.33
5	E	54	GLU	C-N	-8.71	1.23	1.33
1	A	235	LEU	C-N	8.70	1.45	1.34
2	B	461	LEU	C-N	8.69	1.45	1.33
4	D	87	LYS	C-N	8.69	1.45	1.33
8	H	236	VAL	C-N	-8.66	1.23	1.33
2	B	65	LYS	C-N	8.66	1.46	1.34
4	D	187	PHE	C-N	8.62	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	152	LEU	C-N	-8.61	1.22	1.33
1	A	243	PRO	N-CD	-8.60	1.35	1.47
6	F	384	LYS	C-N	-8.58	1.20	1.33
2	B	17	PRO	C-N	8.58	1.44	1.33
2	B	258	GLU	C-N	-8.56	1.22	1.33
7	G	181	LEU	C-N	8.54	1.46	1.33
6	F	363	LYS	C-N	8.53	1.46	1.33
2	B	45	SER	C-N	-8.52	1.21	1.33
5	E	84	LEU	C-N	-8.51	1.22	1.33
4	D	577	PRO	N-CD	-8.50	1.35	1.47
5	E	151	THR	C-N	-8.50	1.23	1.33
2	B	10	THR	C-N	-8.49	1.22	1.33
6	F	172	LYS	C-N	-8.49	1.22	1.33
1	A	53	GLU	C-N	-8.45	1.22	1.33
6	F	281	PRO	N-CD	-8.45	1.35	1.47
4	D	388	GLU	C-N	-8.44	1.22	1.33
1	A	64	ALA	C-N	-8.44	1.22	1.33
4	D	16	GLU	C-N	-8.44	1.22	1.33
5	E	50	GLN	C-N	-8.44	1.22	1.33
3	C	19	GLU	C-N	8.40	1.45	1.34
2	B	38	PRO	N-CD	-8.40	1.35	1.47
5	E	126	SER	C-N	-8.39	1.22	1.33
7	G	322	SER	C-N	8.39	1.44	1.33
1	A	280	PRO	N-CD	-8.38	1.36	1.47
7	G	108	GLN	C-N	-8.37	1.23	1.33
4	D	640	GLY	C-N	8.37	1.45	1.33
8	H	274	ARG	C-N	-8.35	1.23	1.33
1	A	221	LEU	C-N	-8.34	1.23	1.33
6	F	288	ILE	C-N	8.33	1.45	1.33
7	G	221	CYS	C-N	8.33	1.44	1.33
8	H	159	MET	C-N	-8.32	1.23	1.33
1	A	263	GLU	C-N	8.32	1.44	1.33
2	B	184	ALA	C-N	8.32	1.44	1.33
5	E	2	MET	C-N	-8.32	1.22	1.33
6	F	15	HIS	C-N	-8.31	1.23	1.33
1	A	241	LEU	C-N	8.31	1.46	1.33
7	G	73	GLN	C-N	-8.31	1.23	1.33
7	G	285	LEU	C-N	-8.30	1.23	1.33
2	B	314	SER	C-N	-8.30	1.23	1.33
2	B	543	THR	C-N	-8.29	1.23	1.33
3	C	270	ARG	C-N	-8.26	1.22	1.33
5	E	164	ASN	C-N	-8.26	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	68	LEU	C-N	-8.24	1.22	1.33
2	B	181	PRO	C-N	8.23	1.45	1.33
2	B	286	GLY	C-N	-8.17	1.22	1.33
6	F	9	LEU	C-N	8.17	1.44	1.33
3	C	116	LEU	C-N	8.16	1.45	1.33
4	D	498	ASN	C-N	8.13	1.45	1.33
2	B	218	LYS	C-N	-8.12	1.22	1.34
6	F	186	ASN	C-N	-8.09	1.23	1.33
4	D	46	ILE	C-N	-8.07	1.24	1.33
6	F	176	GLN	C-N	-8.07	1.23	1.33
7	G	148	GLU	C-N	-8.06	1.23	1.33
2	B	61	PHE	C-N	8.06	1.44	1.33
4	D	377	ILE	C-N	-8.05	1.23	1.33
5	E	29	SER	C-N	-8.04	1.23	1.34
4	D	21	PRO	C-N	-8.03	1.23	1.34
1	A	275	PHE	C-N	-8.03	1.22	1.33
2	B	247	GLY	C-N	8.03	1.45	1.33
4	D	594	LEU	C-N	8.02	1.45	1.33
5	E	103	ARG	C-N	8.01	1.42	1.33
1	A	259	LEU	C-N	8.00	1.44	1.33
2	B	311	ARG	C-N	-8.00	1.24	1.33
6	F	164	PRO	C-N	-7.98	1.23	1.33
8	H	155	VAL	C-N	-7.98	1.15	1.33
7	G	160	PRO	N-CD	-7.96	1.36	1.47
6	F	111	PRO	N-CD	-7.96	1.36	1.47
4	D	5	SER	C-N	-7.95	1.23	1.33
4	D	657	ALA	C-N	-7.95	1.23	1.33
7	G	236	GLN	C-N	-7.93	1.23	1.33
8	H	177	MET	C-N	-7.90	1.23	1.33
4	D	101	HIS	C-N	7.88	1.44	1.33
2	B	492	GLU	C-N	-7.86	1.24	1.33
3	C	191	ARG	C-N	-7.85	1.24	1.33
4	D	665	ARG	C-N	-7.85	1.22	1.33
4	D	81	GLU	C-N	7.83	1.44	1.33
2	B	151	HIS	C-N	7.82	1.44	1.33
5	E	12	PRO	N-CD	-7.81	1.36	1.47
7	G	26	GLU	C-N	-7.80	1.22	1.33
4	D	210	LEU	C-N	7.78	1.44	1.33
2	B	242	ASN	C-N	-7.78	1.23	1.33
6	F	74	GLU	C-N	7.77	1.43	1.33
5	E	100	ALA	C-N	-7.77	1.24	1.33
8	H	221	ARG	C-N	-7.77	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	660	ARG	C-N	7.76	1.43	1.33
2	B	356	LEU	C-N	-7.75	1.24	1.33
3	C	41	PRO	N-CD	-7.74	1.36	1.47
2	B	183	THR	C-N	7.74	1.44	1.33
5	E	8	SER	C-N	-7.72	1.22	1.33
7	G	296	ALA	C-N	-7.72	1.23	1.33
6	F	198	LEU	C-N	-7.71	1.23	1.33
2	B	42	TRP	C-N	-7.71	1.24	1.33
6	F	81	PRO	N-CD	-7.70	1.37	1.47
6	F	80	TRP	C-N	-7.69	1.19	1.34
7	G	174	PRO	N-CD	-7.68	1.36	1.47
3	C	346	GLN	C-N	-7.68	1.23	1.34
1	A	256	LYS	C-N	7.68	1.44	1.33
4	D	190	PRO	C-N	7.67	1.44	1.33
2	B	462	PHE	C-N	7.66	1.44	1.33
6	F	177	LYS	C-N	-7.66	1.23	1.33
6	F	185	GLU	C-N	-7.66	1.24	1.33
1	A	200	LEU	C-N	-7.65	1.23	1.33
7	G	259	GLU	C-N	7.65	1.44	1.33
8	H	225	LEU	C-N	-7.64	1.24	1.33
2	B	36	LEU	C-N	-7.63	1.22	1.33
4	D	371	ALA	C-N	7.63	1.44	1.33
2	B	224	GLY	C-N	-7.61	1.22	1.33
8	H	252	THR	C-N	-7.58	1.23	1.33
3	C	352	LEU	C-N	7.57	1.46	1.34
7	G	238	LEU	C-N	-7.57	1.24	1.33
8	H	240	LYS	C-N	-7.56	1.23	1.33
5	E	141	PHE	C-N	-7.55	1.24	1.33
2	B	435	PRO	C-N	-7.53	1.23	1.33
6	F	169	ALA	C-N	-7.53	1.24	1.33
4	D	661	ALA	C-N	-7.52	1.20	1.33
6	F	98	TRP	C-N	-7.51	1.24	1.33
6	F	63	LEU	C-N	7.51	1.43	1.33
6	F	179	LEU	C-N	-7.49	1.24	1.33
4	D	47	ILE	C-N	-7.45	1.23	1.33
2	B	595	SER	C-N	7.45	1.44	1.33
2	B	352	GLY	C-N	-7.45	1.24	1.33
4	D	236	SER	C-N	-7.42	1.23	1.33
7	G	30	LEU	C-N	-7.41	1.22	1.33
1	A	219	GLU	C-N	-7.40	1.23	1.33
3	C	151	ARG	C-N	7.40	1.44	1.33
4	D	309	LEU	C-N	-7.39	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	212	ALA	C-N	-7.39	1.24	1.33
5	E	46	ALA	C-N	-7.38	1.23	1.33
7	G	32	ASP	C-N	7.36	1.45	1.33
8	H	170	LEU	C-N	-7.35	1.24	1.33
1	A	224	LEU	C-N	7.35	1.43	1.33
7	G	139	GLU	C-N	7.35	1.44	1.33
4	D	23	GLN	C-N	-7.33	1.23	1.33
2	B	435	PRO	N-CD	-7.33	1.37	1.47
5	E	139	VAL	C-N	-7.32	1.24	1.33
4	D	17	GLU	C-N	7.32	1.44	1.33
6	F	385	TRP	C-N	-7.30	1.24	1.33
8	H	200	ASP	C-N	-7.30	1.24	1.33
2	B	503	HIS	C-N	-7.29	1.24	1.33
6	F	365	GLU	C-N	-7.29	1.24	1.33
2	B	234	GLU	C-N	7.28	1.43	1.33
7	G	346	LEU	C-N	-7.27	1.23	1.33
8	H	307	THR	C-N	-7.27	1.24	1.33
6	F	249	LYS	C-N	-7.25	1.24	1.33
6	F	359	ARG	C-N	7.25	1.43	1.33
3	C	315	SER	C-N	7.25	1.43	1.33
7	G	55	CYS	C-N	7.24	1.43	1.34
4	D	222	GLY	C-N	-7.23	1.22	1.33
1	A	102	LEU	C-N	7.22	1.43	1.33
7	G	106	PHE	C-N	-7.21	1.24	1.33
2	B	463	ARG	C-N	7.21	1.43	1.33
7	G	17	LEU	C-N	-7.20	1.24	1.33
2	B	249	ASP	C-N	7.19	1.44	1.33
5	E	129	ARG	C-N	-7.18	1.24	1.34
8	H	242	PRO	N-CD	-7.18	1.37	1.47
5	E	170	MET	C-N	-7.17	1.24	1.33
4	D	389	CYS	C-N	7.17	1.43	1.33
2	B	23	ASP	C-N	-7.16	1.22	1.33
4	D	593	GLU	C-N	-7.13	1.24	1.34
5	E	89	GLN	C-N	-7.13	1.24	1.33
2	B	457	ASN	C-N	7.13	1.43	1.33
5	E	135	LEU	C-N	-7.12	1.24	1.34
4	D	305	PRO	C-N	-7.11	1.23	1.33
2	B	71	VAL	C-N	7.11	1.43	1.33
1	A	205	MET	C-N	7.09	1.43	1.33
4	D	330	LEU	C-N	-7.08	1.24	1.33
8	H	310	ASP	C-N	-7.08	1.24	1.33
7	G	293	GLU	C-N	-7.08	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	188	LEU	C-N	-7.07	1.21	1.33
7	G	241	ALA	C-N	-7.07	1.24	1.33
2	B	458	THR	C-N	-7.06	1.23	1.33
2	B	338	VAL	C-N	-7.05	1.24	1.33
2	B	225	MET	C-N	-7.05	1.24	1.33
4	D	232	GLN	C-N	-7.04	1.24	1.33
8	H	217	GLN	C-N	-7.02	1.23	1.33
4	D	218	SER	C-N	-7.00	1.24	1.33
1	A	182	LEU	C-N	-6.97	1.24	1.33
7	G	300	GLU	C-N	-6.97	1.25	1.33
6	F	184	LYS	C-N	-6.96	1.24	1.33
2	B	82	LYS	C-N	-6.96	1.23	1.33
4	D	373	LEU	C-N	-6.96	1.25	1.33
5	E	130	PHE	C-N	-6.95	1.24	1.33
2	B	279	LYS	C-N	-6.92	1.25	1.33
6	F	298	ASP	C-N	-6.92	1.24	1.33
8	H	362	PHE	C-N	6.92	1.43	1.33
3	C	325	GLU	C-N	6.91	1.43	1.33
2	B	220	HIS	C-N	-6.89	1.24	1.33
4	D	592	LEU	C-N	-6.89	1.24	1.33
7	G	93	PHE	C-N	6.89	1.42	1.33
3	C	223	ILE	C-N	-6.87	1.23	1.33
4	D	476	LYS	C-N	-6.86	1.24	1.33
5	E	87	LYS	C-N	-6.85	1.24	1.33
2	B	94	GLU	C-N	-6.85	1.24	1.33
6	F	392	CYS	C-N	-6.85	1.25	1.33
3	C	309	THR	C-N	-6.84	1.25	1.33
7	G	171	ASN	C-N	-6.84	1.27	1.33
7	G	292	LEU	C-N	-6.80	1.25	1.33
2	B	240	GLN	C-N	-6.80	1.24	1.33
8	H	230	ASP	C-N	-6.80	1.24	1.34
6	F	78	TYR	C-N	-6.78	1.22	1.33
1	A	143	LYS	C-N	-6.78	1.25	1.33
6	F	116	SER	C-N	6.78	1.41	1.34
1	A	231	ALA	C-N	6.77	1.43	1.33
6	F	382	GLU	C-N	6.77	1.43	1.33
4	D	76	ARG	C-N	6.76	1.42	1.33
4	D	238	ALA	C-N	-6.76	1.25	1.33
6	F	58	VAL	C-N	-6.76	1.25	1.33
2	B	512	TYR	C-N	-6.76	1.24	1.34
4	D	82	GLN	C-N	-6.75	1.24	1.33
8	H	308	ILE	C-N	-6.75	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	ALA	C-N	-6.74	1.23	1.33
8	H	353	GLU	C-N	-6.74	1.25	1.34
3	C	134	LYS	C-N	-6.73	1.24	1.34
2	B	580	LEU	C-N	6.73	1.42	1.33
2	B	300	LYS	C-N	-6.72	1.24	1.33
5	E	48	GLU	C-N	-6.72	1.25	1.33
5	E	132	ALA	C-N	-6.72	1.23	1.33
8	H	198	GLN	C-N	-6.72	1.25	1.33
3	C	129	ILE	C-N	-6.68	1.24	1.33
7	G	291	GLU	C-N	-6.67	1.24	1.33
3	C	142	PRO	C-N	-6.66	1.25	1.33
3	C	310	SER	C-N	-6.66	1.24	1.34
7	G	308	VAL	C-N	-6.66	1.25	1.33
8	H	315	VAL	C-N	-6.65	1.25	1.33
3	C	179	GLU	C-N	6.63	1.42	1.33
3	C	37	PRO	N-CD	-6.62	1.38	1.47
2	B	255	LYS	C-N	6.62	1.42	1.33
2	B	434	LYS	C-N	6.61	1.49	1.33
7	G	42	THR	C-N	-6.60	1.26	1.33
8	H	192	LEU	C-N	-6.60	1.25	1.33
2	B	14	LEU	C-N	6.59	1.43	1.33
4	D	633	CYS	C-N	6.59	1.42	1.33
7	G	223	ASP	C-N	-6.59	1.24	1.33
7	G	120	GLN	C-N	-6.58	1.20	1.33
4	D	375	CYS	C-N	6.58	1.42	1.33
6	F	312	VAL	C-N	-6.58	1.25	1.33
4	D	85	ARG	C-N	-6.57	1.25	1.33
6	F	293	HIS	C-N	-6.56	1.23	1.33
2	B	572	TYR	C-N	-6.55	1.25	1.33
7	G	304	ASN	C-N	-6.55	1.25	1.33
2	B	20	ALA	C-N	6.54	1.43	1.33
7	G	182	ASN	C-N	-6.54	1.25	1.33
3	C	188	LYS	C-N	-6.53	1.26	1.33
6	F	43	PHE	C-N	6.53	1.42	1.32
6	F	18	LEU	C-N	-6.52	1.25	1.33
1	A	7	LYS	C-N	-6.51	1.25	1.33
4	D	94	LEU	C-N	6.50	1.42	1.33
4	D	366	ARG	C-N	-6.50	1.25	1.33
5	E	79	THR	C-N	-6.48	1.23	1.33
5	E	150	LYS	C-N	-6.48	1.25	1.33
5	E	92	GLN	C-N	-6.46	1.25	1.33
7	G	184	GLU	C-N	-6.45	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	149	ASN	C-N	-6.45	1.25	1.33
4	D	440	GLN	C-N	-6.45	1.25	1.33
2	B	228	PHE	C-N	-6.44	1.26	1.34
4	D	623	MET	C-N	-6.43	1.25	1.33
6	F	52	ASN	C-N	-6.42	1.25	1.33
4	D	32	GLN	C-N	6.42	1.42	1.33
4	D	361	VAL	C-N	6.42	1.42	1.33
6	F	226	LYS	C-N	6.41	1.41	1.34
4	D	477	GLU	C-N	-6.41	1.25	1.33
4	D	216	SER	C-N	6.40	1.42	1.33
4	D	516	PRO	N-CD	-6.40	1.38	1.47
6	F	255	VAL	C-N	-6.39	1.25	1.33
7	G	183	ALA	C-N	6.39	1.42	1.33
6	F	96	CYS	C-N	6.39	1.42	1.33
3	C	90	GLY	C-N	6.39	1.42	1.33
8	H	228	LYS	C-N	-6.38	1.24	1.33
4	D	286	GLU	C-N	-6.37	1.25	1.33
5	E	148	TYR	C-N	-6.37	1.25	1.33
6	F	245	MET	C-N	-6.37	1.25	1.33
8	H	277	GLU	C-N	6.36	1.42	1.33
3	C	249	ASP	C-N	-6.36	1.25	1.33
8	H	309	LYS	C-N	-6.34	1.25	1.33
1	A	15	MET	C-N	6.32	1.42	1.33
5	E	83	TYR	C-N	-6.32	1.25	1.34
7	G	284	SER	C-N	-6.31	1.25	1.33
8	H	248	THR	C-N	-6.31	1.25	1.33
4	D	44	LYS	C-N	-6.31	1.25	1.33
7	G	242	LEU	C-N	-6.31	1.25	1.33
2	B	524	GLU	C-N	-6.30	1.25	1.33
1	A	258	GLU	C-N	-6.30	1.25	1.33
4	D	332	ARG	C-N	-6.30	1.25	1.33
2	B	521	THR	C-N	6.28	1.44	1.33
7	G	33	PRO	N-CD	-6.27	1.39	1.47
8	H	337	ASN	C-N	-6.27	1.25	1.33
4	D	409	GLN	C-N	-6.27	1.25	1.33
3	C	203	LEU	C-N	6.26	1.42	1.33
2	B	83	THR	C-N	6.26	1.42	1.33
2	B	523	PRO	N-CD	-6.26	1.39	1.47
3	C	93	THR	C-N	-6.26	1.25	1.33
3	C	186	ALA	C-N	6.25	1.42	1.33
6	F	241	TRP	C-N	-6.25	1.25	1.33
3	C	51	GLU	C-N	-6.24	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	98	ALA	C-N	6.24	1.42	1.33
5	E	144	LYS	C-N	-6.24	1.25	1.33
7	G	35	SER	C-N	6.23	1.41	1.33
7	G	57	ARG	C-N	-6.21	1.25	1.33
2	B	316	LYS	C-N	6.21	1.42	1.33
4	D	19	GLY	C-N	6.21	1.44	1.33
1	A	215	VAL	C-N	-6.20	1.25	1.33
8	H	294	MET	C-N	6.18	1.41	1.33
4	D	48	ARG	C-N	-6.18	1.25	1.33
4	D	42	ILE	C-N	-6.18	1.25	1.34
2	B	525	LEU	C-N	-6.17	1.25	1.33
5	E	44	SER	C-N	-6.17	1.25	1.33
6	F	278	LEU	C-N	6.17	1.42	1.33
1	A	249	LYS	C-N	6.17	1.41	1.33
4	D	310	PRO	N-CD	-6.16	1.39	1.47
5	E	7	TRP	C-N	6.16	1.43	1.33
8	H	203	GLN	C-N	-6.16	1.25	1.33
5	E	99	GLU	C-N	-6.15	1.25	1.33
2	B	48	SER	C-N	-6.15	1.25	1.34
1	A	23	PRO	N-CD	-6.15	1.39	1.47
2	B	91	ALA	C-N	-6.15	1.25	1.33
4	D	157	TYR	C-N	-6.15	1.25	1.33
2	B	120	LYS	C-N	-6.14	1.25	1.33
4	D	658	LEU	C-N	-6.12	1.25	1.34
2	B	375	LEU	C-N	-6.12	1.25	1.33
2	B	239	VAL	C-N	-6.11	1.25	1.33
7	G	65	GLN	C-N	-6.10	1.24	1.33
3	C	142	PRO	N-CD	-6.10	1.39	1.47
8	H	276	LEU	C-N	6.10	1.42	1.33
4	D	382	ARG	C-N	6.09	1.42	1.33
7	G	12	GLU	C-N	-6.09	1.26	1.33
4	D	45	PHE	C-N	-6.08	1.26	1.33
6	F	248	LEU	C-N	-6.07	1.25	1.33
1	A	242	ALA	C-N	-6.07	1.19	1.33
2	B	423	MET	C-N	-6.07	1.25	1.33
2	B	510	PHE	C-N	-6.05	1.24	1.33
2	B	74	GLU	C-N	6.05	1.41	1.33
6	F	303	ALA	C-N	6.05	1.42	1.33
7	G	178	LYS	C-N	6.04	1.41	1.33
6	F	134	ALA	C-N	-6.04	1.26	1.33
2	B	70	PRO	C-N	-6.03	1.27	1.33
3	C	173	HIS	C-N	6.03	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	364	LEU	C-N	6.02	1.41	1.33
2	B	438	ASN	C-N	-6.00	1.26	1.33
2	B	294	ALA	C-N	5.99	1.42	1.33
3	C	58	GLU	C-N	-5.99	1.26	1.33
2	B	507	LEU	C-N	-5.99	1.26	1.33
3	C	209	LYS	C-N	-5.99	1.26	1.33
3	C	133	ASP	C-N	-5.98	1.25	1.34
2	B	39	PHE	C-N	-5.98	1.26	1.33
1	A	228	SER	C-N	-5.96	1.25	1.33
8	H	210	LYS	C-N	-5.96	1.26	1.33
1	A	118	ASP	C-N	5.96	1.41	1.33
2	B	53	VAL	C-N	-5.96	1.25	1.33
4	D	629	PRO	C-N	-5.95	1.27	1.34
8	H	363	ASP	C-N	5.95	1.41	1.34
6	F	201	LYS	C-N	-5.95	1.25	1.33
2	B	13	LYS	C-N	-5.95	1.25	1.33
1	A	146	GLU	C-N	-5.95	1.25	1.33
3	C	287	LEU	C-N	-5.95	1.26	1.33
4	D	225	ASP	C-N	-5.94	1.25	1.34
2	B	464	THR	C-N	-5.94	1.25	1.33
2	B	576	ASN	C-N	5.94	1.41	1.33
6	F	238	ARG	C-N	-5.94	1.26	1.33
8	H	305	PHE	C-N	-5.94	1.25	1.33
2	B	412	GLU	C-N	-5.93	1.26	1.33
6	F	315	LEU	C-N	-5.93	1.26	1.33
7	G	9	ALA	C-N	-5.91	1.26	1.33
2	B	92	ILE	C-N	-5.91	1.25	1.33
6	F	348	GLU	C-N	-5.90	1.26	1.33
5	E	28	LEU	C-N	-5.90	1.25	1.33
2	B	132	CYS	C-N	5.89	1.42	1.33
2	B	471	VAL	C-N	-5.89	1.26	1.33
4	D	499	LEU	C-N	-5.89	1.24	1.33
3	C	344	MET	C-N	-5.88	1.26	1.33
6	F	160	LYS	C-N	5.88	1.40	1.33
6	F	109	GLY	C-N	-5.88	1.22	1.33
5	E	171	ARG	C-N	-5.88	1.26	1.33
6	F	289	GLU	C-N	5.87	1.42	1.34
4	D	469	ARG	C-N	-5.87	1.25	1.33
2	B	359	ALA	C-N	-5.87	1.26	1.33
4	D	1	MET	C-N	-5.87	1.26	1.33
2	B	499	LYS	C-N	-5.87	1.26	1.33
4	D	384	ALA	C-N	-5.86	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	81	LEU	C-N	5.86	1.41	1.34
5	E	101	VAL	C-N	-5.86	1.25	1.33
6	F	254	GLU	C-N	-5.85	1.26	1.33
3	C	330	GLU	C-N	-5.85	1.26	1.33
4	D	585	SER	C-N	-5.85	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	328	SER	C-N	-5.84	1.26	1.33
8	H	326	PHE	C-N	-5.83	1.26	1.33
2	B	251	THR	C-N	-5.83	1.25	1.33
6	F	87	ARG	C-N	-5.83	1.26	1.33
6	F	90	GLU	C-N	5.83	1.41	1.33
8	H	173	LEU	C-N	-5.82	1.26	1.33
1	A	168	GLU	C-N	-5.82	1.26	1.33
3	C	62	GLN	C-N	-5.82	1.26	1.33
2	B	133	LEU	C-N	-5.81	1.26	1.33
6	F	138	MET	C-N	-5.81	1.26	1.33
4	D	643	THR	C-N	5.81	1.41	1.33
4	D	628	GLN	C-N	-5.81	1.27	1.34
1	A	79	PRO	N-CD	-5.80	1.39	1.47
7	G	202	ASN	C-N	-5.80	1.26	1.33
6	F	171	ASN	C-N	-5.80	1.26	1.33
7	G	218	LYS	C-N	-5.79	1.25	1.34
4	D	93	ILE	C-N	5.78	1.41	1.33
6	F	26	GLU	C-N	-5.78	1.26	1.33
6	F	178	TYR	C-N	-5.78	1.26	1.33
6	F	168	LEU	C-N	-5.77	1.26	1.33
6	F	57	TYR	C-N	-5.76	1.26	1.33
7	G	123	ASP	C-N	-5.76	1.25	1.33
7	G	4	GLY	C-N	5.76	1.41	1.33
6	F	280	ILE	C-N	-5.75	1.25	1.33
4	D	437	SER	C-N	-5.75	1.26	1.33
7	G	59	TYR	C-N	5.75	1.40	1.33
5	E	45	HIS	C-N	-5.75	1.26	1.33
1	A	214	LEU	C-N	-5.74	1.26	1.33
1	A	225	LYS	C-N	-5.74	1.26	1.33
1	A	251	LYS	C-N	-5.74	1.26	1.33
2	B	261	ARG	C-N	-5.73	1.26	1.33
3	C	29	GLY	C-N	5.73	1.41	1.33
4	D	586	LEU	C-N	-5.72	1.26	1.33
2	B	290	ALA	C-N	-5.72	1.26	1.34
3	C	80	LEU	C-N	-5.71	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	101	GLY	C-N	5.70	1.41	1.33
7	G	69	LEU	C-N	5.70	1.41	1.33
7	G	110	SER	C-N	-5.69	1.26	1.33
3	C	312	GLN	C-N	5.68	1.41	1.33
8	H	258	ARG	C-N	-5.68	1.25	1.33
6	F	158	GLN	C-N	5.68	1.41	1.33
8	H	257	THR	C-N	-5.68	1.25	1.33
5	E	13	SER	C-N	-5.67	1.26	1.33
3	C	71	VAL	C-N	-5.67	1.26	1.33
2	B	431	SER	C-N	5.66	1.41	1.33
5	E	189	TRP	C-N	-5.65	1.26	1.33
4	D	290	PRO	C-N	-5.65	1.25	1.33
7	G	294	SER	C-N	-5.65	1.26	1.33
6	F	47	MET	C-N	5.65	1.41	1.33
2	B	467	GLY	C-N	-5.64	1.26	1.33
5	E	159	PRO	C-N	-5.64	1.26	1.33
2	B	55	ASP	C-N	-5.63	1.26	1.33
2	B	354	TYR	C-N	-5.63	1.26	1.33
3	C	25	ASN	C-N	5.63	1.41	1.33
4	D	27	SER	C-N	-5.63	1.25	1.33
8	H	214	THR	C-N	-5.63	1.26	1.33
1	A	238	TYR	C-N	5.61	1.42	1.33
6	F	14	GLU	C-N	-5.60	1.26	1.34
6	F	182	LEU	C-N	-5.59	1.26	1.33
2	B	588	GLU	C-N	5.58	1.41	1.33
7	G	34	GLN	C-N	5.58	1.41	1.33
2	B	80	VAL	C-N	-5.58	1.26	1.34
6	F	212	ALA	C-N	-5.57	1.26	1.34
3	C	143	PRO	N-CD	-5.57	1.40	1.47
3	C	222	GLU	C-N	5.56	1.40	1.33
6	F	101	LYS	C-N	5.56	1.40	1.33
2	B	347	MET	C-N	5.55	1.41	1.34
5	E	216	SER	C-N	-5.54	1.27	1.34
7	G	84	LEU	C-N	-5.54	1.26	1.33
4	D	578	ASP	C-N	5.54	1.41	1.33
4	D	177	ALA	C-N	-5.53	1.26	1.33
5	E	77	ASP	C-N	-5.53	1.27	1.33
7	G	334	LEU	C-N	-5.52	1.26	1.33
7	G	70	LYS	C-N	-5.49	1.26	1.33
1	A	175	ARG	C-N	-5.49	1.26	1.33
3	C	351	SER	C-N	5.48	1.45	1.33
8	H	189	GLU	C-N	-5.48	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	56	ARG	C-N	-5.48	1.26	1.33
7	G	245	PHE	C-N	-5.47	1.26	1.33
2	B	451	GLN	C-N	-5.46	1.26	1.33
4	D	397	ALA	C-N	5.46	1.41	1.33
3	C	302	LYS	C-N	-5.46	1.25	1.33
2	B	254	ASP	C-N	-5.46	1.26	1.33
7	G	215	LYS	C-N	-5.46	1.26	1.33
2	B	485	GLN	C-N	-5.45	1.26	1.33
4	D	71	HIS	C-N	-5.44	1.26	1.33
5	E	56	LYS	C-N	-5.43	1.26	1.33
2	B	378	GLN	C-N	-5.43	1.26	1.33
3	C	317	TYR	C-N	-5.43	1.26	1.33
2	B	358	MET	C-N	-5.42	1.26	1.33
4	D	136	ALA	C-N	-5.41	1.26	1.33
5	E	43	PHE	C-N	-5.41	1.26	1.33
7	G	297	GLN	C-N	-5.41	1.26	1.33
7	G	24	CYS	C-N	-5.41	1.25	1.33
6	F	342	HIS	C-N	5.40	1.40	1.33
2	B	69	LYS	C-N	-5.39	1.27	1.33
2	B	539	LEU	C-N	-5.38	1.26	1.34
6	F	356	ARG	C-N	5.38	1.41	1.33
1	A	80	SER	C-N	5.38	1.41	1.33
4	D	517	TYR	C-N	-5.37	1.27	1.33
4	D	426	HIS	C-N	-5.37	1.27	1.33
6	F	3	SER	C-N	-5.37	1.25	1.33
5	E	55	ILE	C-N	-5.37	1.26	1.33
4	D	436	SER	C-N	-5.36	1.26	1.33
8	H	211	ARG	C-N	-5.36	1.26	1.33
2	B	271	HIS	C-N	-5.36	1.26	1.33
6	F	165	GLN	C-N	-5.35	1.26	1.33
5	E	155	ILE	C-N	5.35	1.40	1.34
7	G	307	ASP	C-N	-5.35	1.27	1.33
7	G	330	LYS	C-N	-5.35	1.26	1.33
4	D	329	GLU	C-N	-5.35	1.27	1.33
2	B	84	PHE	C-N	-5.35	1.25	1.33
4	D	182	LEU	C-N	5.35	1.41	1.33
7	G	116	LEU	C-N	-5.34	1.26	1.33
2	B	257	LYS	C-N	-5.34	1.26	1.33
3	C	73	TYR	C-N	-5.32	1.26	1.33
1	A	60	ALA	C-N	-5.32	1.26	1.33
4	D	607	GLN	C-N	-5.31	1.26	1.33
1	A	252	ILE	C-N	5.31	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	SER	C-N	-5.31	1.26	1.33
7	G	169	GLU	C-N	-5.30	1.26	1.33
1	A	210	THR	C-N	5.29	1.40	1.33
1	A	139	SER	C-N	-5.28	1.26	1.33
1	A	127	GLU	C-N	5.28	1.41	1.33
7	G	147	ARG	C-N	-5.28	1.27	1.33
3	C	336	ASP	C-N	5.28	1.41	1.33
6	F	376	ASP	C-N	-5.28	1.26	1.33
6	F	139	LEU	C-N	5.28	1.41	1.34
3	C	177	THR	C-N	5.26	1.41	1.33
4	D	199	VAL	C-N	5.26	1.41	1.33
4	D	183	SER	C-N	5.26	1.41	1.33
5	E	19	LEU	C-N	-5.25	1.27	1.33
4	D	3	ARG	C-N	-5.25	1.27	1.33
7	G	180	LEU	C-N	-5.24	1.26	1.33
4	D	505	LEU	C-N	-5.24	1.26	1.34
1	A	68	TYR	C-N	-5.24	1.26	1.33
2	B	581	LYS	C-N	-5.22	1.26	1.33
7	G	131	LEU	C-N	-5.22	1.26	1.33
7	G	239	ARG	C-N	-5.22	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
6	F	305	LYS	C-N	-5.21	1.25	1.33
4	D	664	SER	C-N	5.21	1.41	1.33
2	B	268	CYS	C-N	-5.21	1.26	1.33
7	G	60	PRO	C-N	5.20	1.40	1.33
8	H	199	LYS	C-N	-5.20	1.26	1.33
4	D	462	GLU	C-N	-5.20	1.27	1.33
1	A	250	VAL	C-N	5.19	1.41	1.34
4	D	509	ARG	C-N	5.19	1.40	1.33
2	B	201	LYS	C-N	-5.19	1.27	1.33
2	B	419	GLU	C-N	-5.18	1.26	1.33
3	C	238	ALA	C-N	-5.18	1.26	1.33
1	A	167	PHE	C-N	-5.17	1.26	1.33
4	D	146	GLU	C-N	-5.16	1.26	1.33
4	D	92	GLU	C-N	-5.16	1.27	1.33
6	F	333	GLY	C-N	-5.16	1.27	1.33
2	B	153	LEU	C-N	5.16	1.40	1.33
4	D	568	GLN	C-N	5.15	1.41	1.33
8	H	313	ASN	C-N	-5.15	1.27	1.33
6	F	123	GLY	C-N	-5.15	1.26	1.34
6	F	370	ILE	C-N	-5.14	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	70	ARG	C-N	-5.14	1.26	1.33
7	G	128	ASN	C-N	5.14	1.40	1.33
2	B	202	TYR	C-N	-5.14	1.27	1.33
1	A	233	GLU	C-N	-5.13	1.26	1.33
2	B	384	LEU	C-N	-5.12	1.27	1.33
6	F	204	ARG	C-N	-5.12	1.26	1.33
8	H	316	LEU	C-N	-5.11	1.26	1.33
1	A	202	SER	C-N	-5.11	1.25	1.33
2	B	146	PHE	C-N	5.11	1.41	1.34
7	G	212	SER	C-N	-5.11	1.26	1.34
8	H	183	ARG	C-N	-5.10	1.27	1.33
2	B	531	GLN	C-N	-5.10	1.27	1.33
1	A	132	GLU	C-N	-5.10	1.26	1.33
5	E	63	SER	C-N	-5.09	1.27	1.33
3	C	210	HIS	C-N	-5.09	1.27	1.33
7	G	298	PHE	C-N	-5.08	1.27	1.33
5	E	41	PRO	C-N	5.07	1.40	1.33
8	H	235	PRO	N-CD	-5.07	1.40	1.47
7	G	40	LEU	C-N	5.07	1.41	1.33
6	F	83	LEU	C-N	5.06	1.40	1.33
8	H	273	HIS	C-N	-5.05	1.27	1.33
6	F	219	LEU	C-N	5.05	1.41	1.33
3	C	256	GLU	C-N	-5.04	1.27	1.33
2	B	230	GLU	C-N	5.04	1.40	1.33
2	B	25	GLU	C-N	5.04	1.40	1.33
2	B	299	ASP	C-N	-5.03	1.26	1.33
4	D	603	ARG	C-N	-5.03	1.27	1.33
6	F	115	ALA	C-N	5.01	1.40	1.34
2	B	38	PRO	C-N	-5.01	1.27	1.33
2	B	325	HIS	C-N	-5.01	1.27	1.33
8	H	347	ALA	C-N	-5.00	1.27	1.33

All (880) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	122	PRO	O-C-N	-34.35	80.93	121.46
4	D	301	THR	O-C-N	-31.89	90.60	122.18
4	D	178	VAL	O-C-N	-30.38	84.60	122.57
4	D	221	PRO	O-C-N	-29.47	82.85	122.64
4	D	304	ASP	O-C-N	-28.47	88.58	121.32
7	G	130	ILE	O-C-N	-27.98	87.59	122.57
3	C	352	LEU	O-C-N	-27.89	89.25	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	228	VAL	O-C-N	-25.93	90.15	122.57
3	C	117	THR	O-C-N	-25.91	88.14	122.59
4	D	286	GLU	O-C-N	-25.90	88.14	122.59
6	F	1	MET	CA-C-N	24.40	168.14	121.54
6	F	1	MET	C-N-CA	24.40	168.14	121.54
4	D	306	GLN	O-C-N	-22.75	92.34	122.59
1	A	275	PHE	O-C-N	-22.52	97.71	122.03
1	A	282	LYS	O-C-N	-22.30	92.93	122.59
2	B	591	THR	O-C-N	-22.26	93.48	122.19
4	D	216	SER	O-C-N	-21.74	90.42	121.72
7	G	137	SER	O-C-N	-21.66	93.78	122.59
4	D	284	LEU	O-C-N	-21.65	93.80	122.59
2	B	234	GLU	O-C-N	-21.03	94.62	122.59
1	A	283	ARG	O-C-N	-21.00	89.40	123.00
1	A	284	ARG	CA-C-N	20.79	158.14	122.79
1	A	284	ARG	C-N-CA	20.79	158.14	122.79
5	E	221	HIS	O-C-N	-20.39	99.99	121.60
1	A	277	VAL	O-C-N	-20.37	97.88	121.10
4	D	186	THR	O-C-N	-19.60	96.52	122.59
2	B	88	LYS	O-C-N	-18.66	97.77	122.59
3	C	119	ASP	O-C-N	-17.93	98.75	122.59
2	B	594	GLY	O-C-N	-17.77	99.59	122.70
4	D	175	PHE	O-C-N	-16.84	103.01	123.05
2	B	245	SER	O-C-N	-16.84	102.96	122.15
2	B	236	PHE	O-C-N	-16.62	100.49	122.59
2	B	596	SER	O-C-N	-16.49	100.66	122.59
2	B	231	GLY	O-C-N	-16.43	101.35	122.70
6	F	295	LEU	O-C-N	-16.32	104.11	122.55
7	G	127	SER	O-C-N	-16.22	93.14	122.34
1	A	280	PRO	CA-C-N	16.10	146.63	122.65
1	A	280	PRO	C-N-CA	16.10	146.63	122.65
2	B	222	PHE	O-C-N	-15.96	101.28	122.83
1	A	283	ARG	CA-C-N	15.81	149.38	122.82
1	A	283	ARG	C-N-CA	15.81	149.38	122.82
5	E	39	GLU	O-C-N	-15.41	102.27	122.61
2	B	249	ASP	O-C-N	-15.38	102.08	122.38
1	A	281	SER	O-C-N	15.22	141.00	123.19
2	B	84	PHE	O-C-N	-15.22	103.35	122.68
2	B	238	LEU	O-C-N	-15.22	102.35	122.59
1	A	278	PRO	O-C-N	-15.19	102.13	122.64
2	B	246	PHE	O-C-N	-15.04	102.58	122.59
2	B	16	TYR	O-C-N	-14.98	108.28	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	123	ASP	O-C-N	-14.97	102.67	122.59
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
2	B	92	ILE	O-C-N	-14.80	104.08	122.57
3	C	122	PRO	CA-C-N	-14.74	101.42	119.84
3	C	122	PRO	C-N-CA	-14.74	101.42	119.84
4	D	662	THR	O-C-N	-14.32	101.11	121.72
2	B	181	PRO	O-C-N	-14.30	103.33	122.64
5	E	220	LEU	O-C-N	-14.26	103.62	122.59
4	D	184	SER	O-C-N	-14.21	103.30	122.33
7	G	129	VAL	CA-C-N	14.12	147.38	121.97
7	G	129	VAL	C-N-CA	14.12	147.38	121.97
1	A	277	VAL	CA-C-N	-13.99	102.36	119.84
1	A	277	VAL	C-N-CA	-13.99	102.36	119.84
2	B	95	VAL	O-C-N	-13.83	105.28	122.57
2	B	16	TYR	CA-C-N	13.55	135.19	119.47
2	B	16	TYR	C-N-CA	13.55	135.19	119.47
6	F	6	ARG	O-C-N	-13.52	105.77	121.32
2	B	592	GLY	O-C-N	-13.31	105.40	122.70
1	A	242	ALA	O-C-N	-13.23	110.53	121.38
4	D	302	HIS	O-C-N	-12.97	107.42	122.20
4	D	279	GLY	CA-C-N	12.92	135.99	119.84
4	D	279	GLY	C-N-CA	12.92	135.99	119.84
7	G	133	SER	O-C-N	-12.91	105.42	122.59
2	B	223	GLU	CA-C-N	12.77	142.56	122.51
2	B	223	GLU	C-N-CA	12.77	142.56	122.51
4	D	280	PRO	O-C-N	-12.76	105.42	122.64
3	C	118	ALA	O-C-N	-12.67	105.74	122.59
3	C	351	SER	O-C-N	-12.66	106.06	122.39
4	D	219	VAL	O-C-N	-12.63	106.78	122.57
2	B	225	MET	O-C-N	-12.56	105.12	122.46
7	G	196	LYS	CA-C-N	12.56	146.02	121.41
7	G	196	LYS	C-N-CA	12.56	146.02	121.41
7	G	124	THR	CA-C-N	12.52	144.51	121.97
7	G	124	THR	C-N-CA	12.52	144.51	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
2	B	23	ASP	CA-C-N	12.33	135.66	120.13
2	B	23	ASP	C-N-CA	12.33	135.66	120.13
2	B	432	ALA	CA-C-N	-12.15	101.93	121.26
2	B	432	ALA	C-N-CA	-12.15	101.93	121.26
3	C	123	PRO	O-C-N	-12.08	106.33	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	593	GLY	O-C-N	-12.06	107.02	122.70
1	A	276	VAL	CA-C-N	12.03	144.38	122.13
1	A	276	VAL	C-N-CA	12.03	144.38	122.13
6	F	224	ASP	O-C-N	-11.96	107.39	122.34
7	G	130	ILE	CA-C-N	11.89	137.18	120.29
7	G	130	ILE	C-N-CA	11.89	137.18	120.29
4	D	183	SER	O-C-N	-11.77	106.94	122.59
4	D	287	PHE	CA-C-N	11.62	143.73	121.54
4	D	287	PHE	C-N-CA	11.62	143.73	121.54
4	D	663	GLY	CA-C-N	-11.62	103.67	122.26
4	D	663	GLY	C-N-CA	-11.62	103.67	122.26
6	F	3	SER	O-C-N	-11.61	110.33	122.64
4	D	289	GLU	CA-C-N	11.59	134.33	119.84
4	D	289	GLU	C-N-CA	11.59	134.33	119.84
1	A	244	ASN	CA-C-N	11.49	132.42	119.32
1	A	244	ASN	C-N-CA	11.49	132.42	119.32
2	B	242	ASN	O-C-N	-11.48	107.31	122.59
1	A	281	SER	CA-C-N	-11.45	99.67	121.54
1	A	281	SER	C-N-CA	-11.45	99.67	121.54
4	D	280	PRO	CA-C-N	-11.42	102.32	120.60
4	D	280	PRO	C-N-CA	-11.42	102.32	120.60
7	G	183	ALA	CA-C-N	11.39	137.34	121.05
7	G	183	ALA	C-N-CA	11.39	137.34	121.05
7	G	230	ASP	O-C-N	-11.30	107.56	122.59
3	C	344	MET	O-C-N	-11.29	109.89	122.09
6	F	146	ALA	O-C-N	-11.22	108.82	122.96
4	D	220	HIS	CA-C-N	11.20	133.84	119.84
4	D	220	HIS	C-N-CA	11.20	133.84	119.84
2	B	93	GLU	O-C-N	-11.19	107.71	122.59
6	F	223	VAL	O-C-N	-11.18	111.27	122.23
1	A	284	ARG	O-C-N	-11.18	107.63	122.94
3	C	320	LEU	CA-C-N	11.16	139.39	121.87
3	C	320	LEU	C-N-CA	11.16	139.39	121.87
2	B	96	ALA	O-C-N	-11.10	107.83	122.59
6	F	225	ARG	O-C-N	-11.10	110.35	122.12
5	E	43	PHE	CA-C-N	11.06	135.10	120.28
5	E	43	PHE	C-N-CA	11.06	135.10	120.28
1	A	236	ASN	O-C-N	-10.96	109.39	122.22
4	D	218	SER	O-C-N	-10.92	108.07	122.59
8	H	156	PRO	O-C-N	-10.90	107.93	122.64
7	G	272	SER	O-C-N	-10.89	110.39	121.28
2	B	242	ASN	CA-C-N	10.85	141.50	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	ASN	C-N-CA	10.85	141.50	121.97
3	C	320	LEU	O-C-N	-10.84	104.97	122.42
2	B	237	GLN	CA-C-N	10.81	142.19	121.54
2	B	237	GLN	C-N-CA	10.81	142.19	121.54
5	E	2	MET	O-C-N	-10.70	108.36	122.59
6	F	159	SER	O-C-N	-10.60	108.36	122.57
2	B	2	SER	O-C-N	-10.55	108.98	123.01
2	B	223	GLU	O-C-N	-10.54	110.41	123.06
3	C	344	MET	CA-C-N	10.42	134.24	120.28
3	C	344	MET	C-N-CA	10.42	134.24	120.28
4	D	177	ALA	O-C-N	-10.35	109.25	123.01
2	B	456	ASP	O-C-N	-10.32	108.73	122.57
2	B	229	VAL	O-C-N	-10.31	108.54	122.05
6	F	8	HIS	O-C-N	-10.29	108.26	122.46
3	C	119	ASP	CA-C-N	-10.18	103.67	120.87
3	C	119	ASP	C-N-CA	-10.18	103.67	120.87
7	G	128	ASN	O-C-N	-10.17	109.06	122.59
6	F	6	ARG	CA-C-N	10.17	132.55	119.84
6	F	6	ARG	C-N-CA	10.17	132.55	119.84
6	F	227	ILE	O-C-N	-10.13	108.77	122.05
7	G	132	GLU	O-C-N	-10.00	109.30	122.59
6	F	228	SER	O-C-N	-9.96	109.34	122.59
1	A	234	LYS	O-C-N	-9.95	109.09	122.43
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
2	B	88	LYS	CA-C-N	-9.93	103.77	122.13
2	B	88	LYS	C-N-CA	-9.93	103.77	122.13
3	C	348	LEU	O-C-N	-9.90	110.87	122.15
6	F	2	GLN	CA-C-N	9.85	138.09	123.12
6	F	2	GLN	C-N-CA	9.85	138.09	123.12
3	C	342	ARG	O-C-N	9.83	133.36	122.15
2	B	595	SER	O-C-N	-9.82	109.53	122.59
2	B	240	GLN	O-C-N	-9.81	109.54	122.59
2	B	230	GLU	O-C-N	-9.79	109.57	122.59
1	A	238	TYR	O-C-N	-9.76	110.67	122.48
3	C	280	CYS	O-C-N	-9.71	109.61	122.23
2	B	241	LEU	O-C-N	-9.68	109.72	122.59
4	D	386	MET	O-C-N	9.66	132.36	122.12
2	B	591	THR	CA-C-N	9.64	140.31	121.41
2	B	591	THR	C-N-CA	9.64	140.31	121.41
4	D	576	ASN	O-C-N	9.63	130.57	120.85
6	F	108	ALA	O-C-N	-9.58	109.25	122.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	ASP	O-C-N	-9.56	112.13	123.13
4	D	175	PHE	CA-C-N	9.53	134.67	121.05
4	D	175	PHE	C-N-CA	9.53	134.67	121.05
3	C	321	GLY	CA-C-N	9.52	129.75	119.28
3	C	321	GLY	C-N-CA	9.52	129.75	119.28
7	G	226	SER	CA-C-N	9.51	135.09	121.02
7	G	226	SER	C-N-CA	9.51	135.09	121.02
1	A	215	VAL	O-C-N	9.49	131.08	121.87
7	G	272	SER	CA-C-N	9.39	131.58	119.84
7	G	272	SER	C-N-CA	9.39	131.58	119.84
4	D	628	GLN	CA-C-N	9.32	129.56	119.87
4	D	628	GLN	C-N-CA	9.32	129.56	119.87
4	D	665	ARG	CA-C-N	-9.31	104.94	121.70
4	D	665	ARG	C-N-CA	-9.31	104.94	121.70
1	A	241	LEU	O-C-N	-9.27	111.45	123.13
2	B	556	MET	O-C-N	-9.24	112.32	122.12
7	G	197	GLY	O-C-N	-9.24	110.69	122.70
4	D	404	LYS	O-C-N	9.20	131.88	122.12
7	G	199	ASP	O-C-N	-9.20	109.85	122.46
1	A	228	SER	O-C-N	-9.20	111.67	122.15
8	H	255	ASP	O-C-N	-9.18	111.48	122.22
1	A	217	LEU	CA-C-N	9.15	132.55	120.28
1	A	217	LEU	C-N-CA	9.15	132.55	120.28
5	E	42	CYS	CA-C-N	9.13	135.67	122.35
5	E	42	CYS	C-N-CA	9.13	135.67	122.35
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
2	B	458	THR	O-C-N	-9.12	110.47	122.59
5	E	42	CYS	O-C-N	-9.11	111.65	123.21
7	G	28	VAL	O-C-N	-9.07	109.92	122.62
4	D	176	SER	CA-C-N	9.06	134.42	121.02
4	D	176	SER	C-N-CA	9.06	134.42	121.02
5	E	43	PHE	O-C-N	-9.05	110.53	122.47
3	C	347	GLU	O-C-N	-8.99	111.21	122.27
4	D	288	SER	O-C-N	-8.99	110.63	122.59
4	D	308	THR	O-C-N	-8.91	110.74	122.59
5	E	4	ALA	O-C-N	-8.90	110.75	122.59
1	A	191	TYR	O-C-N	-8.89	112.01	122.15
1	A	279	GLU	O-C-N	-8.89	108.77	123.00
2	B	459	GLN	O-C-N	-8.89	110.77	122.59
2	B	250	GLY	CA-C-N	8.88	133.42	120.90
2	B	250	GLY	C-N-CA	8.88	133.42	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	SER	CA-C-N	-8.87	109.64	122.77
2	B	188	SER	C-N-CA	-8.87	109.64	122.77
4	D	221	PRO	CA-C-N	8.82	138.70	121.41
4	D	221	PRO	C-N-CA	8.82	138.70	121.41
2	B	82	LYS	O-C-N	8.81	132.53	122.22
1	A	221	LEU	O-C-N	-8.79	112.81	122.12
6	F	3	SER	CA-C-N	8.76	138.57	121.41
6	F	3	SER	C-N-CA	8.76	138.57	121.41
4	D	216	SER	CA-C-N	8.74	138.24	121.54
4	D	216	SER	C-N-CA	8.74	138.24	121.54
6	F	216	GLN	CA-C-N	8.67	132.61	120.29
6	F	216	GLN	C-N-CA	8.67	132.61	120.29
1	A	274	GLU	O-C-N	-8.66	111.89	122.11
1	A	228	SER	CA-C-N	8.61	132.52	120.29
1	A	228	SER	C-N-CA	8.61	132.52	120.29
7	G	70	LYS	CA-C-N	8.61	132.17	120.38
7	G	70	LYS	C-N-CA	8.61	132.17	120.38
4	D	279	GLY	O-C-N	-8.60	113.17	121.77
6	F	76	PHE	CA-C-N	8.60	132.16	120.38
6	F	76	PHE	C-N-CA	8.60	132.16	120.38
3	C	316	SER	CA-C-N	8.56	132.45	120.29
3	C	316	SER	C-N-CA	8.56	132.45	120.29
4	D	665	ARG	O-C-N	-8.56	111.20	122.59
1	A	191	TYR	CA-C-N	8.53	133.27	120.31
1	A	191	TYR	C-N-CA	8.53	133.27	120.31
1	A	221	LEU	CA-C-N	8.53	131.71	120.28
1	A	221	LEU	C-N-CA	8.53	131.71	120.28
2	B	240	GLN	CA-C-N	8.52	137.81	121.54
2	B	240	GLN	C-N-CA	8.52	137.81	121.54
6	F	220	ALA	O-C-N	-8.49	111.20	122.23
6	F	5	SER	O-C-N	-8.48	111.31	122.59
4	D	359	SER	O-C-N	-8.47	113.13	123.04
8	H	258	ARG	O-C-N	-8.41	110.47	122.41
6	F	216	GLN	O-C-N	-8.40	112.58	122.15
7	G	275	GLY	CA-C-N	8.36	128.06	119.19
7	G	275	GLY	C-N-CA	8.36	128.06	119.19
1	A	234	LYS	CA-C-N	8.35	134.85	120.58
1	A	234	LYS	C-N-CA	8.35	134.85	120.58
1	A	285	LEU	O-C-N	-8.35	110.68	122.03
2	B	228	PHE	O-C-N	-8.34	110.86	122.37
4	D	458	PRO	O-C-N	-8.31	110.98	122.37
1	A	217	LEU	O-C-N	-8.29	112.70	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	348	LEU	CA-C-N	8.29	131.21	120.44
3	C	348	LEU	C-N-CA	8.29	131.21	120.44
5	E	5	ASN	O-C-N	-8.26	111.83	121.32
2	B	47	ALA	O-C-N	-8.25	113.03	122.93
6	F	209	GLU	CA-C-N	8.23	131.31	120.28
6	F	209	GLU	C-N-CA	8.23	131.31	120.28
2	B	186	GLU	O-C-N	-8.21	111.67	122.59
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	-8.17	112.84	122.15
4	D	290	PRO	CA-C-N	-8.15	107.31	121.97
4	D	290	PRO	C-N-CA	-8.15	107.31	121.97
4	D	455	LYS	O-C-N	-8.12	111.48	122.36
1	A	202	SER	O-C-N	-8.10	112.31	122.27
1	A	224	LEU	O-C-N	-8.09	112.92	122.15
4	D	223	LYS	O-C-N	-8.08	111.22	122.37
1	A	224	LEU	CA-C-N	8.07	131.10	120.28
1	A	224	LEU	C-N-CA	8.07	131.10	120.28
5	E	3	ALA	O-C-N	-8.06	111.87	122.59
2	B	185	CYS	CA-C-N	-8.05	106.17	121.54
2	B	185	CYS	C-N-CA	-8.05	106.17	121.54
4	D	176	SER	O-C-N	-8.05	113.40	123.06
4	D	575	THR	O-C-N	-8.02	112.05	122.39
2	B	235	ASN	CA-C-N	8.01	136.84	121.54
2	B	235	ASN	C-N-CA	8.01	136.84	121.54
7	G	274	MET	O-C-N	-7.94	111.58	122.46
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	-7.93	113.53	122.09
6	F	146	ALA	CA-C-N	7.91	132.45	120.82
6	F	146	ALA	C-N-CA	7.91	132.45	120.82
2	B	91	ALA	O-C-N	-7.89	112.10	122.59
7	G	275	GLY	O-C-N	-7.88	113.89	121.77
1	A	274	GLU	CA-C-N	7.88	131.34	120.63
1	A	274	GLU	C-N-CA	7.88	131.34	120.63
4	D	535	ALA	CA-C-N	7.85	127.56	119.56
4	D	535	ALA	C-N-CA	7.85	127.56	119.56
3	C	293	ARG	O-C-N	7.84	131.09	122.15
1	A	237	SER	O-C-N	-7.83	111.65	122.46
2	B	86	ILE	CA-C-N	-7.82	109.45	121.02
2	B	86	ILE	C-N-CA	-7.82	109.45	121.02
4	D	576	ASN	C-N-CD	-7.78	103.48	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	515	ALA	CA-C-N	7.77	127.82	119.28
4	D	515	ALA	C-N-CA	7.77	127.82	119.28
5	E	38	LEU	CA-C-N	-7.76	110.73	122.21
5	E	38	LEU	C-N-CA	-7.76	110.73	122.21
3	C	181	GLY	CA-C-N	7.74	131.43	120.28
3	C	181	GLY	C-N-CA	7.74	131.43	120.28
4	D	5	SER	O-C-N	-7.73	114.11	122.07
2	B	432	ALA	O-C-N	-7.72	112.33	122.59
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
5	E	217	ILE	O-C-N	-7.66	113.33	122.06
4	D	282	CYS	CA-C-N	7.63	131.97	121.05
4	D	282	CYS	C-N-CA	7.63	131.97	121.05
7	G	196	LYS	O-C-N	-7.63	112.34	122.57
3	C	120	SER	CA-C-N	7.59	136.18	122.13
3	C	120	SER	C-N-CA	7.59	136.18	122.13
2	B	182	GLU	O-C-N	-7.55	112.54	122.59
8	H	305	PHE	O-C-N	-7.54	114.25	122.09
7	G	59	TYR	CA-C-N	7.54	128.14	120.38
7	G	59	TYR	C-N-CA	7.54	128.14	120.38
2	B	304	LYS	O-C-N	-7.53	113.00	123.01
7	G	146	ILE	O-C-N	7.52	129.28	121.91
1	A	231	ALA	CA-C-N	7.50	130.94	120.29
1	A	231	ALA	C-N-CA	7.50	130.94	120.29
4	D	281	SER	O-C-N	-7.50	112.64	122.39
7	G	70	LYS	O-C-N	-7.48	114.04	122.86
8	H	232	VAL	O-C-N	-7.47	114.91	122.23
7	G	135	SER	CA-C-N	-7.46	110.30	120.82
7	G	135	SER	C-N-CA	-7.46	110.30	120.82
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
4	D	38	GLN	CA-C-N	7.44	131.61	120.31
4	D	38	GLN	C-N-CA	7.44	131.61	120.31
4	D	5	SER	CA-C-N	7.43	130.24	120.28
4	D	5	SER	C-N-CA	7.43	130.24	120.28
2	B	549	ASP	CA-C-N	7.43	130.84	120.29
2	B	549	ASP	C-N-CA	7.43	130.84	120.29
6	F	276	ALA	O-C-N	-7.42	113.62	122.46
4	D	17	GLU	O-C-N	-7.42	113.20	122.17
7	G	133	SER	CA-C-N	7.41	135.69	121.54
7	G	133	SER	C-N-CA	7.41	135.69	121.54
5	E	41	PRO	O-C-N	7.38	131.50	123.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	205	LYS	O-C-N	7.33	129.89	122.12
7	G	126	SER	CA-C-N	-7.31	107.70	122.55
7	G	126	SER	C-N-CA	-7.31	107.70	122.55
4	D	119	LEU	CA-C-N	-7.29	111.69	122.41
4	D	119	LEU	C-N-CA	-7.29	111.69	122.41
2	B	184	ALA	CA-C-N	-7.27	110.53	120.28
2	B	184	ALA	C-N-CA	-7.27	110.53	120.28
1	A	243	PRO	O-C-N	-7.27	112.83	122.64
7	G	273	PRO	O-C-N	-7.27	112.83	122.64
3	C	338	ILE	O-C-N	7.22	128.88	121.87
7	G	178	LYS	O-C-N	7.22	127.50	120.71
7	G	127	SER	CA-C-N	-7.21	107.76	121.54
7	G	127	SER	C-N-CA	-7.21	107.76	121.54
4	D	184	SER	CA-C-N	-7.21	107.77	121.54
4	D	184	SER	C-N-CA	-7.21	107.77	121.54
7	G	167	SER	O-C-N	7.16	127.26	121.17
2	B	556	MET	CA-C-N	7.13	132.81	120.68
2	B	556	MET	C-N-CA	7.13	132.81	120.68
2	B	250	GLY	O-C-N	-7.13	113.43	122.70
4	D	386	MET	CA-C-N	-7.13	111.17	120.44
4	D	386	MET	C-N-CA	-7.13	111.17	120.44
6	F	84	ASP	CA-C-N	7.12	129.82	120.28
6	F	84	ASP	C-N-CA	7.12	129.82	120.28
6	F	229	ASP	O-C-N	-7.12	112.65	122.19
1	A	194	HIS	O-C-N	7.08	131.43	122.23
2	B	222	PHE	CA-C-N	7.02	131.09	121.05
2	B	222	PHE	C-N-CA	7.02	131.09	121.05
4	D	217	SER	O-C-N	-6.99	113.30	122.59
2	B	244	ASN	O-C-N	-6.99	113.68	122.27
2	B	256	CYS	O-C-N	6.95	129.49	122.12
2	B	431	SER	CA-C-N	6.94	134.80	121.54
2	B	431	SER	C-N-CA	6.94	134.80	121.54
6	F	366	ASP	O-C-N	-6.94	114.60	122.09
1	A	78	GLY	CA-C-N	6.92	127.07	119.87
1	A	78	GLY	C-N-CA	6.92	127.07	119.87
2	B	521	THR	O-C-N	6.92	131.06	123.10
3	C	347	GLU	CA-C-N	6.91	130.10	120.29
3	C	347	GLU	C-N-CA	6.91	130.10	120.29
1	A	236	ASN	CA-C-N	6.90	134.85	121.18
1	A	236	ASN	C-N-CA	6.90	134.85	121.18
4	D	177	ALA	CA-C-N	6.89	134.37	121.97
4	D	177	ALA	C-N-CA	6.89	134.37	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	HIS	O-C-N	6.87	129.40	122.12
7	G	74	THR	O-C-N	-6.86	114.84	122.12
3	C	268	LYS	O-C-N	6.82	129.46	122.09
4	D	303	LEU	CA-C-N	-6.82	105.17	121.80
4	D	303	LEU	C-N-CA	-6.82	105.17	121.80
4	D	425	LYS	O-C-N	-6.81	114.90	122.12
7	G	184	GLU	O-C-N	-6.81	114.89	123.06
7	G	20	LEU	CA-C-N	6.80	132.05	122.46
7	G	20	LEU	C-N-CA	6.80	132.05	122.46
6	F	333	GLY	CA-C-N	6.77	130.18	120.98
6	F	333	GLY	C-N-CA	6.77	130.18	120.98
8	H	324	ARG	O-C-N	6.75	129.03	122.07
8	H	363	ASP	CA-C-N	6.75	131.48	123.44
8	H	363	ASP	C-N-CA	6.75	131.48	123.44
4	D	201	LYS	O-C-N	6.75	129.02	122.07
4	D	631	GLN	O-C-N	-6.74	113.40	122.43
2	B	552	LEU	CA-C-N	6.73	129.84	120.29
2	B	552	LEU	C-N-CA	6.73	129.84	120.29
1	A	244	ASN	O-C-N	-6.72	113.46	121.12
1	A	231	ALA	O-C-N	-6.72	113.49	122.23
2	B	433	SER	O-C-N	-6.71	113.87	123.07
4	D	82	GLN	CA-C-N	6.71	129.57	120.44
4	D	82	GLN	C-N-CA	6.71	129.57	120.44
4	D	397	ALA	O-C-N	6.69	129.78	122.15
2	B	126	SER	O-C-N	6.66	129.75	122.15
6	F	1	MET	O-C-N	-6.64	112.37	123.00
4	D	379	ARG	O-C-N	6.64	129.16	122.12
2	B	547	LEU	O-C-N	6.63	129.71	122.15
1	A	199	GLN	CA-C-N	6.63	129.70	120.29
1	A	199	GLN	C-N-CA	6.63	129.70	120.29
6	F	209	GLU	O-C-N	-6.62	114.61	122.15
2	B	311	ARG	O-C-N	-6.61	115.26	122.07
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
4	D	62	ASN	O-C-N	6.57	129.08	122.12
6	F	106	VAL	O-C-N	-6.56	114.38	121.80
2	B	457	ASN	CA-C-N	-6.55	109.04	121.54
2	B	457	ASN	C-N-CA	-6.55	109.04	121.54
2	B	544	VAL	O-C-N	6.54	128.56	121.83
3	C	342	ARG	CA-C-N	-6.54	111.52	120.28
3	C	342	ARG	C-N-CA	-6.54	111.52	120.28
2	B	304	LYS	CA-C-N	6.54	134.02	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	LYS	C-N-CA	6.54	134.02	121.54
6	F	321	LEU	O-C-N	6.52	129.03	122.12
3	C	125	ASP	CA-C-N	-6.51	113.51	122.30
3	C	125	ASP	C-N-CA	-6.51	113.51	122.30
2	B	299	ASP	O-C-N	-6.51	113.48	122.46
5	E	213	SER	CA-C-N	-6.51	110.42	120.31
5	E	213	SER	C-N-CA	-6.51	110.42	120.31
8	H	271	ASN	CA-C-N	6.51	129.29	120.38
8	H	271	ASN	C-N-CA	6.51	129.29	120.38
5	E	5	ASN	CA-C-N	6.50	127.96	119.84
5	E	5	ASN	C-N-CA	6.50	127.96	119.84
2	B	90	PRO	O-C-N	-6.49	113.88	122.64
4	D	21	PRO	CA-C-N	6.48	129.84	120.38
4	D	21	PRO	C-N-CA	6.48	129.84	120.38
2	B	295	SER	CA-C-N	6.48	131.27	120.64
2	B	295	SER	C-N-CA	6.48	131.27	120.64
8	H	214	THR	O-C-N	-6.47	114.77	122.15
7	G	101	GLY	O-C-N	-6.46	114.69	122.38
3	C	340	ASP	O-C-N	-6.45	115.43	122.07
7	G	129	VAL	O-C-N	-6.45	114.51	122.57
8	H	305	PHE	CA-C-N	6.45	129.44	120.29
8	H	305	PHE	C-N-CA	6.45	129.44	120.29
7	G	228	VAL	CA-C-N	-6.43	111.83	120.90
7	G	228	VAL	C-N-CA	-6.43	111.83	120.90
2	B	65	LYS	O-C-N	6.43	128.94	122.12
7	G	339	GLU	O-C-N	6.43	129.48	122.15
2	B	85	SER	O-C-N	-6.41	114.48	123.01
2	B	185	CYS	O-C-N	-6.39	115.35	122.12
2	B	593	GLY	CA-C-N	6.39	133.93	121.41
2	B	593	GLY	C-N-CA	6.39	133.93	121.41
2	B	48	SER	CA-C-N	6.38	129.47	120.28
2	B	48	SER	C-N-CA	6.38	129.47	120.28
4	D	425	LYS	CA-C-N	6.38	129.34	120.29
4	D	425	LYS	C-N-CA	6.38	129.34	120.29
8	H	304	SER	CA-C-N	6.37	129.13	120.54
8	H	304	SER	C-N-CA	6.37	129.13	120.54
4	D	185	SER	CA-C-N	6.35	133.66	121.54
4	D	185	SER	C-N-CA	6.35	133.66	121.54
7	G	274	MET	CA-C-N	6.35	131.83	121.87
7	G	274	MET	C-N-CA	6.35	131.83	121.87
5	E	41	PRO	CA-C-N	-6.34	113.73	122.93
5	E	41	PRO	C-N-CA	-6.34	113.73	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	124	GLU	CA-C-N	6.34	129.42	120.28
5	E	124	GLU	C-N-CA	6.34	129.42	120.28
5	E	58	GLU	CA-C-N	6.33	129.13	120.46
5	E	58	GLU	C-N-CA	6.33	129.13	120.46
8	H	238	THR	O-C-N	-6.32	114.50	122.27
2	B	299	ASP	CA-C-N	6.32	132.20	121.14
2	B	299	ASP	C-N-CA	6.32	132.20	121.14
6	F	213	LEU	CA-C-N	6.31	128.74	120.28
6	F	213	LEU	C-N-CA	6.31	128.74	120.28
2	B	539	LEU	CA-C-N	6.30	129.35	120.28
2	B	539	LEU	C-N-CA	6.30	129.35	120.28
7	G	122	PRO	O-C-N	-6.29	114.14	122.64
7	G	3	GLY	O-C-N	-6.28	114.53	122.70
1	A	238	TYR	CA-C-N	6.28	131.32	120.58
1	A	238	TYR	C-N-CA	6.28	131.32	120.58
6	F	58	VAL	CA-C-N	6.28	129.07	120.46
6	F	58	VAL	C-N-CA	6.28	129.07	120.46
1	A	280	PRO	O-C-N	6.28	130.80	123.01
5	E	103	ARG	O-C-N	-6.27	114.88	122.22
2	B	549	ASP	O-C-N	-6.26	115.48	122.12
7	G	184	GLU	CA-C-N	6.24	133.46	121.54
7	G	184	GLU	C-N-CA	6.24	133.46	121.54
4	D	38	GLN	O-C-N	-6.23	114.08	122.43
4	D	404	LYS	CA-C-N	-6.23	111.93	120.28
4	D	404	LYS	C-N-CA	-6.23	111.93	120.28
6	F	304	GLY	O-C-N	-6.23	114.43	122.34
6	F	163	ASP	O-C-N	-6.20	116.21	121.23
2	B	588	GLU	CA-C-N	6.19	128.57	120.28
2	B	588	GLU	C-N-CA	6.19	128.57	120.28
4	D	35	PHE	O-C-N	6.19	129.87	122.26
8	H	200	ASP	O-C-N	-6.19	115.10	122.15
5	E	58	GLU	O-C-N	-6.18	115.56	122.12
2	B	101	GLU	O-C-N	6.17	128.67	122.12
7	G	242	LEU	O-C-N	6.16	129.17	122.15
4	D	151	SER	CA-C-N	6.15	128.52	120.28
4	D	151	SER	C-N-CA	6.15	128.52	120.28
6	F	224	ASP	CA-C-N	-6.15	112.04	120.28
6	F	224	ASP	C-N-CA	-6.15	112.04	120.28
4	D	25	ALA	CA-C-N	6.15	126.16	119.89
4	D	25	ALA	C-N-CA	6.15	126.16	119.89
3	C	269	LEU	CA-C-N	6.14	129.01	120.29
3	C	269	LEU	C-N-CA	6.14	129.01	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	282	ASN	O-C-N	6.14	128.63	122.12
4	D	181	ASP	CA-C-N	-6.14	109.82	121.54
4	D	181	ASP	C-N-CA	-6.14	109.82	121.54
6	F	76	PHE	O-C-N	-6.13	114.95	122.25
6	F	64	PHE	O-C-N	6.13	128.62	122.12
2	B	388	GLY	O-C-N	-6.11	116.24	122.17
2	B	491	GLN	O-C-N	6.11	129.11	122.15
3	C	313	ILE	CA-C-N	6.11	129.07	120.28
3	C	313	ILE	C-N-CA	6.11	129.07	120.28
8	H	285	ILE	O-C-N	6.10	128.11	121.83
7	G	198	LYS	O-C-N	-6.08	114.50	122.59
7	G	74	THR	CA-C-N	6.08	128.43	120.28
7	G	74	THR	C-N-CA	6.08	128.43	120.28
4	D	25	ALA	O-C-N	-6.08	116.14	121.31
4	D	188	LEU	CA-C-N	6.07	131.85	121.35
4	D	188	LEU	C-N-CA	6.07	131.85	121.35
6	F	77	ARG	CA-C-N	-6.07	112.53	122.54
6	F	77	ARG	C-N-CA	-6.07	112.53	122.54
4	D	173	VAL	O-C-N	-6.07	115.25	122.77
2	B	539	LEU	O-C-N	-6.06	115.70	122.12
3	C	340	ASP	CA-C-N	6.05	128.39	120.28
3	C	340	ASP	C-N-CA	6.05	128.39	120.28
4	D	286	GLU	CA-C-N	-6.03	112.15	120.71
4	D	286	GLU	C-N-CA	-6.03	112.15	120.71
2	B	311	ARG	CA-C-N	6.03	128.38	120.60
2	B	311	ARG	C-N-CA	6.03	128.38	120.60
6	F	296	GLN	O-C-N	-6.01	114.59	122.59
4	D	593	GLU	O-C-N	-6.01	115.30	122.15
5	E	220	LEU	CA-C-N	-6.01	111.42	121.03
5	E	220	LEU	C-N-CA	-6.01	111.42	121.03
5	E	216	SER	O-C-N	-6.01	114.58	122.39
2	B	541	HIS	O-C-N	6.00	128.99	122.15
4	D	411	GLN	O-C-N	5.99	128.47	122.12
4	D	648	ARG	O-C-N	5.99	128.47	122.12
7	G	243	THR	CA-C-N	5.99	128.22	120.44
7	G	243	THR	C-N-CA	5.99	128.22	120.44
6	F	389	LEU	O-C-N	-5.99	114.47	122.49
2	B	251	THR	O-C-N	-5.98	115.67	122.97
3	C	312	GLN	CA-C-N	5.98	128.91	120.42
3	C	312	GLN	C-N-CA	5.98	128.91	120.42
4	D	181	ASP	O-C-N	-5.98	115.78	122.12
6	F	114	VAL	O-C-N	-5.97	117.05	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	319	PHE	O-C-N	-5.97	114.44	122.43
4	D	358	GLY	O-C-N	-5.96	115.13	122.23
6	F	11	TRP	O-C-N	-5.96	115.24	122.22
2	B	235	ASN	O-C-N	-5.95	114.67	122.59
4	D	147	ALA	O-C-N	-5.95	115.37	122.15
3	C	308	SER	CA-C-N	5.95	128.53	120.44
3	C	308	SER	C-N-CA	5.95	128.53	120.44
2	B	295	SER	O-C-N	-5.94	114.26	122.46
1	A	259	LEU	CA-C-N	5.93	128.71	120.29
1	A	259	LEU	C-N-CA	5.93	128.71	120.29
4	D	63	LEU	O-C-N	5.93	128.18	122.07
7	G	30	LEU	O-C-N	-5.93	116.46	123.22
6	F	77	ARG	O-C-N	5.93	128.40	122.12
2	B	91	ALA	CA-C-N	-5.92	111.32	121.97
2	B	91	ALA	C-N-CA	-5.92	111.32	121.97
2	B	552	LEU	O-C-N	-5.91	115.71	122.09
4	D	664	SER	O-C-N	-5.91	114.58	122.38
1	A	203	ALA	CA-C-N	5.90	131.44	120.87
1	A	203	ALA	C-N-CA	5.90	131.44	120.87
1	A	163	GLU	O-C-N	5.90	128.88	122.15
3	C	301	LYS	CA-C-N	5.90	128.19	120.28
3	C	301	LYS	C-N-CA	5.90	128.19	120.28
1	A	259	LEU	O-C-N	-5.89	115.44	122.15
3	C	298	ALA	CA-C-N	5.88	126.47	120.00
3	C	298	ALA	C-N-CA	5.88	126.47	120.00
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
6	F	37	THR	CA-C-N	5.87	129.99	120.60
6	F	37	THR	C-N-CA	5.87	129.99	120.60
2	B	546	ILE	CA-C-N	5.86	128.62	120.29
2	B	546	ILE	C-N-CA	5.86	128.62	120.29
7	G	199	ASP	CA-C-N	5.86	130.50	120.71
7	G	199	ASP	C-N-CA	5.86	130.50	120.71
4	D	290	PRO	O-C-N	-5.86	114.73	122.64
8	H	214	THR	CA-C-N	5.84	128.59	120.29
8	H	214	THR	C-N-CA	5.84	128.59	120.29
4	D	70	GLN	O-C-N	5.84	128.16	122.09
4	D	87	LYS	O-C-N	5.84	128.31	122.12
3	C	305	GLN	CA-C-N	5.83	128.10	120.28
3	C	305	GLN	C-N-CA	5.83	128.10	120.28
4	D	394	GLU	O-C-N	5.83	128.31	122.12
2	B	123	MET	O-C-N	5.83	128.39	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ALA	O-C-N	-5.82	113.78	122.39
6	F	79	CYS	O-C-N	-5.81	115.89	122.23
2	B	112	ASN	O-C-N	5.80	128.27	122.12
4	D	630	VAL	O-C-N	-5.80	114.45	122.05
4	D	185	SER	O-C-N	-5.78	114.90	122.59
3	C	180	GLU	CA-C-N	5.76	127.04	120.53
3	C	180	GLU	C-N-CA	5.76	127.04	120.53
4	D	220	HIS	O-C-N	-5.75	114.71	121.32
6	F	6	ARG	C-N-CD	-5.75	101.43	125.00
7	G	124	THR	O-C-N	-5.73	114.97	122.59
4	D	630	VAL	CA-C-N	5.73	130.28	120.72
4	D	630	VAL	C-N-CA	5.73	130.28	120.72
1	A	202	SER	CA-C-N	5.72	133.37	121.94
1	A	202	SER	C-N-CA	5.72	133.37	121.94
5	E	158	ILE	O-C-N	-5.71	116.01	120.07
6	F	191	GLU	CA-C-N	5.71	127.94	120.28
6	F	191	GLU	C-N-CA	5.71	127.94	120.28
4	D	158	ARG	CA-C-N	5.70	127.92	120.28
4	D	158	ARG	C-N-CA	5.70	127.92	120.28
6	F	333	GLY	O-C-N	-5.70	115.29	122.70
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
6	F	114	VAL	CA-C-N	5.69	128.47	120.28
6	F	114	VAL	C-N-CA	5.69	128.47	120.28
3	C	280	CYS	CA-C-N	5.69	132.69	123.37
3	C	280	CYS	C-N-CA	5.69	132.69	123.37
2	B	358	MET	O-C-N	5.68	128.14	122.12
4	D	147	ALA	CA-C-N	5.67	128.34	120.29
4	D	147	ALA	C-N-CA	5.67	128.34	120.29
2	B	234	GLU	CA-C-N	5.67	132.36	121.54
2	B	234	GLU	C-N-CA	5.67	132.36	121.54
2	B	572	TYR	CA-C-N	5.66	127.87	120.28
2	B	572	TYR	C-N-CA	5.66	127.87	120.28
4	D	538	SER	CA-C-N	5.66	127.69	120.56
4	D	538	SER	C-N-CA	5.66	127.69	120.56
2	B	581	LYS	O-C-N	5.65	128.11	122.12
2	B	431	SER	O-C-N	5.64	130.09	122.59
3	C	223	ILE	CA-C-N	5.64	127.81	120.26
3	C	223	ILE	C-N-CA	5.64	127.81	120.26
8	H	273	HIS	O-C-N	5.64	128.58	122.15
1	A	270	VAL	CA-C-N	5.63	128.09	120.44
1	A	270	VAL	C-N-CA	5.63	128.09	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	76	ALA	O-C-N	-5.62	115.74	122.15
4	D	19	GLY	O-C-N	-5.62	115.76	122.33
1	A	270	VAL	O-C-N	-5.61	114.43	121.84
2	B	247	GLY	O-C-N	-5.61	115.41	122.70
4	D	48	ARG	O-C-N	-5.61	114.04	122.28
6	F	36	LYS	O-C-N	-5.61	116.63	123.19
8	H	255	ASP	CA-C-N	5.60	132.28	121.18
8	H	255	ASP	C-N-CA	5.60	132.28	121.18
8	H	176	LYS	CA-C-N	5.60	127.72	120.44
8	H	176	LYS	C-N-CA	5.60	127.72	120.44
3	C	293	ARG	CA-C-N	-5.60	112.78	120.28
3	C	293	ARG	C-N-CA	-5.60	112.78	120.28
2	B	155	VAL	O-C-N	5.59	127.71	121.90
4	D	35	PHE	CA-C-N	-5.59	115.16	122.37
4	D	35	PHE	C-N-CA	-5.59	115.16	122.37
7	G	106	PHE	O-C-N	5.59	128.04	122.12
3	C	39	LEU	O-C-N	-5.59	116.68	123.27
2	B	178	PHE	O-C-N	-5.58	115.11	122.42
3	C	244	LEU	CA-C-N	-5.57	115.81	122.44
3	C	244	LEU	C-N-CA	-5.57	115.81	122.44
3	C	331	TYR	O-C-N	5.57	128.02	122.12
2	B	52	VAL	O-C-N	-5.56	116.15	122.94
7	G	282	HIS	O-C-N	-5.56	116.25	122.03
3	C	15	LEU	CA-C-N	-5.56	113.44	122.34
3	C	15	LEU	C-N-CA	-5.56	113.44	122.34
4	D	593	GLU	CA-C-N	5.56	128.76	120.31
4	D	593	GLU	C-N-CA	5.56	128.76	120.31
7	G	3	GLY	CA-C-N	5.56	132.31	121.41
7	G	3	GLY	C-N-CA	5.56	132.31	121.41
1	A	160	LYS	O-C-N	5.55	128.00	122.12
6	F	226	LYS	O-C-N	-5.55	112.35	122.34
1	A	279	GLU	CA-C-N	-5.54	114.07	119.78
1	A	279	GLU	C-N-CA	-5.54	114.07	119.78
6	F	58	VAL	O-C-N	-5.54	116.13	121.90
6	F	123	GLY	CA-C-N	5.54	125.20	119.05
6	F	123	GLY	C-N-CA	5.54	125.20	119.05
6	F	207	ARG	O-C-N	5.54	128.47	122.15
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	235	LEU	CA-C-N	5.53	128.24	120.28
1	A	235	LEU	C-N-CA	5.53	128.24	120.28
2	B	233	ASP	O-C-N	-5.53	115.23	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	329	GLU	CA-C-N	5.52	127.62	120.44
4	D	329	GLU	C-N-CA	5.52	127.62	120.44
6	F	110	PHE	CA-C-N	5.52	125.47	119.78
6	F	110	PHE	C-N-CA	5.52	125.47	119.78
4	D	627	GLU	O-C-N	-5.52	114.53	122.36
1	A	237	SER	CA-C-N	5.51	131.15	122.11
1	A	237	SER	C-N-CA	5.51	131.15	122.11
4	D	440	GLN	CA-C-N	5.51	128.01	120.46
4	D	440	GLN	C-N-CA	5.51	128.01	120.46
2	B	459	GLN	CA-C-N	-5.51	112.87	121.02
2	B	459	GLN	C-N-CA	-5.51	112.87	121.02
5	E	150	LYS	O-C-N	5.51	127.96	122.12
4	D	623	MET	CA-C-N	5.50	127.65	120.28
4	D	623	MET	C-N-CA	5.50	127.65	120.28
4	D	631	GLN	CA-C-N	5.50	131.18	122.60
4	D	631	GLN	C-N-CA	5.50	131.18	122.60
2	B	105	LYS	O-C-N	5.50	128.42	122.15
4	D	188	LEU	O-C-N	-5.50	116.03	122.96
6	F	137	VAL	O-C-N	-5.50	116.54	121.87
7	G	172	PRO	O-C-N	-5.50	113.73	122.52
5	E	76	ALA	CA-C-N	5.49	129.39	120.60
5	E	76	ALA	C-N-CA	5.49	129.39	120.60
8	H	304	SER	O-C-N	-5.49	114.88	122.46
6	F	10	ALA	O-C-N	-5.49	116.17	122.09
6	F	250	GLU	O-C-N	-5.47	115.09	122.43
3	C	313	ILE	O-C-N	-5.47	116.19	121.83
8	H	344	SER	CA-C-N	5.47	127.55	120.44
8	H	344	SER	C-N-CA	5.47	127.55	120.44
1	A	199	GLN	O-C-N	-5.47	115.54	122.27
2	B	388	GLY	CA-C-N	5.47	128.05	120.29
2	B	388	GLY	C-N-CA	5.47	128.05	120.29
4	D	626	TRP	O-C-N	-5.46	115.13	122.23
7	G	178	LYS	CA-C-N	-5.46	113.28	119.28
7	G	178	LYS	C-N-CA	-5.46	113.28	119.28
7	G	273	PRO	CA-C-N	5.46	131.26	121.66
7	G	273	PRO	C-N-CA	5.46	131.26	121.66
8	H	200	ASP	CA-C-N	5.45	128.03	120.29
8	H	200	ASP	C-N-CA	5.45	128.03	120.29
2	B	584	VAL	CA-C-N	5.43	126.00	119.98
2	B	584	VAL	C-N-CA	5.43	126.00	119.98
5	E	31	ASN	O-C-N	5.42	127.87	122.12
7	G	60	PRO	O-C-N	-5.42	115.06	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	11	TRP	CA-C-N	5.42	127.55	120.28
6	F	11	TRP	C-N-CA	5.42	127.55	120.28
7	G	282	HIS	CA-C-N	5.42	127.55	120.28
7	G	282	HIS	C-N-CA	5.42	127.55	120.28
6	F	137	VAL	CA-C-N	5.42	127.49	120.44
6	F	137	VAL	C-N-CA	5.42	127.49	120.44
1	A	206	GLU	CA-C-N	5.42	126.86	120.09
1	A	206	GLU	C-N-CA	5.42	126.86	120.09
1	A	215	VAL	CA-C-N	-5.42	113.02	120.28
1	A	215	VAL	C-N-CA	-5.42	113.02	120.28
2	B	548	GLY	O-C-N	5.42	127.39	122.19
6	F	52	ASN	CA-C-N	5.42	127.98	120.29
6	F	52	ASN	C-N-CA	5.42	127.98	120.29
1	A	255	ALA	CA-C-N	5.41	127.98	120.29
1	A	255	ALA	C-N-CA	5.41	127.98	120.29
2	B	355	ASP	O-C-N	5.41	127.86	122.12
4	D	515	ALA	O-C-N	-5.41	115.73	121.30
4	D	71	HIS	O-C-N	5.41	127.85	122.12
4	D	283	GLN	CA-C-N	5.40	131.86	121.54
4	D	283	GLN	C-N-CA	5.40	131.86	121.54
2	B	553	LYS	CA-C-N	5.40	127.95	120.29
2	B	553	LYS	C-N-CA	5.40	127.95	120.29
4	D	211	HIS	CA-C-N	5.39	127.50	120.28
4	D	211	HIS	C-N-CA	5.39	127.50	120.28
5	E	95	ASN	O-C-N	5.38	127.62	122.07
3	C	308	SER	O-C-N	-5.38	116.01	122.15
7	G	28	VAL	CA-C-N	5.38	131.10	123.14
7	G	28	VAL	C-N-CA	5.38	131.10	123.14
2	B	239	VAL	CA-C-N	5.38	131.81	121.54
2	B	239	VAL	C-N-CA	5.38	131.81	121.54
7	G	22	CYS	CA-C-N	5.36	125.03	119.56
7	G	22	CYS	C-N-CA	5.36	125.03	119.56
5	E	219	ASN	O-C-N	-5.36	104.69	122.06
2	B	532	LEU	CA-C-N	5.35	125.92	119.98
2	B	532	LEU	C-N-CA	5.35	125.92	119.98
8	H	333	SER	CA-C-N	5.35	127.71	120.65
8	H	333	SER	C-N-CA	5.35	127.71	120.65
2	B	545	GLU	CA-C-N	5.34	128.01	120.42
2	B	545	GLU	C-N-CA	5.34	128.01	120.42
4	D	570	ALA	CA-C-N	5.34	127.88	120.29
4	D	570	ALA	C-N-CA	5.34	127.88	120.29
6	F	37	THR	O-C-N	-5.34	116.96	123.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	535	GLN	O-C-N	-5.34	116.46	122.12
1	A	193	ILE	O-C-N	-5.33	115.77	121.80
8	H	257	THR	O-C-N	-5.33	115.43	122.42
4	D	390	ARG	O-C-N	5.33	127.77	122.12
2	B	546	ILE	O-C-N	-5.32	116.35	121.83
2	B	92	ILE	CA-C-N	-5.32	111.38	121.54
2	B	92	ILE	C-N-CA	-5.32	111.38	121.54
3	C	309	THR	CA-C-N	5.32	127.41	120.28
3	C	309	THR	C-N-CA	5.32	127.41	120.28
6	F	34	ALA	O-C-N	-5.32	115.53	122.39
7	G	174	PRO	CA-C-N	5.32	127.84	120.29
7	G	174	PRO	C-N-CA	5.32	127.84	120.29
4	D	473	SER	O-C-N	-5.32	116.48	122.12
4	D	29	GLU	O-C-N	5.31	128.21	122.15
6	F	38	LEU	O-C-N	-5.31	115.48	122.39
5	E	39	GLU	CA-C-N	-5.31	114.23	121.61
5	E	39	GLU	C-N-CA	-5.31	114.23	121.61
6	F	211	VAL	O-C-N	5.31	127.30	121.83
4	D	306	GLN	CA-C-N	-5.29	111.43	121.54
4	D	306	GLN	C-N-CA	-5.29	111.43	121.54
7	G	132	GLU	CA-C-N	5.29	131.64	121.54
7	G	132	GLU	C-N-CA	5.29	131.64	121.54
3	C	180	GLU	O-C-N	-5.29	117.02	123.10
2	B	180	THR	O-C-N	-5.28	116.44	121.20
7	G	135	SER	O-C-N	-5.28	113.96	122.41
5	E	78	ILE	CA-C-N	-5.28	111.45	121.54
5	E	78	ILE	C-N-CA	-5.28	111.45	121.54
3	C	276	VAL	CA-C-N	5.28	127.79	120.29
3	C	276	VAL	C-N-CA	5.28	127.79	120.29
6	F	84	ASP	O-C-N	-5.28	115.39	122.94
3	C	15	LEU	O-C-N	5.28	129.51	123.02
6	F	191	GLU	O-C-N	-5.28	116.53	122.12
4	D	151	SER	O-C-N	-5.26	116.55	122.12
4	D	223	LYS	CA-C-N	5.25	129.48	120.71
4	D	223	LYS	C-N-CA	5.25	129.48	120.71
4	D	30	MET	CA-C-N	5.25	129.48	120.72
4	D	30	MET	C-N-CA	5.25	129.48	120.72
2	B	49	GLU	O-C-N	-5.25	116.08	122.22
3	C	287	LEU	CA-C-N	5.24	127.17	120.56
3	C	287	LEU	C-N-CA	5.24	127.17	120.56
1	A	250	VAL	O-C-N	5.24	127.22	121.83
4	D	58	LYS	O-C-N	5.24	127.47	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	26	GLU	O-C-N	-5.23	116.05	123.01
4	D	156	GLN	O-C-N	5.23	127.66	122.12
2	B	17	PRO	O-C-N	-5.22	115.85	122.17
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
7	G	177	PHE	CA-C-N	5.21	126.61	120.09
7	G	177	PHE	C-N-CA	5.21	126.61	120.09
3	C	312	GLN	O-C-N	-5.21	116.21	122.15
4	D	6	LEU	O-C-N	5.20	127.64	122.12
4	D	225	ASP	O-C-N	-5.20	116.61	122.12
5	E	20	GLU	O-C-N	5.20	127.63	122.12
6	F	366	ASP	CA-C-N	5.19	128.21	120.31
6	F	366	ASP	C-N-CA	5.19	128.21	120.31
4	D	399	LYS	CA-C-N	5.19	127.23	120.28
4	D	399	LYS	C-N-CA	5.19	127.23	120.28
4	D	397	ALA	CA-C-N	-5.18	113.66	120.14
4	D	397	ALA	C-N-CA	-5.18	113.66	120.14
2	B	350	VAL	O-C-N	5.18	127.28	121.90
3	C	243	ARG	O-C-N	-5.16	115.92	122.17
3	C	57	ARG	O-C-N	5.16	128.03	122.15
4	D	646	GLN	O-C-N	5.16	128.03	122.15
4	D	305	PRO	O-C-N	-5.16	115.68	122.64
3	C	68	ARG	O-C-N	5.16	127.38	122.07
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
2	B	488	VAL	O-C-N	5.15	126.96	121.91
6	F	213	LEU	O-C-N	-5.15	115.93	122.27
3	C	198	ASP	O-C-N	5.13	127.56	122.12
2	B	126	SER	CA-C-N	-5.13	114.29	119.98
2	B	126	SER	C-N-CA	-5.13	114.29	119.98
2	B	513	PRO	O-C-N	-5.13	116.08	122.23
2	B	566	GLU	O-C-N	5.12	127.55	122.12
2	B	535	GLN	CA-C-N	5.12	128.10	120.31
2	B	535	GLN	C-N-CA	5.12	128.10	120.31
7	G	26	GLU	CA-C-N	5.10	131.83	121.93
7	G	26	GLU	C-N-CA	5.10	131.83	121.93
4	D	135	ARG	O-C-N	5.09	127.32	122.07
3	C	181	GLY	O-C-N	-5.09	115.16	122.69
1	A	43	ALA	CA-C-N	5.09	127.52	120.29
1	A	43	ALA	C-N-CA	5.09	127.52	120.29
8	H	225	LEU	CA-C-N	5.08	127.64	120.42
8	H	225	LEU	C-N-CA	5.08	127.64	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	205	ASP	CA-C-N	5.08	127.51	120.29
6	F	205	ASP	C-N-CA	5.08	127.51	120.29
2	B	553	LYS	O-C-N	-5.08	116.36	122.15
2	B	249	ASP	CA-C-N	5.08	131.36	121.41
2	B	249	ASP	C-N-CA	5.08	131.36	121.41
3	C	336	ASP	CA-C-N	5.08	127.50	120.29
3	C	336	ASP	C-N-CA	5.08	127.50	120.29
2	B	22	LEU	O-C-N	-5.07	117.44	123.22
2	B	186	GLU	CA-C-N	5.06	131.21	121.54
2	B	186	GLU	C-N-CA	5.06	131.21	121.54
8	H	296	SER	O-C-N	-5.06	116.30	122.22
6	F	46	ASN	CA-C-N	5.06	127.56	120.28
6	F	46	ASN	C-N-CA	5.06	127.56	120.28
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	194	HIS	CA-C-N	-5.05	113.52	120.28
1	A	194	HIS	C-N-CA	-5.05	113.52	120.28
2	B	588	GLU	O-C-N	-5.04	116.07	122.17
4	D	30	MET	O-C-N	-5.04	116.41	122.15
8	H	258	ARG	CA-C-N	5.03	130.76	121.70
8	H	258	ARG	C-N-CA	5.03	130.76	121.70
6	F	246	GLN	CA-C-N	5.02	127.01	120.28
6	F	246	GLN	C-N-CA	5.02	127.01	120.28
4	D	417	CYS	N-CA-C	-5.02	105.70	111.07
2	B	354	TYR	O-C-N	5.02	127.24	122.07
4	D	225	ASP	CA-C-N	5.01	127.93	120.31
4	D	225	ASP	C-N-CA	5.01	127.93	120.31
6	F	202	GLN	CA-C-N	5.01	127.54	120.42
6	F	202	GLN	C-N-CA	5.01	127.54	120.42
3	C	150	VAL	CA-C-N	5.01	127.40	120.29
3	C	150	VAL	C-N-CA	5.01	127.40	120.29
4	D	198	GLU	O-C-N	5.01	127.23	122.07
7	G	131	LEU	O-C-N	-5.01	116.44	122.15

There are no chirality outliers.

All (193) 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	269	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	D	177	ALA	Mainchain
4	D	178	VAL	Mainchain
4	D	180	PRO	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	216	SER	Mainchain
4	D	217	SER	Mainchain
4	D	218	SER	Mainchain
4	D	219	VAL	Mainchain
4	D	220	HIS	Mainchain
4	D	221	PRO	Mainchain
4	D	279	GLY	Peptide
4	D	281	SER	Mainchain
4	D	284	LEU	Mainchain
4	D	286	GLU	Mainchain
4	D	288	SER	Peptide,Mainchain
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	222	0
2	B	4771	0	4789	442	0
3	C	2885	0	2956	249	0
4	D	5415	0	5449	505	0
5	E	1717	0	1726	144	0
6	F	3171	0	3250	276	0
7	G	2687	0	2656	227	0
8	H	1671	0	1682	225	0
All	All	24599	0	24868	1461	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 30.

All (1461) 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	1.57
1:A:278:PRO:HB2	1:A:279:GLU:CB	1.31	1.57
6:F:335:ARG:CZ	8:H:259:HIS:CB	1.81	1.53
2:B:490:GLU:CA	4:D:560:ARG:NH2	1.71	1.52
6:F:335:ARG:CZ	8:H:259:HIS:HB3	1.37	1.51
1:A:283:ARG:C	1:A:284:ARG:N	1.70	1.49
6:F:247:MET:HB2	8:H:240:LYS:NZ	1.23	1.48
1:A:281:SER:CB	1:A:283:ARG:HD2	1.41	1.47
2:B:402:GLU:OE2	4:D:158:ARG:CZ	1.64	1.45
1:A:280:PRO:C	1:A:281:SER:N	1.75	1.45
6:F:335:ARG:NH2	8:H:259:HIS:CG	1.86	1.44
1:A:284:ARG:C	1:A:285:LEU:N	1.69	1.44
8:H:294:MET:HE1	8:H:298:ALA:CB	1.46	1.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:HB3	3:C:114:ARG:NH2	1.18	1.43
6:F:326:ARG:NH1	8:H:295:PRO:HD3	1.30	1.42
1:A:278:PRO:CG	1:A:279:GLU:HB2	1.51	1.41
1:A:189:TYR:CD1	3:C:271:MET:HE1	1.54	1.41
6:F:335:ARG:HH21	8:H:259:HIS:CA	1.34	1.41
5:E:155:ILE:CG2	6:F:334:VAL:CG2	1.99	1.40
1:A:277:VAL:C	1:A:278:PRO:N	1.79	1.38
2:B:223:GLU:C	2:B:224:GLY:N	1.81	1.38
5:E:189:TRP:CZ3	8:H:340:ILE:HD12	1.58	1.38
2:B:131:MET:CE	3:C:85:VAL:HG21	1.51	1.38
6:F:335:ARG:NH2	8:H:259:HIS:CA	1.85	1.37
2:B:138:LYS:CD	3:C:84:GLN:NE2	1.86	1.36
4:D:307:GLU:CD	7:G:324:ILE:HD11	1.50	1.36
2:B:138:LYS:CE	3:C:84:GLN:HE22	1.37	1.35
5:E:189:TRP:CH2	8:H:340:ILE:CD1	2.09	1.34
3:C:63:ARG:NH2	4:D:535:ALA:HB2	1.43	1.33
8:H:259:HIS:C	8:H:300:GLU:OE2	1.72	1.33
1:A:138:THR:OG1	2:B:92:ILE:CD1	1.75	1.32
5:E:155:ILE:HG23	6:F:334:VAL:CG2	1.55	1.32
5:E:189:TRP:CZ3	8:H:340:ILE:CD1	2.09	1.32
1:A:58:LYS:NZ	4:D:506:SER:OG	1.62	1.32
2:B:404:GLY:HA2	4:D:459:TRP:CH2	1.63	1.32
6:F:326:ARG:HH12	8:H:295:PRO:CD	1.41	1.31
4:D:296:SER:HB3	4:D:301:THR:CG2	1.57	1.31
1:A:145:THR:HG21	4:D:69:LEU:CD1	1.61	1.31
5:E:189:TRP:CH2	8:H:340:ILE:HD12	1.64	1.30
1:A:278:PRO:CB	1:A:279:GLU:CB	2.07	1.30
4:D:662:THR:C	4:D:664:SER:H	1.32	1.29
3:C:118:ALA:C	3:C:120:SER:H	1.40	1.29
2:B:222:PHE:CD1	2:B:241:LEU:HD13	1.68	1.29
1:A:277:VAL:O	1:A:278:PRO:C	1.74	1.29
2:B:138:LYS:HD2	3:C:84:GLN:CD	1.56	1.29
6:F:377:ARG:HH12	8:H:343:GLN:CB	1.45	1.28
4:D:214:SER:OG	4:D:426:HIS:CE1	1.86	1.28
6:F:247:MET:SD	8:H:240:LYS:HG3	1.73	1.28
1:A:152:LYS:NZ	2:B:73:ASP:OD2	1.66	1.27
2:B:80:VAL:CG1	4:D:65:TRP:CZ3	2.16	1.27
1:A:278:PRO:CB	1:A:279:GLU:HB2	1.62	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:132:CYS:SG	4:D:119:LEU:HG	1.74	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LYS:NZ	3:C:84:GLN:OE1	1.69	1.25
2:B:120:LYS:NZ	3:C:171:SER:O	1.70	1.25
4:D:307:GLU:CD	7:G:324:ILE:CD1	2.08	1.25
1:A:278:PRO:CB	1:A:279:GLU:HG3	1.67	1.24
6:F:335:ARG:HH22	8:H:259:HIS:CG	1.51	1.24
4:D:296:SER:CB	4:D:301:THR:HG23	1.66	1.24
2:B:97:ILE:HD12	4:D:82:GLN:CD	1.61	1.23
4:D:307:GLU:OE2	7:G:324:ILE:HD12	1.39	1.22
8:H:359:GLN:HG2	8:H:363:ASP:OD2	1.07	1.22
5:E:60:ASN:HB3	8:H:207:HIS:CE1	1.72	1.22
3:C:63:ARG:HH22	4:D:535:ALA:CB	1.51	1.22
6:F:260:ALA:HB1	8:H:258:ARG:NH1	1.55	1.21
1:A:281:SER:OG	1:A:283:ARG:CD	1.89	1.20
2:B:138:LYS:HE3	3:C:84:GLN:NE2	1.52	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:148:LEU:HD13	2:B:80:VAL:CG2	1.72	1.20
6:F:260:ALA:CB	8:H:258:ARG:HH12	1.55	1.20
6:F:173:LEU:HD12	7:G:118:VAL:HG21	1.19	1.19
6:F:53:LYS:HE2	6:F:57:TYR:OH	1.37	1.19
2:B:132:CYS:CA	4:D:119:LEU:HD21	1.72	1.18
2:B:77:LEU:HD21	4:D:61:GLY:HA3	1.20	1.18
4:D:352:HIS:CB	4:D:366:ARG:HH21	1.56	1.18
2:B:138:LYS:CD	3:C:84:GLN:HE22	1.49	1.17
6:F:260:ALA:CB	8:H:258:ARG:NH1	2.06	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
4:D:307:GLU:OE2	7:G:324:ILE:CD1	1.92	1.16
4:D:352:HIS:HB3	4:D:366:ARG:NH2	1.59	1.16
6:F:250:GLU:OE2	8:H:244:LYS:NZ	1.77	1.16
1:A:148:LEU:CD1	2:B:80:VAL:CG2	2.23	1.16
2:B:138:LYS:HE3	3:C:84:GLN:HE22	1.04	1.16
6:F:53:LYS:CE	6:F:57:TYR:OH	1.92	1.16
6:F:359:ARG:HG3	8:H:328:GLN:OE1	1.43	1.15
7:G:143:VAL:CG2	8:H:159:MET:HE1	1.76	1.15
1:A:71:ASP:CB	3:C:114:ARG:NH2	2.09	1.15
1:A:278:PRO:CB	1:A:279:GLU:CG	2.17	1.15
2:B:132:CYS:SG	4:D:119:LEU:CG	2.33	1.15
2:B:55:ASP:OD1	4:D:49:HIS:CE1	1.99	1.15
3:C:118:ALA:O	3:C:120:SER:N	1.77	1.15
2:B:138:LYS:CE	3:C:84:GLN:NE2	1.98	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:377:ARG:NH1	8:H:343:GLN:CA	2.10	1.14
1:A:148:LEU:CD1	2:B:80:VAL:HG22	1.78	1.14
6:F:44:GLY:H	6:F:47:MET:HE2	1.03	1.14
6:F:377:ARG:HH12	8:H:343:GLN:CA	1.60	1.14
2:B:490:GLU:HA	4:D:560:ARG:NH2	0.81	1.14
2:B:55:ASP:CG	4:D:49:HIS:HE1	1.56	1.13
4:D:662:THR:C	4:D:664:SER:N	1.96	1.13
2:B:132:CYS:HA	4:D:119:LEU:CD2	1.77	1.13
4:D:214:SER:OG	4:D:426:HIS:HE1	1.22	1.12
2:B:80:VAL:CG1	4:D:65:TRP:CH2	2.32	1.12
4:D:189:GLU:OE1	4:D:197:ARG:CZ	1.98	1.12
1:A:278:PRO:HB2	1:A:279:GLU:CA	1.78	1.11
6:F:10:ALA:O	6:F:13:ARG:HG2	1.49	1.11
7:G:312:ARG:HH12	8:H:323:ALA:HB2	1.07	1.11
2:B:138:LYS:CD	3:C:84:GLN:CD	2.20	1.11
1:A:189:TYR:CD1	3:C:271:MET:CE	2.34	1.11
1:A:278:PRO:HB3	1:A:279:GLU:HG3	1.29	1.11
1:A:145:THR:HG21	4:D:69:LEU:HD11	1.24	1.10
7:G:59:TYR:HD1	7:G:62:VAL:HG23	1.00	1.10
7:G:143:VAL:HG22	8:H:159:MET:CE	1.81	1.10
1:A:152:LYS:NZ	2:B:73:ASP:CG	2.09	1.09
8:H:259:HIS:CA	8:H:300:GLU:OE2	2.00	1.09
2:B:138:LYS:CG	3:C:84:GLN:NE2	2.15	1.08
4:D:8:GLN:HG3	4:D:28:GLU:OE1	1.53	1.08
4:D:352:HIS:HB3	4:D:366:ARG:HH21	0.95	1.08
6:F:377:ARG:NH1	8:H:343:GLN:HA	1.62	1.08
3:C:63:ARG:NH2	4:D:535:ALA:CB	2.13	1.08
6:F:206:MET:CE	8:H:199:LYS:HG3	1.84	1.07
2:B:80:VAL:HG12	4:D:65:TRP:CZ3	1.85	1.07
2:B:97:ILE:HD11	4:D:82:GLN:CB	1.84	1.07
8:H:359:GLN:CG	8:H:363:ASP:OD2	2.00	1.07
1:A:281:SER:CB	1:A:283:ARG:CD	2.30	1.07
2:B:175:MET:HG3	4:D:460:PRO:HG3	1.27	1.07
6:F:377:ARG:NH1	8:H:343:GLN:CB	2.18	1.07
3:C:131:GLY:O	4:D:140:LYS:NZ	1.86	1.07
6:F:206:MET:HE1	8:H:199:LYS:CG	1.83	1.07
8:H:294:MET:CE	8:H:298:ALA:CB	2.29	1.07
2:B:567:LYS:NZ	4:D:626:TRP:O	1.88	1.07
5:E:60:ASN:HB3	8:H:207:HIS:NE2	1.68	1.07
2:B:80:VAL:HG11	4:D:65:TRP:CH2	1.89	1.06
6:F:325:GLU:OE2	6:F:325:GLU:HA	1.39	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:NZ	4:D:506:SER:CB	2.18	1.06
2:B:97:ILE:HD11	4:D:82:GLN:HB3	1.10	1.06
6:F:247:MET:CB	8:H:240:LYS:NZ	2.18	1.06
2:B:443:ASP:OD1	4:D:509:ARG:NH2	1.88	1.05
2:B:490:GLU:HA	4:D:560:ARG:CZ	1.85	1.05
7:G:280:PHE:CE1	8:H:287:LYS:HG3	1.90	1.05
1:A:278:PRO:HG2	1:A:279:GLU:HB2	1.07	1.05
6:F:173:LEU:HD12	7:G:118:VAL:CG2	1.86	1.05
2:B:77:LEU:HD21	4:D:61:GLY:CA	1.87	1.05
6:F:173:LEU:CD1	7:G:118:VAL:HG21	1.86	1.05
7:G:130:ILE:HG22	7:G:131:LEU:N	1.72	1.05
1:A:149:VAL:HG13	2:B:70:PRO:HG2	1.35	1.04
1:A:58:LYS:HZ3	4:D:506:SER:CB	1.71	1.04
2:B:138:LYS:CE	3:C:84:GLN:CD	2.31	1.04
2:B:138:LYS:HG3	3:C:84:GLN:NE2	1.73	1.04
2:B:483:ARG:HH21	4:D:549:GLN:NE2	1.57	1.03
4:D:4:ARG:HG3	4:D:32:GLN:NE2	1.73	1.03
2:B:55:ASP:CG	4:D:49:HIS:CE1	2.36	1.03
2:B:131:MET:HE3	3:C:85:VAL:HG21	1.40	1.03
5:E:155:ILE:HG21	6:F:334:VAL:CG2	1.86	1.03
5:E:189:TRP:CH2	8:H:340:ILE:HD13	1.88	1.02
7:G:143:VAL:HG22	8:H:159:MET:HE1	1.04	1.02
6:F:377:ARG:HH12	8:H:343:GLN:CG	1.72	1.02
7:G:124:THR:HG22	7:G:125:ILE:HG13	1.39	1.02
4:D:296:SER:CB	4:D:301:THR:CG2	2.28	1.02
5:E:102:LEU:CD2	7:G:255:ILE:HD12	1.88	1.02
3:C:63:ARG:HH22	4:D:535:ALA:HB2	0.99	1.01
2:B:77:LEU:CD2	4:D:61:GLY:HA3	1.89	1.01
2:B:132:CYS:HA	4:D:119:LEU:HD21	1.04	1.01
2:B:94:GLU:O	2:B:96:ALA:N	1.93	1.01
1:A:128:LEU:HD22	4:D:97:ARG:NH2	1.74	1.00
1:A:145:THR:HG21	4:D:69:LEU:HD13	1.40	1.00
2:B:138:LYS:CE	3:C:84:GLN:OE1	2.09	1.00
6:F:227:ILE:HA	8:H:223:ARG:NH2	1.75	1.00
2:B:407:VAL:HG21	4:D:459:TRP:CZ3	1.95	1.00
3:C:118:ALA:C	3:C:120:SER:N	2.07	1.00
5:E:49:LEU:HD23	8:H:196:ASN:HD22	1.24	1.00
3:C:273:GLU:OE2	4:D:614:TYR:OH	1.79	1.00
4:D:305:PRO:O	4:D:307:GLU:N	1.93	1.00
3:C:236:ARG:HH12	4:D:575:THR:HA	1.22	1.00
3:C:63:ARG:NH1	4:D:537:GLU:OE2	1.94	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:LEU:HD21	4:D:571:LEU:HD12	1.43	0.99
6:F:227:ILE:HA	8:H:223:ARG:HH22	1.27	0.99
1:A:113:ILE:HG23	3:C:172:PHE:CZ	1.96	0.99
1:A:279:GLU:CB	1:A:280:PRO:HD3	1.92	0.99
2:B:135:SER:OG	4:D:121:CYS:SG	2.10	0.99
4:D:509:ARG:HD3	4:D:521:PHE:CE2	1.98	0.99
1:A:266:LEU:HD12	3:C:345:LEU:HG	1.42	0.99
5:E:102:LEU:HD22	7:G:255:ILE:HD12	1.43	0.98
2:B:55:ASP:OD1	4:D:49:HIS:HE1	1.39	0.98
7:G:274:MET:HE1	8:H:280:GLN:N	1.78	0.98
2:B:138:LYS:CG	3:C:84:GLN:HE22	1.75	0.98
6:F:260:ALA:HB1	8:H:258:ARG:HH12	0.82	0.98
2:B:424:LEU:HD22	4:D:484:ILE:CD1	1.94	0.98
4:D:290:PRO:O	4:D:291:ILE:C	1.99	0.98
2:B:404:GLY:HA2	4:D:459:TRP:HH2	1.25	0.97
2:B:131:MET:CE	3:C:85:VAL:CG2	2.42	0.97
2:B:443:ASP:CG	4:D:509:ARG:HH22	1.72	0.97
1:A:138:THR:OG1	2:B:92:ILE:HD13	1.64	0.97
1:A:279:GLU:HB3	1:A:280:PRO:HD3	1.44	0.97
6:F:359:ARG:CG	8:H:328:GLN:OE1	2.11	0.97
4:D:509:ARG:NH1	4:D:521:PHE:HZ	1.61	0.96
6:F:326:ARG:NH1	8:H:295:PRO:CD	2.12	0.96
2:B:407:VAL:CG2	4:D:459:TRP:HZ3	1.77	0.96
4:D:137:PHE:CE2	4:D:141:ARG:NH1	2.33	0.96
1:A:278:PRO:CG	1:A:279:GLU:CB	2.39	0.96
1:A:278:PRO:HG2	1:A:279:GLU:CB	1.95	0.96
2:B:297:VAL:HG11	4:D:355:LEU:HD11	1.47	0.96
1:A:281:SER:OG	1:A:283:ARG:HD2	1.56	0.96
4:D:189:GLU:OE1	4:D:197:ARG:NH1	1.98	0.96
1:A:138:THR:OG1	2:B:92:ILE:HD12	1.62	0.96
1:A:281:SER:HB3	1:A:283:ARG:HD2	1.00	0.96
1:A:12:LEU:HB3	1:A:21:LEU:HD21	1.48	0.95
1:A:71:ASP:HB3	3:C:114:ARG:HH22	1.16	0.95
4:D:374:ARG:NH1	5:E:218:GLU:OE1	1.99	0.95
2:B:490:GLU:HG2	4:D:560:ARG:CZ	1.97	0.95
7:G:59:TYR:HD1	7:G:62:VAL:CG2	1.79	0.95
2:B:80:VAL:HG11	4:D:65:TRP:CZ3	1.97	0.94
6:F:247:MET:CE	8:H:243:PHE:HD1	1.81	0.94
1:A:189:TYR:HD1	3:C:271:MET:CE	1.77	0.94
7:G:62:VAL:HG12	7:G:66:LEU:CD1	1.96	0.94
1:A:1:MET:HE1	1:A:28:THR:HG22	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:SER:CB	4:D:152:ASN:HD21	1.80	0.94
6:F:57:TYR:OH	6:F:88:ASP:OD1	1.84	0.94
7:G:62:VAL:HG12	7:G:66:LEU:HD12	1.47	0.94
7:G:47:ARG:NH1	7:G:108:GLN:OE1	2.00	0.94
2:B:443:ASP:CG	4:D:509:ARG:NH2	2.26	0.93
4:D:137:PHE:HE2	4:D:141:ARG:NH1	1.67	0.93
2:B:84:PHE:HE2	4:D:65:TRP:CE3	1.86	0.93
2:B:120:LYS:HZ1	3:C:175:PRO:HA	1.34	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:189:GLU:CD	4:D:197:ARG:HH12	1.77	0.93
2:B:91:ALA:O	2:B:93:GLU:N	2.01	0.93
7:G:131:LEU:O	7:G:132:GLU:C	2.04	0.93
2:B:402:GLU:OE2	4:D:158:ARG:NH1	2.01	0.93
2:B:522:THR:HG23	4:D:590:TYR:CE2	2.03	0.92
4:D:658:LEU:O	4:D:662:THR:OG1	1.85	0.92
5:E:181:GLU:CD	7:G:335:ARG:HH12	1.77	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
4:D:214:SER:HG	4:D:426:HIS:CE1	1.87	0.92
6:F:260:ALA:HB3	8:H:258:ARG:NH1	1.84	0.92
1:A:152:LYS:HZ1	2:B:73:ASP:CG	1.72	0.92
2:B:2:SER:OG	2:B:28:ASP:OD1	1.88	0.92
7:G:92:HIS:HE1	7:G:93:PHE:CE1	1.88	0.92
2:B:181:PRO:HG3	2:B:189:SER:OG	1.70	0.92
2:B:166:SER:OG	4:D:152:ASN:ND2	2.02	0.92
2:B:407:VAL:CG2	4:D:459:TRP:CZ3	2.53	0.92
4:D:189:GLU:CD	4:D:197:ARG:NH1	2.28	0.92
4:D:298:ASN:O	4:D:299:GLU:HB2	1.68	0.92
2:B:132:CYS:SG	4:D:119:LEU:CD2	2.59	0.91
7:G:38:GLU:O	7:G:42:THR:OG1	1.87	0.91
7:G:274:MET:HE1	8:H:280:GLN:HB2	1.51	0.91
6:F:206:MET:HE1	8:H:199:LYS:HG3	0.95	0.91
7:G:130:ILE:HG22	7:G:131:LEU:H	1.27	0.91
2:B:134:LYS:CD	3:C:85:VAL:HG13	2.00	0.91
4:D:176:SER:O	4:D:256:ARG:NH2	2.04	0.91
5:E:49:LEU:HD23	8:H:196:ASN:ND2	1.85	0.91
2:B:263:GLN:NE2	2:B:346:ASN:ND2	2.19	0.91
2:B:483:ARG:HH21	4:D:549:GLN:HE22	1.04	0.91
6:F:335:ARG:CZ	8:H:259:HIS:HB2	1.69	0.91
1:A:189:TYR:HD1	3:C:271:MET:HE1	0.86	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PHE:CE1	2:B:241:LEU:HD13	2.05	0.91
4:D:76:ARG:O	4:D:79:GLU:HB2	1.70	0.91
4:D:122:GLU:HG3	4:D:512:ASN:HD21	1.35	0.91
4:D:183:SER:OG	4:D:184:SER:N	2.03	0.90
5:E:189:TRP:CZ3	8:H:340:ILE:HD11	2.06	0.90
2:B:347:MET:HE2	4:D:403:MET:SD	2.11	0.90
2:B:35:ASP:HB3	4:D:30:MET:CE	2.01	0.90
7:G:312:ARG:NH1	8:H:323:ALA:HB2	1.85	0.90
3:C:18:ASP:OD1	3:C:21:ASP:CG	2.15	0.90
2:B:97:ILE:CD1	4:D:82:GLN:HB3	2.01	0.90
1:A:1:MET:CE	1:A:28:THR:HG22	2.02	0.90
2:B:507:LEU:CD1	4:D:579:THR:HG22	2.01	0.90
3:C:5:LEU:HD12	3:C:22:LEU:CD1	2.01	0.90
2:B:500:LEU:HD21	4:D:571:LEU:CD1	2.03	0.89
6:F:173:LEU:CD1	7:G:118:VAL:CG2	2.47	0.89
3:C:4:THR:HG23	3:C:33:ILE:HD11	1.54	0.89
5:E:77:ASP:OD2	6:F:238:ARG:NE	2.05	0.89
2:B:424:LEU:CD2	4:D:484:ILE:CD1	2.50	0.89
5:E:155:ILE:HG21	6:F:334:VAL:HG23	1.54	0.89
2:B:132:CYS:CB	4:D:119:LEU:HD21	2.02	0.89
2:B:404:GLY:CA	4:D:459:TRP:CH2	2.52	0.89
7:G:92:HIS:CE1	7:G:93:PHE:CE1	2.60	0.89
2:B:97:ILE:CD1	4:D:82:GLN:CD	2.44	0.89
2:B:507:LEU:HD12	4:D:579:THR:HG22	1.55	0.89
1:A:145:THR:HG23	4:D:65:TRP:CZ2	2.07	0.88
2:B:264:LEU:HD13	6:F:381:TRP:CH2	2.07	0.88
1:A:149:VAL:HG13	2:B:70:PRO:CG	2.02	0.88
6:F:241:TRP:CZ2	7:G:238:LEU:HD21	2.08	0.88
6:F:313:GLN:HE21	8:H:282:HIS:CE1	1.90	0.88
1:A:281:SER:HB3	1:A:283:ARG:CD	1.95	0.88
2:B:74:GLU:OE1	4:D:54:ARG:HG3	1.73	0.88
2:B:249:ASP:O	2:B:250:GLY:O	1.92	0.88
2:B:376:MET:HE1	4:D:211:HIS:HB2	1.54	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
2:B:134:LYS:HD3	3:C:85:VAL:HG13	1.56	0.88
6:F:247:MET:CB	8:H:240:LYS:HZ2	1.80	0.88
2:B:138:LYS:HD2	3:C:84:GLN:NE2	1.69	0.88
1:A:145:THR:HG1	4:D:65:TRP:HZ2	1.22	0.87
3:C:236:ARG:NH2	4:D:579:THR:OG1	2.07	0.87
4:D:189:GLU:OE1	4:D:197:ARG:NH2	2.06	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:662:THR:O	4:D:664:SER:N	2.07	0.87
6:F:247:MET:HB2	8:H:240:LYS:HZ1	1.08	0.87
4:D:528:VAL:HG13	4:D:546:MET:SD	2.15	0.87
8:H:359:GLN:HG2	8:H:363:ASP:CG	1.98	0.87
3:C:63:ARG:HH12	4:D:535:ALA:HB1	1.39	0.87
2:B:424:LEU:HD22	4:D:484:ILE:HD12	1.56	0.87
4:D:304:ASP:C	4:D:306:GLN:H	1.83	0.86
6:F:44:GLY:N	6:F:47:MET:HE2	1.89	0.86
6:F:224:ASP:OD2	8:H:216:LEU:HD21	1.75	0.86
3:C:129:ILE:CD1	4:D:489:LEU:HD13	2.06	0.86
6:F:377:ARG:HH22	8:H:343:GLN:CD	1.83	0.86
5:E:97:HIS:NE2	8:H:247:TYR:OH	1.92	0.86
1:A:71:ASP:HB3	3:C:114:ARG:HH21	1.37	0.86
6:F:326:ARG:NH2	7:G:291:GLU:OE2	2.07	0.86
6:F:53:LYS:HE3	6:F:57:TYR:OH	1.75	0.85
6:F:247:MET:HE1	8:H:243:PHE:HD1	1.41	0.85
4:D:219:VAL:O	4:D:221:PRO:HD3	1.76	0.85
2:B:138:LYS:HD2	3:C:84:GLN:OE1	1.75	0.85
4:D:509:ARG:NH1	4:D:521:PHE:CZ	2.38	0.85
4:D:352:HIS:CG	4:D:366:ARG:HH21	1.95	0.85
1:A:148:LEU:HD13	2:B:80:VAL:HG21	1.58	0.85
5:E:181:GLU:CG	7:G:335:ARG:HH12	1.88	0.85
1:A:145:THR:CG2	4:D:69:LEU:HD11	2.05	0.85
2:B:138:LYS:CD	3:C:84:GLN:OE1	2.23	0.85
4:D:352:HIS:CG	4:D:366:ARG:HE	1.94	0.85
1:A:128:LEU:HD22	4:D:97:ARG:HH21	1.42	0.84
2:B:132:CYS:SG	4:D:119:LEU:HD21	2.16	0.84
1:A:283:ARG:O	1:A:284:ARG:N	2.09	0.84
4:D:46:ILE:HG23	4:D:50:ILE:HD12	1.58	0.84
2:B:483:ARG:NH2	4:D:549:GLN:HE22	1.73	0.84
3:C:229:LEU:CD2	4:D:571:LEU:HD12	2.07	0.84
3:C:227:VAL:HG22	3:C:230:ARG:HH21	1.41	0.84
7:G:249:THR:HG23	8:H:243:PHE:CD2	2.12	0.84
2:B:522:THR:OG1	4:D:593:GLU:OE2	1.95	0.84
6:F:247:MET:CB	8:H:240:LYS:HZ1	1.84	0.84
2:B:507:LEU:CD1	4:D:579:THR:CG2	2.55	0.84
5:E:148:TYR:OH	7:G:289:PHE:CD1	2.30	0.84
7:G:41:CYS:HA	7:G:47:ARG:HH12	1.40	0.84
1:A:71:ASP:C	3:C:114:ARG:HH21	1.86	0.84
4:D:352:HIS:CD2	4:D:366:ARG:HE	1.94	0.84
6:F:325:GLU:OE2	6:F:325:GLU:CA	2.25	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:CYS:HB3	3:C:67:MET:HE2	1.58	0.83
2:B:96:ALA:C	2:B:98:GLU:H	1.86	0.83
2:B:402:GLU:OE2	4:D:158:ARG:NH2	2.12	0.83
6:F:230:LYS:HE3	8:H:222:LEU:HD23	1.60	0.83
2:B:222:PHE:CD1	2:B:241:LEU:CD1	2.58	0.83
7:G:274:MET:HE1	8:H:280:GLN:CB	2.08	0.83
1:A:58:LYS:HZ1	4:D:506:SER:HB2	1.43	0.83
4:D:4:ARG:HG3	4:D:32:GLN:HE21	1.43	0.82
2:B:94:GLU:CD	4:D:79:GLU:OE2	2.17	0.82
2:B:490:GLU:CB	4:D:560:ARG:NH2	2.41	0.82
1:A:171:LYS:HE2	1:A:175:ARG:NH2	1.94	0.82
2:B:456:ASP:C	2:B:458:THR:H	1.87	0.82
2:B:97:ILE:CD1	4:D:82:GLN:CG	2.57	0.82
3:C:270:ARG:HD2	4:D:614:TYR:OH	1.79	0.82
1:A:77:LEU:HD22	3:C:154:LEU:CD2	2.10	0.82
1:A:266:LEU:CD1	3:C:345:LEU:HG	2.09	0.82
2:B:30:LEU:CD2	4:D:34:LEU:HD23	2.09	0.82
6:F:92:ARG:NH1	6:F:118:PHE:O	2.13	0.82
7:G:280:PHE:CD1	8:H:287:LYS:HG3	2.15	0.82
3:C:5:LEU:HD12	3:C:22:LEU:HD12	1.61	0.82
2:B:96:ALA:C	2:B:98:GLU:N	2.34	0.81
1:A:172:VAL:HG13	3:C:253:ILE:HG21	1.61	0.81
2:B:216:PHE:HD2	4:D:269:GLN:HG2	1.44	0.81
2:B:550:LEU:HD11	3:C:276:VAL:HG21	1.59	0.81
5:E:179:MET:HG2	8:H:329:ILE:HD11	1.62	0.81
6:F:377:ARG:HH22	8:H:343:GLN:CG	1.92	0.81
7:G:139:GLU:HG3	8:H:155:VAL:HG22	1.61	0.81
1:A:145:THR:OG1	4:D:65:TRP:CZ2	2.34	0.81
7:G:274:MET:SD	8:H:280:GLN:HB2	2.19	0.81
5:E:181:GLU:CD	7:G:335:ARG:NH1	2.37	0.81
6:F:326:ARG:HH11	8:H:295:PRO:HD3	1.45	0.81
4:D:122:GLU:HG3	4:D:512:ASN:ND2	1.96	0.81
5:E:97:HIS:HE2	8:H:247:TYR:HH	0.81	0.81
2:B:84:PHE:HE2	4:D:65:TRP:CZ3	1.97	0.81
3:C:18:ASP:OD1	3:C:21:ASP:OD2	1.98	0.81
1:A:141:ARG:HG3	3:C:220:GLN:NE2	1.96	0.80
1:A:235:LEU:HD11	3:C:313:ILE:CG2	2.11	0.80
2:B:376:MET:CE	4:D:211:HIS:HB2	2.10	0.80
4:D:296:SER:HB3	4:D:301:THR:HG23	0.84	0.80
4:D:453:GLN:HA	4:D:457:LEU:HD12	1.62	0.80
6:F:247:MET:SD	8:H:240:LYS:CG	2.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:274:MET:HE1	8:H:280:GLN:H	1.43	0.80
1:A:141:ARG:HG3	3:C:220:GLN:HE22	1.46	0.80
1:A:1:MET:HE1	1:A:28:THR:CG2	2.11	0.80
1:A:124:VAL:HG21	2:B:110:GLN:NE2	1.97	0.80
3:C:229:LEU:HD21	4:D:571:LEU:CD1	2.11	0.80
2:B:193:PHE:HB3	2:B:392:GLU:OE1	1.81	0.80
2:B:407:VAL:HG21	4:D:459:TRP:CE3	2.17	0.80
2:B:329:ILE:HD13	4:D:386:MET:SD	2.21	0.80
6:F:377:ARG:HH22	8:H:343:GLN:HG3	1.46	0.80
7:G:249:THR:HG23	8:H:243:PHE:CG	2.17	0.80
1:A:281:SER:OG	1:A:283:ARG:CZ	2.30	0.80
1:A:58:LYS:NZ	4:D:506:SER:HB2	1.96	0.79
2:B:80:VAL:HG13	4:D:65:TRP:CH2	2.15	0.79
1:A:277:VAL:C	1:A:278:PRO:CA	2.55	0.79
7:G:274:MET:HE1	8:H:280:GLN:CA	2.12	0.79
1:A:148:LEU:HD11	2:B:80:VAL:HG22	1.62	0.79
1:A:152:LYS:HZ2	2:B:73:ASP:CG	1.85	0.79
6:F:326:ARG:HH12	8:H:295:PRO:HD3	0.89	0.79
3:C:236:ARG:NH1	4:D:575:THR:HA	1.96	0.79
6:F:377:ARG:HH12	8:H:343:GLN:HG3	1.44	0.79
7:G:239:ARG:HG3	8:H:232:VAL:HG21	1.63	0.79
2:B:131:MET:HE2	3:C:85:VAL:HG21	1.61	0.79
2:B:500:LEU:HD21	4:D:571:LEU:HD13	1.62	0.79
1:A:211:HIS:HA	4:D:630:VAL:HG23	1.65	0.79
2:B:513:PRO:HG2	2:B:519:MET:CE	2.13	0.79
2:B:30:LEU:HD21	4:D:34:LEU:HD23	1.65	0.78
2:B:276:MET:HE3	4:D:334:GLN:HG2	1.65	0.78
2:B:566:GLU:HA	2:B:569:LEU:HD12	1.66	0.78
2:B:80:VAL:HG11	4:D:65:TRP:CZ2	2.18	0.78
2:B:97:ILE:HD12	4:D:82:GLN:CG	2.13	0.78
2:B:289:TRP:CE2	2:B:293:ASN:ND2	2.52	0.78
6:F:359:ARG:HG3	8:H:328:GLN:CD	2.07	0.78
2:B:43:PHE:CZ	4:D:46:ILE:HD13	2.18	0.78
1:A:277:VAL:O	1:A:278:PRO:CA	2.31	0.78
3:C:141:LEU:HG	3:C:142:PRO:HD2	1.65	0.78
6:F:241:TRP:HZ2	7:G:238:LEU:HD21	1.48	0.78
6:F:335:ARG:HH21	8:H:259:HIS:CG	1.73	0.78
4:D:189:GLU:OE2	4:D:197:ARG:NH1	2.16	0.78
3:C:180:GLU:OE1	3:C:188:LYS:NZ	2.17	0.77
1:A:145:THR:HG23	4:D:65:TRP:HZ2	1.48	0.77
4:D:117:GLN:O	4:D:119:LEU:N	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:211:HIS:CE1	4:D:215:ILE:HD11	2.19	0.77
5:E:9:PRO:CB	6:F:197:GLN:OE1	2.32	0.77
5:E:148:TYR:HH	7:G:289:PHE:HD1	1.30	0.77
1:A:240:ASP:O	1:A:251:LYS:NZ	2.17	0.77
5:E:221:HIS:HB3	5:E:222:PRO:O	1.85	0.77
3:C:5:LEU:CD1	3:C:22:LEU:HD12	2.15	0.77
7:G:131:LEU:O	7:G:132:GLU:O	2.01	0.77
2:B:399:VAL:HA	4:D:158:ARG:NH1	1.99	0.77
2:B:522:THR:HG22	2:B:524:GLU:OE2	1.85	0.77
6:F:166:LYS:NZ	7:G:87:ASP:OD2	2.13	0.77
6:F:247:MET:HB2	8:H:240:LYS:HZ2	0.96	0.77
5:E:9:PRO:HB3	6:F:197:GLN:OE1	1.85	0.77
6:F:227:ILE:CA	8:H:223:ARG:HH22	1.97	0.77
3:C:14:MET:SD	4:D:552:PHE:HA	2.25	0.77
4:D:280:PRO:O	4:D:281:SER:C	2.09	0.77
5:E:102:LEU:HD22	7:G:255:ILE:CD1	2.15	0.76
6:F:377:ARG:NH1	8:H:343:GLN:CG	2.48	0.76
6:F:377:ARG:NH1	8:H:343:GLN:HG3	2.01	0.76
1:A:5:SER:HA	1:A:31:MET:HE1	1.68	0.76
2:B:94:GLU:OE1	4:D:79:GLU:OE2	2.04	0.76
4:D:290:PRO:O	4:D:291:ILE:O	2.02	0.76
4:D:528:VAL:CG1	4:D:546:MET:SD	2.73	0.76
3:C:123:PRO:C	3:C:125:ASP:H	1.93	0.76
1:A:277:VAL:HG12	1:A:278:PRO:HA	1.68	0.76
2:B:87:SER:C	2:B:89:VAL:H	1.93	0.76
2:B:88:LYS:O	2:B:90:PRO:HD3	1.86	0.76
6:F:326:ARG:HH12	8:H:295:PRO:CG	1.99	0.76
2:B:424:LEU:CD2	4:D:484:ILE:HD11	2.15	0.76
6:F:9:LEU:HD22	6:F:124:PRO:HB3	1.68	0.76
1:A:138:THR:OG1	2:B:92:ILE:HD11	1.82	0.76
2:B:451:GLN:HG3	2:B:463:ARG:HH12	1.50	0.76
8:H:294:MET:HE1	8:H:298:ALA:HB3	0.77	0.76
1:A:189:TYR:HA	3:C:271:MET:CE	2.15	0.76
2:B:490:GLU:HG2	4:D:560:ARG:NH1	2.01	0.76
2:B:490:GLU:CG	4:D:560:ARG:CZ	2.64	0.76
4:D:68:GLN:O	4:D:72:THR:OG1	2.04	0.76
3:C:133:ASP:OD1	3:C:136:ASP:CG	2.28	0.75
4:D:296:SER:OG	4:D:300:SER:N	2.19	0.75
4:D:305:PRO:C	4:D:307:GLU:H	1.91	0.75
2:B:42:TRP:CE2	4:D:20:LEU:HD13	2.21	0.75
5:E:121:LEU:CD2	8:H:276:LEU:HD21	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:GLU:CD	3:C:188:LYS:HZ2	1.95	0.75
6:F:234:ILE:HG12	8:H:226:ILE:HD11	1.68	0.75
2:B:386:GLN:HE22	4:D:440:GLN:CD	1.95	0.75
2:B:458:THR:O	2:B:460:LYS:N	2.20	0.75
6:F:171:ASN:OD1	7:G:149:ASN:ND2	2.19	0.75
3:C:121:VAL:CG1	3:C:122:PRO:HD2	2.17	0.75
6:F:377:ARG:NH1	8:H:343:GLN:HB2	2.00	0.75
1:A:141:ARG:HE	3:C:220:GLN:NE2	1.85	0.75
2:B:87:SER:O	2:B:89:VAL:N	2.16	0.75
3:C:63:ARG:NH1	4:D:535:ALA:HB1	2.02	0.75
4:D:199:VAL:HG21	4:D:241:VAL:HG21	1.68	0.75
2:B:120:LYS:NZ	3:C:171:SER:C	2.45	0.74
2:B:490:GLU:HA	4:D:560:ARG:HH22	1.41	0.74
4:D:202:LEU:HD22	4:D:237:MET:CE	2.17	0.74
2:B:507:LEU:HD12	4:D:579:THR:CG2	2.15	0.74
2:B:287:LEU:HD21	4:D:343:HIS:HD2	1.52	0.74
2:B:297:VAL:CG1	4:D:355:LEU:HD11	2.17	0.74
3:C:116:LEU:HD12	3:C:137:LEU:CD1	2.16	0.74
6:F:224:ASP:CG	6:F:227:ILE:HD11	2.12	0.74
2:B:216:PHE:CD2	4:D:269:GLN:HG2	2.22	0.74
1:A:33:ILE:HG23	3:C:15:LEU:HD22	1.68	0.74
1:A:145:THR:CG2	4:D:65:TRP:CZ2	2.70	0.74
1:A:148:LEU:HD13	2:B:80:VAL:HG23	1.68	0.74
3:C:303:GLU:OE2	3:C:303:GLU:HA	1.88	0.74
7:G:274:MET:CE	8:H:280:GLN:CB	2.58	0.74
2:B:443:ASP:OD2	4:D:509:ARG:NH2	2.21	0.74
4:D:571:LEU:O	4:D:575:THR:HG23	1.88	0.74
2:B:222:PHE:CE1	2:B:241:LEU:CD1	2.70	0.74
6:F:377:ARG:NH2	8:H:343:GLN:HG3	2.02	0.74
2:B:42:TRP:CD2	4:D:20:LEU:HD13	2.23	0.73
2:B:84:PHE:CE2	4:D:65:TRP:CZ3	2.76	0.73
5:E:141:PHE:CA	7:G:289:PHE:HZ	2.01	0.73
1:A:145:THR:CG2	4:D:65:TRP:HZ2	2.01	0.73
1:A:211:HIS:HA	4:D:630:VAL:CG2	2.17	0.73
5:E:148:TYR:OH	7:G:289:PHE:CE1	2.39	0.73
6:F:92:ARG:NH1	6:F:119:LEU:HA	2.04	0.73
2:B:132:CYS:SG	4:D:119:LEU:CD1	2.76	0.73
2:B:166:SER:CB	4:D:152:ASN:ND2	2.50	0.73
6:F:60:PHE:HE1	6:F:99:LEU:HD11	1.54	0.73
3:C:116:LEU:CD1	3:C:137:LEU:HD11	2.19	0.72
4:D:307:GLU:CG	7:G:324:ILE:HD11	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:CYS:CB	3:C:67:MET:HE2	2.18	0.72
2:B:194:LEU:HA	2:B:197:LEU:HG	1.70	0.72
2:B:521:THR:HG22	3:C:251:ASP:OD2	1.89	0.72
2:B:402:GLU:OE2	4:D:158:ARG:NE	2.20	0.72
6:F:297:MET:HE1	6:F:314:LEU:HG	1.69	0.72
1:A:172:VAL:HG13	3:C:253:ILE:CG2	2.20	0.72
2:B:424:LEU:HD22	4:D:484:ILE:HD11	1.70	0.72
2:B:77:LEU:HD23	2:B:81:LEU:HD11	1.71	0.72
2:B:120:LYS:NZ	3:C:171:SER:OG	2.20	0.72
6:F:247:MET:CE	8:H:243:PHE:CD1	2.70	0.71
2:B:386:GLN:NE2	4:D:440:GLN:CD	2.48	0.71
1:A:113:ILE:HB	1:A:114:PRO:HD3	1.72	0.71
2:B:209:SER:HA	4:D:262:THR:HG23	1.71	0.71
1:A:279:GLU:CB	1:A:280:PRO:CD	2.56	0.71
2:B:347:MET:HB3	2:B:348:PRO:HD3	1.72	0.71
3:C:129:ILE:CD1	4:D:489:LEU:CD1	2.68	0.71
6:F:163:ASP:OD2	7:G:59:TYR:OH	2.03	0.71
6:F:287:ARG:HD3	6:F:321:LEU:HD21	1.71	0.71
6:F:338:LEU:HD12	8:H:304:SER:HB3	1.71	0.71
2:B:456:ASP:C	2:B:458:THR:N	2.47	0.71
6:F:157:LEU:N	6:F:170:ARG:HH22	1.89	0.71
1:A:228:SER:HA	3:C:307:LEU:HD12	1.71	0.71
2:B:266:TYR:CG	2:B:345:LEU:HD11	2.25	0.71
6:F:176:GLN:OE1	7:G:117:ASP:HB3	1.91	0.71
2:B:87:SER:C	2:B:89:VAL:N	2.48	0.70
4:D:601:MET:CE	4:D:604:LEU:HD12	2.21	0.70
1:A:64:ALA:HB1	4:D:492:VAL:CG1	2.21	0.70
3:C:63:ARG:HH22	4:D:535:ALA:HB1	1.53	0.70
4:D:307:GLU:OE1	7:G:324:ILE:HD11	1.90	0.70
7:G:274:MET:HE2	8:H:280:GLN:HB2	1.72	0.70
2:B:131:MET:HE1	3:C:85:VAL:CG2	2.13	0.70
5:E:108:LEU:HD22	8:H:254:LEU:HD11	1.72	0.70
2:B:213:LEU:HD13	4:D:265:LEU:HD11	1.73	0.70
6:F:173:LEU:HD21	7:G:90:LEU:HD21	1.72	0.70
6:F:257:VAL:HG11	8:H:255:ASP:HB2	1.72	0.70
1:A:133:MET:SD	3:C:217:LEU:HD22	2.31	0.70
2:B:94:GLU:CB	4:D:79:GLU:OE1	2.40	0.70
4:D:317:GLN:HA	8:H:334:PHE:CE2	2.27	0.70
7:G:56:SER:OG	7:G:63:GLN:OE1	2.01	0.70
1:A:275:PHE:O	1:A:276:VAL:C	2.32	0.70
7:G:7:LEU:HD21	7:G:34:GLN:OE1	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:HB3	1:A:280:PRO:CD	2.08	0.70
2:B:94:GLU:HB3	4:D:79:GLU:OE1	1.92	0.70
2:B:522:THR:HG23	4:D:590:TYR:HE2	1.53	0.69
6:F:377:ARG:HH12	8:H:343:GLN:HA	1.32	0.69
7:G:124:THR:HG22	7:G:125:ILE:H	1.55	0.69
5:E:141:PHE:HB2	7:G:289:PHE:CZ	2.28	0.69
1:A:172:VAL:CG1	3:C:253:ILE:HG21	2.22	0.69
2:B:536:LEU:HD21	3:C:261:LYS:HG2	1.72	0.69
6:F:335:ARG:NH2	8:H:259:HIS:CB	0.54	0.69
7:G:130:ILE:CG2	7:G:131:LEU:N	2.49	0.69
3:C:75:LEU:HD11	3:C:162:LEU:HD23	1.74	0.69
5:E:59:ILE:HG23	7:G:210:ILE:HD12	1.75	0.69
6:F:28:GLY:HA2	6:F:38:LEU:HD11	1.73	0.69
4:D:631:GLN:HB3	4:D:648:ARG:NH2	2.07	0.69
5:E:97:HIS:CD2	8:H:247:TYR:HH	2.11	0.69
6:F:261:VAL:HG21	8:H:254:LEU:HD23	1.74	0.69
7:G:92:HIS:CE1	7:G:93:PHE:CD1	2.80	0.69
7:G:62:VAL:HG12	7:G:66:LEU:HD11	1.75	0.69
4:D:265:LEU:O	4:D:269:GLN:HG3	1.94	0.68
6:F:175:ARG:CZ	7:G:152:LEU:HD22	2.22	0.68
2:B:70:PRO:O	4:D:66:TYR:OH	2.10	0.68
2:B:577:GLU:OE1	4:D:640:GLY:N	2.26	0.68
4:D:202:LEU:HD22	4:D:237:MET:HE1	1.75	0.68
5:E:4:ALA:O	5:E:6:PRO:HD3	1.93	0.68
2:B:220:HIS:CE1	4:D:276:LEU:HD11	2.27	0.68
4:D:4:ARG:HG3	4:D:32:GLN:HE22	1.57	0.68
5:E:47:GLU:HG3	6:F:195:LYS:HZ3	1.57	0.68
5:E:190:ARG:CZ	6:F:370:ILE:HG12	2.24	0.68
2:B:138:LYS:HE3	3:C:84:GLN:CD	2.09	0.68
3:C:123:PRO:C	3:C:125:ASP:N	2.50	0.68
5:E:148:TYR:HH	7:G:289:PHE:HE1	1.36	0.68
6:F:16:MET:SD	6:F:130:LEU:HD23	2.33	0.68
6:F:247:MET:HE1	8:H:243:PHE:CD1	2.27	0.68
2:B:134:LYS:HD2	3:C:85:VAL:HG13	1.74	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:279:GLU:HB2	1:A:280:PRO:HD3	1.75	0.68
2:B:80:VAL:CG1	4:D:65:TRP:CE3	2.75	0.68
3:C:129:ILE:HD11	4:D:489:LEU:HD22	1.76	0.68
1:A:240:ASP:OD2	3:C:335:LYS:NZ	2.27	0.68
2:B:84:PHE:CE2	4:D:65:TRP:CE3	2.77	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:73:LYS:NZ	7:G:220:GLU:OE2	2.26	0.68
2:B:334:LEU:HB3	2:B:335:PRO:HD3	1.76	0.68
1:A:270:VAL:HA	1:A:273:MET:HE3	1.77	0.67
3:C:116:LEU:HD12	3:C:137:LEU:HD12	1.75	0.67
2:B:536:LEU:HD22	3:C:261:LYS:HD3	1.77	0.67
5:E:137:LEU:HD23	7:G:285:LEU:HD23	1.76	0.67
5:E:179:MET:HG2	8:H:329:ILE:CD1	2.24	0.67
1:A:12:LEU:HB3	1:A:21:LEU:CD2	2.23	0.67
2:B:35:ASP:HB3	4:D:30:MET:HE1	1.76	0.67
3:C:141:LEU:HD23	3:C:147:VAL:HG21	1.75	0.67
7:G:37:TYR:OH	7:G:105:PRO:HG3	1.94	0.67
3:C:63:ARG:CZ	4:D:535:ALA:CB	2.71	0.67
5:E:189:TRP:HZ3	8:H:340:ILE:HD12	1.50	0.67
6:F:227:ILE:HG12	8:H:223:ARG:HH22	1.60	0.67
2:B:490:GLU:CA	4:D:560:ARG:HH22	2.03	0.66
6:F:335:ARG:HH21	8:H:259:HIS:CB	0.66	0.66
8:H:234:THR:HB	8:H:235:PRO:HD3	1.77	0.66
3:C:351:SER:O	3:C:353:PRO:HD2	1.94	0.66
6:F:227:ILE:HG12	8:H:223:ARG:NH2	2.11	0.66
2:B:74:GLU:CD	4:D:54:ARG:HG3	2.21	0.66
4:D:184:SER:O	4:D:185:SER:C	2.29	0.66
2:B:513:PRO:HG2	2:B:519:MET:HE2	1.75	0.66
4:D:275:ASP:HA	4:D:278:LYS:HE3	1.78	0.66
1:A:128:LEU:CD2	4:D:97:ARG:HH21	2.08	0.66
1:A:138:THR:HG1	2:B:92:ILE:CD1	2.04	0.66
6:F:192:TYR:OH	7:G:173:TRP:NE1	2.27	0.66
6:F:377:ARG:HH11	8:H:343:GLN:CA	2.07	0.66
4:D:352:HIS:CG	4:D:366:ARG:NE	2.64	0.66
6:F:9:LEU:HD21	6:F:124:PRO:O	1.96	0.66
6:F:224:ASP:O	6:F:225:ARG:C	2.25	0.66
4:D:17:GLU:O	4:D:52:SER:HB3	1.96	0.66
6:F:259:ASP:HB3	6:F:263:ARG:NH2	2.10	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	0.66
2:B:95:VAL:HG13	2:B:99:LYS:HB3	1.78	0.66
5:E:189:TRP:CZ2	8:H:340:ILE:HD13	2.31	0.66
2:B:376:MET:HE1	4:D:211:HIS:CB	2.25	0.65
5:E:9:PRO:HB2	6:F:197:GLN:OE1	1.96	0.65
4:D:206:PHE:CD2	4:D:230:SER:OG	2.49	0.65
6:F:44:GLY:O	6:F:47:MET:HE3	1.95	0.65
7:G:235:ILE:HD11	8:H:225:LEU:HD22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:CB	1:A:21:LEU:HD21	2.24	0.65
2:B:88:LYS:O	2:B:90:PRO:CD	2.43	0.65
2:B:175:MET:CG	4:D:460:PRO:HG3	2.16	0.65
2:B:120:LYS:HZ2	3:C:171:SER:C	1.96	0.65
2:B:513:PRO:HG2	2:B:519:MET:HE3	1.77	0.65
4:D:631:GLN:HB2	4:D:648:ARG:HH22	1.61	0.65
1:A:77:LEU:HD22	3:C:154:LEU:HD22	1.77	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:77:LEU:HD21	4:D:61:GLY:C	2.21	0.65
2:B:577:GLU:OE1	4:D:640:GLY:CA	2.45	0.65
4:D:631:GLN:CB	4:D:648:ARG:NH2	2.60	0.65
4:D:296:SER:HB2	4:D:301:THR:CG2	2.25	0.65
5:E:186:ILE:HG12	7:G:338:TYR:CZ	2.32	0.65
5:E:221:HIS:HB3	5:E:222:PRO:C	2.22	0.65
4:D:317:GLN:HG3	8:H:334:PHE:CD2	2.32	0.65
3:C:128:SER:OG	3:C:132:LEU:O	2.12	0.65
7:G:301:THR:HG23	8:H:312:GLU:HB2	1.78	0.65
2:B:138:LYS:HG3	3:C:84:GLN:HE21	1.62	0.64
2:B:272:LYS:HE3	2:B:276:MET:HE2	1.79	0.64
2:B:319:THR:HG23	4:D:378:LEU:HD12	1.78	0.64
5:E:42:CYS:SG	6:F:187:LEU:HD23	2.37	0.64
6:F:176:GLN:CD	7:G:117:ASP:HB3	2.22	0.64
8:H:259:HIS:N	8:H:300:GLU:OE2	2.15	0.64
2:B:97:ILE:HD11	4:D:82:GLN:CG	2.22	0.64
2:B:383:GLU:OE2	4:D:203:ARG:NE	2.30	0.64
6:F:359:ARG:CG	8:H:328:GLN:CD	2.70	0.64
1:A:77:LEU:HD22	3:C:154:LEU:HD21	1.80	0.64
4:D:352:HIS:CG	4:D:366:ARG:NH2	2.63	0.64
7:G:123:ASP:O	7:G:124:THR:O	2.15	0.64
1:A:215:VAL:HG21	4:D:629:PRO:HB2	1.79	0.64
4:D:157:TYR:CE1	4:D:161:GLN:NE2	2.64	0.64
5:E:155:ILE:HG23	6:F:334:VAL:HG21	0.65	0.64
2:B:42:TRP:CE2	4:D:20:LEU:CD1	2.80	0.64
2:B:507:LEU:HD11	4:D:579:THR:HG22	1.77	0.64
5:E:141:PHE:CA	7:G:289:PHE:CZ	2.81	0.64
2:B:36:LEU:CD2	4:D:34:LEU:HD21	2.28	0.64
2:B:81:LEU:O	2:B:84:PHE:HB2	1.98	0.64
6:F:295:LEU:HD21	6:F:317:GLU:OE1	1.98	0.64
7:G:81:ILE:HG22	7:G:99:ILE:HD12	1.78	0.64
2:B:2:SER:OG	2:B:28:ASP:CG	2.40	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ALA:C	2:B:93:GLU:N	2.56	0.64
2:B:383:GLU:OE2	4:D:203:ARG:NH2	2.31	0.64
2:B:420:ARG:NE	4:D:477:GLU:OE1	2.30	0.64
2:B:424:LEU:HD23	4:D:484:ILE:CD1	2.27	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
2:B:245:SER:O	2:B:246:PHE:C	2.32	0.64
2:B:536:LEU:CD2	3:C:261:LYS:HD3	2.27	0.64
2:B:570:TYR:CG	4:D:631:GLN:HG2	2.33	0.64
2:B:507:LEU:HD21	4:D:582:LEU:HD23	1.79	0.63
4:D:317:GLN:HA	8:H:334:PHE:CD2	2.33	0.63
5:E:76:ALA:HB1	7:G:224:LEU:HD21	1.80	0.63
1:A:64:ALA:HB1	4:D:492:VAL:HG12	1.80	0.63
2:B:166:SER:HB3	4:D:152:ASN:ND2	2.12	0.63
2:B:190:GLN:OE1	4:D:169:SER:O	2.16	0.63
2:B:344:LEU:HD13	4:D:399:LYS:HD2	1.80	0.63
3:C:86:ARG:CB	3:C:92:LEU:HD12	2.28	0.63
3:C:133:ASP:OD1	3:C:136:ASP:OD2	2.16	0.63
5:E:60:ASN:CB	8:H:207:HIS:NE2	2.54	0.63
7:G:130:ILE:CG2	7:G:131:LEU:H	2.00	0.63
2:B:120:LYS:NZ	3:C:175:PRO:HA	2.11	0.63
2:B:588:GLU:OE2	4:D:650:ARG:NH2	2.30	0.63
2:B:132:CYS:SG	4:D:119:LEU:HD11	2.37	0.63
6:F:185:GLU:OE1	7:G:168:PRO:HB3	1.99	0.63
5:E:60:ASN:HB3	8:H:207:HIS:CD2	2.33	0.63
8:H:359:GLN:O	8:H:363:ASP:HB2	1.98	0.63
2:B:35:ASP:CB	4:D:30:MET:CE	2.75	0.62
2:B:376:MET:HE1	4:D:207:LEU:O	1.98	0.62
2:B:482:MET:HE3	4:D:554:ARG:HG2	1.79	0.62
6:F:227:ILE:CG1	8:H:223:ARG:HH22	2.11	0.62
2:B:263:GLN:NE2	2:B:346:ASN:HD21	1.98	0.62
2:B:510:PHE:CE1	4:D:586:LEU:HB3	2.33	0.62
5:E:179:MET:CG	8:H:329:ILE:CD1	2.77	0.62
5:E:139:VAL:HG22	6:F:278:LEU:HD12	1.80	0.62
1:A:130:ASN:HB3	3:C:213:MET:HE1	1.81	0.62
3:C:4:THR:CG2	3:C:33:ILE:HD11	2.26	0.62
5:E:60:ASN:CB	8:H:207:HIS:CE1	2.66	0.62
6:F:92:ARG:HH11	6:F:119:LEU:HA	1.61	0.62
1:A:145:THR:HG23	4:D:65:TRP:CE2	2.34	0.62
1:A:217:LEU:O	1:A:220:THR:OG1	2.17	0.62
2:B:453:LEU:HB3	2:B:471:VAL:HG12	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:485:CYS:SG	4:D:487:PRO:HD2	2.39	0.62
4:D:598:VAL:HB	4:D:599:PRO:HD3	1.82	0.62
3:C:5:LEU:CD1	3:C:22:LEU:CD1	2.76	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
1:A:145:THR:CG2	4:D:69:LEU:CD1	2.57	0.62
4:D:457:LEU:N	4:D:458:PRO:CD	2.62	0.62
2:B:329:ILE:CD1	4:D:386:MET:SD	2.88	0.62
3:C:116:LEU:HD11	3:C:137:LEU:HD11	1.82	0.62
4:D:306:GLN:C	4:D:307:GLU:O	2.43	0.62
5:E:186:ILE:HG12	7:G:338:TYR:CE2	2.34	0.62
1:A:134:GLU:HG3	3:C:213:MET:SD	2.40	0.62
2:B:194:LEU:O	2:B:197:LEU:HB2	2.00	0.62
4:D:601:MET:HE2	4:D:604:LEU:HD12	1.79	0.62
5:E:64:LEU:HD13	8:H:211:ARG:HG3	1.80	0.62
6:F:288:ILE:HD11	6:F:314:LEU:CD2	2.30	0.62
1:A:277:VAL:C	1:A:278:PRO:C	2.64	0.61
2:B:84:PHE:HE2	4:D:65:TRP:HE3	1.43	0.61
2:B:88:LYS:O	2:B:90:PRO:N	2.33	0.61
4:D:184:SER:O	4:D:186:THR:N	2.33	0.61
2:B:407:VAL:CB	4:D:459:TRP:HZ3	2.13	0.61
5:E:158:ILE:HD12	6:F:334:VAL:HG11	1.81	0.61
7:G:14:TYR:HB2	7:G:36:ILE:CG2	2.31	0.61
2:B:406:ILE:HD13	4:D:155:ILE:HD11	1.82	0.61
5:E:189:TRP:HZ3	8:H:336:VAL:HG12	1.65	0.61
3:C:116:LEU:CD1	3:C:137:LEU:CD1	2.78	0.61
3:C:129:ILE:HD13	4:D:489:LEU:CD1	2.30	0.61
4:D:535:ALA:HB1	4:D:537:GLU:OE2	2.00	0.61
2:B:80:VAL:HG11	4:D:65:TRP:CE3	2.32	0.61
4:D:307:GLU:CD	7:G:324:ILE:HD12	1.97	0.61
5:E:57:ALA:HB2	8:H:203:GLN:NE2	2.15	0.61
5:E:78:ILE:CD1	6:F:234:ILE:HG23	2.31	0.61
1:A:78:GLY:O	1:A:81:TYR:HD1	1.84	0.61
6:F:163:ASP:OD1	6:F:164:PRO:HD2	2.00	0.61
6:F:335:ARG:NH2	8:H:259:HIS:HB2	0.95	0.61
3:C:86:ARG:HB2	3:C:92:LEU:HD12	1.81	0.61
3:C:282:THR:HB	3:C:283:PRO:HD2	1.83	0.61
5:E:141:PHE:HA	7:G:289:PHE:CZ	2.36	0.61
2:B:293:ASN:O	2:B:297:VAL:HG23	2.01	0.61
4:D:314:SER:OG	7:G:321:GLY:N	2.29	0.61
4:D:416:ALA:HA	4:D:419:LEU:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:377:ARG:CZ	8:H:343:GLN:HG3	2.30	0.61
5:E:69:LEU:HB3	7:G:217:LEU:HD23	1.82	0.60
6:F:92:ARG:HH12	6:F:119:LEU:C	2.08	0.60
6:F:319:LEU:O	8:H:293:ILE:HD11	2.01	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
5:E:21:LYS:NZ	7:G:159:SER:HA	2.17	0.60
1:A:71:ASP:HB3	3:C:114:ARG:CZ	2.19	0.60
2:B:536:LEU:HD21	3:C:261:LYS:CG	2.30	0.60
4:D:157:TYR:CZ	4:D:161:GLN:NE2	2.69	0.60
5:E:9:PRO:CA	6:F:197:GLN:HE22	2.14	0.60
5:E:175:LEU:HD21	7:G:328:CYS:SG	2.41	0.60
2:B:35:ASP:CB	4:D:30:MET:HE3	2.31	0.60
4:D:264:GLU:HA	4:D:267:LYS:HD2	1.83	0.60
3:C:129:ILE:HD11	4:D:489:LEU:CD2	2.31	0.60
3:C:167:PHE:HB3	3:C:185:ARG:NH2	2.16	0.60
5:E:62:LYS:NZ	7:G:211:SER:OG	2.21	0.60
2:B:490:GLU:CG	4:D:560:ARG:NH2	2.65	0.60
4:D:509:ARG:HD3	4:D:521:PHE:CZ	2.36	0.60
1:A:33:ILE:HG23	3:C:15:LEU:CD2	2.31	0.60
1:A:130:ASN:CB	3:C:213:MET:HE1	2.31	0.60
2:B:96:ALA:O	2:B:99:LYS:N	2.34	0.60
5:E:59:ILE:HG23	7:G:210:ILE:CD1	2.31	0.60
1:A:207:GLU:N	1:A:208:PRO:CD	2.64	0.60
4:D:210:LEU:HD21	4:D:227:ARG:HD3	1.83	0.60
5:E:135:LEU:HB3	5:E:136:PRO:CD	2.29	0.60
6:F:44:GLY:H	6:F:47:MET:CE	1.95	0.60
7:G:123:ASP:O	7:G:124:THR:C	2.42	0.60
6:F:326:ARG:NH1	8:H:295:PRO:CG	2.62	0.59
2:B:273:LEU:HA	4:D:330:LEU:HD13	1.84	0.59
5:E:97:HIS:CE1	6:F:255:VAL:HG13	2.37	0.59
7:G:41:CYS:CA	7:G:47:ARG:NH1	2.65	0.59
1:A:5:SER:HA	1:A:31:MET:CE	2.32	0.59
2:B:171:VAL:HG21	4:D:463:ILE:HD13	1.85	0.59
4:D:268:LEU:HB3	4:D:272:GLN:HE21	1.67	0.59
4:D:383:ASP:O	4:D:387:GLN:HG3	2.01	0.59
6:F:116:SER:HA	6:F:119:LEU:HD12	1.83	0.59
1:A:99:CYS:HB3	3:C:67:MET:CE	2.32	0.59
5:E:78:ILE:HD11	6:F:234:ILE:HG23	1.85	0.59
6:F:234:ILE:HG12	8:H:226:ILE:CD1	2.33	0.59
2:B:97:ILE:HD12	4:D:82:GLN:NE2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:MET:CE	4:D:207:LEU:O	2.50	0.59
2:B:588:GLU:CD	4:D:650:ARG:HH21	2.11	0.59
4:D:631:GLN:OE1	4:D:648:ARG:NH2	2.35	0.59
6:F:377:ARG:HH11	8:H:343:GLN:HA	1.59	0.59
2:B:391:LEU:HD11	4:D:239:GLU:HG2	1.83	0.59
2:B:490:GLU:C	4:D:560:ARG:NH2	2.59	0.59
4:D:130:ARG:NH2	4:D:484:ILE:O	2.35	0.59
4:D:291:ILE:O	4:D:292:THR:C	2.45	0.59
6:F:173:LEU:CD2	7:G:90:LEU:HD21	2.33	0.59
7:G:14:TYR:CE1	7:G:18:GLN:NE2	2.70	0.59
5:E:141:PHE:CB	7:G:289:PHE:CZ	2.86	0.58
5:E:158:ILE:HD11	7:G:295:ILE:HG23	1.86	0.58
7:G:2:THR:HG21	7:G:37:TYR:CE1	2.39	0.58
2:B:550:LEU:HD11	3:C:276:VAL:CG2	2.31	0.58
4:D:211:HIS:CE1	4:D:215:ILE:CD1	2.85	0.58
5:E:148:TYR:OH	7:G:289:PHE:HD1	1.75	0.58
6:F:168:LEU:CD1	7:G:145:CYS:SG	2.91	0.58
1:A:266:LEU:HD12	3:C:345:LEU:CG	2.24	0.58
2:B:344:LEU:HD22	2:B:347:MET:CE	2.34	0.58
2:B:483:ARG:NH2	4:D:549:GLN:NE2	2.37	0.58
6:F:60:PHE:CE1	6:F:99:LEU:HD11	2.37	0.58
2:B:385:LEU:HD12	4:D:254:LEU:CD1	2.33	0.58
1:A:93:ASN:OD1	3:C:68:ARG:NH1	2.36	0.58
2:B:92:ILE:O	2:B:94:GLU:N	2.37	0.58
4:D:202:LEU:HD22	4:D:237:MET:HE3	1.85	0.58
1:A:145:THR:OG1	4:D:65:TRP:HZ2	1.78	0.58
4:D:631:GLN:HB3	4:D:648:ARG:HH21	1.68	0.58
5:E:72:GLU:OE1	8:H:218:ARG:NH1	2.36	0.58
5:E:76:ALA:CB	7:G:224:LEU:HD21	2.33	0.58
6:F:326:ARG:HD2	8:H:293:ILE:HG23	1.86	0.58
2:B:80:VAL:HG12	4:D:65:TRP:CE3	2.34	0.58
4:D:10:LEU:HD23	4:D:31:LEU:HD22	1.86	0.58
2:B:139:GLU:OE1	4:D:123:ARG:HD3	2.03	0.57
4:D:631:GLN:CB	4:D:648:ARG:HH22	2.17	0.57
1:A:189:TYR:CA	3:C:271:MET:HE2	2.30	0.57
2:B:37:LYS:HB3	2:B:38:PRO:HD3	1.85	0.57
5:E:139:VAL:HG22	6:F:278:LEU:CD1	2.34	0.57
8:H:358:ARG:HH21	8:H:366:LEU:CD1	2.18	0.57
1:A:141:ARG:HE	3:C:220:GLN:HE22	1.51	0.57
1:A:278:PRO:HG2	1:A:280:PRO:HD3	1.86	0.57
1:A:113:ILE:HG21	2:B:121:LEU:HD11	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ARG:NH2	4:D:535:ALA:HB1	2.11	0.57
7:G:249:THR:CG2	8:H:243:PHE:HB2	2.35	0.57
1:A:141:ARG:CG	3:C:220:GLN:NE2	2.66	0.57
1:A:171:LYS:HE2	1:A:175:ARG:HH21	1.67	0.57
2:B:429:LEU:HB3	4:D:484:ILE:HG23	1.85	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:171:VAL:HG11	4:D:463:ILE:HD12	1.86	0.57
7:G:62:VAL:CG1	7:G:66:LEU:CD1	2.75	0.57
6:F:6:ARG:C	6:F:8:HIS:H	2.12	0.57
2:B:125:GLU:CD	4:D:113:GLU:OE2	2.46	0.57
3:C:280:CYS:HB2	4:D:625:TRP:HD1	1.69	0.57
4:D:601:MET:HE2	4:D:601:MET:HA	1.85	0.57
2:B:418:GLU:O	2:B:422:THR:HG23	2.05	0.57
5:E:87:LYS:HD3	6:F:241:TRP:CE3	2.40	0.57
1:A:141:ARG:CG	3:C:220:GLN:HE22	2.14	0.56
1:A:113:ILE:CG2	2:B:121:LEU:HD11	2.35	0.56
2:B:507:LEU:HD11	4:D:579:THR:CG2	2.32	0.56
5:E:166:ASP:OD1	6:F:340:TYR:OH	2.23	0.56
7:G:142:VAL:HG13	8:H:163:ILE:HD11	1.86	0.56
1:A:148:LEU:HD12	2:B:80:VAL:HG22	1.80	0.56
2:B:72:LEU:HB2	2:B:77:LEU:HD12	1.88	0.56
2:B:500:LEU:HD21	4:D:571:LEU:HD11	1.84	0.56
7:G:146:ILE:HG12	8:H:163:ILE:HG13	1.86	0.56
4:D:661:ALA:C	4:D:663:GLY:H	2.14	0.56
6:F:377:ARG:NH2	8:H:343:GLN:CD	2.60	0.56
6:F:261:VAL:HG21	8:H:254:LEU:CD2	2.34	0.56
1:A:141:ARG:NE	3:C:220:GLN:HE22	2.04	0.56
2:B:251:THR:C	2:B:253:GLU:N	2.63	0.56
2:B:399:VAL:HA	4:D:158:ARG:HH12	1.70	0.56
2:B:522:THR:CG2	4:D:590:TYR:CE2	2.84	0.56
4:D:216:SER:O	4:D:218:SER:N	2.38	0.56
6:F:9:LEU:HD22	6:F:124:PRO:CB	2.33	0.56
1:A:138:THR:HG1	2:B:92:ILE:HD11	1.67	0.56
4:D:304:ASP:C	4:D:306:GLN:N	2.45	0.56
5:E:47:GLU:HG3	6:F:195:LYS:NZ	2.20	0.56
8:H:294:MET:CE	8:H:298:ALA:HB2	2.28	0.56
2:B:134:LYS:HD2	3:C:85:VAL:CG1	2.35	0.55
2:B:177:PHE:HD1	2:B:192:ILE:CD1	2.18	0.55
6:F:227:ILE:HG22	6:F:227:ILE:O	2.05	0.55
2:B:96:ALA:O	2:B:98:GLU:N	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:GLU:HB3	3:C:127:THR:HG21	1.86	0.55
6:F:135:ARG:HG3	8:H:168:LEU:CD2	2.36	0.55
7:G:93:PHE:CE2	7:G:94:ASP:CG	2.85	0.55
6:F:241:TRP:CH2	7:G:238:LEU:HD21	2.40	0.55
2:B:94:GLU:O	2:B:95:VAL:C	2.48	0.55
4:D:577:PRO:HG2	4:D:582:LEU:HD13	1.89	0.55
1:A:228:SER:CA	3:C:307:LEU:HD12	2.36	0.55
4:D:216:SER:C	4:D:218:SER:H	2.14	0.55
6:F:192:TYR:CE1	7:G:172:PRO:CD	2.89	0.55
2:B:97:ILE:HD12	4:D:82:GLN:OE1	2.02	0.55
6:F:10:ALA:O	6:F:13:ARG:CG	2.39	0.55
6:F:259:ASP:HB3	6:F:263:ARG:HH21	1.71	0.55
1:A:71:ASP:CB	3:C:114:ARG:HH21	1.98	0.55
2:B:157:ASN:HA	4:D:474:ILE:HD12	1.89	0.55
3:C:12:LEU:HB3	3:C:15:LEU:HD12	1.88	0.55
3:C:351:SER:C	3:C:353:PRO:HD2	2.32	0.55
4:D:305:PRO:C	4:D:307:GLU:N	2.52	0.55
4:D:486:LEU:N	4:D:487:PRO:CD	2.69	0.55
6:F:175:ARG:HD3	7:G:121:TYR:OH	2.07	0.55
1:A:241:LEU:HD13	3:C:328:VAL:HG22	1.88	0.55
6:F:338:LEU:HD12	8:H:304:SER:CB	2.37	0.55
4:D:528:VAL:HG12	4:D:528:VAL:O	2.07	0.54
3:C:129:ILE:HD13	4:D:489:LEU:HD11	1.89	0.54
3:C:259:GLU:HG3	4:D:604:LEU:HD21	1.88	0.54
2:B:402:GLU:CD	4:D:158:ARG:NH2	2.65	0.54
3:C:239:ALA:HB1	4:D:586:LEU:HD11	1.90	0.54
4:D:601:MET:HE1	4:D:604:LEU:HD12	1.90	0.54
5:E:181:GLU:CG	7:G:335:ARG:NH1	2.66	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	2.43	0.54
6:F:23:LEU:O	6:F:66:LYS:HE3	2.08	0.54
6:F:170:ARG:HG2	7:G:89:MET:HE2	1.88	0.54
2:B:511:MET:C	2:B:513:PRO:HD3	2.33	0.54
3:C:116:LEU:HD12	3:C:137:LEU:HD11	1.83	0.54
5:E:141:PHE:HB2	7:G:289:PHE:HZ	1.73	0.54
6:F:157:LEU:HG	6:F:170:ARG:NH2	2.22	0.54
8:H:257:THR:O	8:H:300:GLU:OE1	2.26	0.54
1:A:278:PRO:HB3	1:A:279:GLU:CG	2.09	0.54
3:C:5:LEU:HD12	3:C:22:LEU:HD11	1.85	0.54
6:F:92:ARG:NH1	6:F:119:LEU:CA	2.70	0.54
6:F:170:ARG:NE	7:G:89:MET:HG3	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:LEU:O	7:G:11:VAL:HG23	2.07	0.54
7:G:142:VAL:HG13	8:H:163:ILE:CD1	2.38	0.54
1:A:64:ALA:HB1	4:D:492:VAL:HG11	1.88	0.54
1:A:277:VAL:HG12	1:A:278:PRO:CA	2.36	0.54
2:B:42:TRP:CD2	4:D:20:LEU:CD1	2.90	0.54
2:B:121:LEU:HD12	3:C:172:PHE:HE2	1.73	0.54
4:D:575:THR:O	4:D:577:PRO:C	2.51	0.54
7:G:16:ARG:NH2	7:G:120:GLN:OE1	2.40	0.54
2:B:77:LEU:HD23	2:B:81:LEU:CD1	2.37	0.54
3:C:95:GLU:HB3	3:C:153:ARG:HH12	1.73	0.54
2:B:536:LEU:CD2	3:C:261:LYS:CD	2.86	0.54
4:D:122:GLU:CG	4:D:512:ASN:HD21	2.15	0.54
5:E:49:LEU:HD23	8:H:196:ASN:HB3	1.90	0.54
3:C:115:LEU:HD23	4:D:490:LEU:HG	1.89	0.53
3:C:121:VAL:HG13	3:C:122:PRO:HD2	1.89	0.53
4:D:263:GLN:HA	4:D:266:LYS:HD2	1.90	0.53
5:E:10:VAL:HG13	6:F:193:GLN:OE1	2.07	0.53
5:E:75:THR:O	5:E:79:THR:OG1	2.13	0.53
5:E:17:LEU:HD13	7:G:161:HIS:CE1	2.43	0.53
5:E:102:LEU:HD23	7:G:255:ILE:HD12	1.86	0.53
5:E:141:PHE:CB	7:G:289:PHE:HZ	2.20	0.53
3:C:63:ARG:NH1	4:D:535:ALA:CB	2.70	0.53
3:C:63:ARG:NH1	4:D:537:GLU:CD	2.66	0.53
6:F:335:ARG:NE	8:H:259:HIS:HB3	2.12	0.53
7:G:59:TYR:CD1	7:G:62:VAL:CG2	2.66	0.53
6:F:283:LEU:HD23	6:F:321:LEU:HD13	1.91	0.53
7:G:150:GLU:HG2	8:H:166:GLN:NE2	2.24	0.53
1:A:244:ASN:OD1	1:A:245:PRO:HD2	2.08	0.53
2:B:41:ASP:O	2:B:45:SER:OG	2.25	0.53
2:B:93:GLU:O	2:B:94:GLU:C	2.50	0.53
2:B:264:LEU:CD1	6:F:381:TRP:CH2	2.87	0.53
2:B:347:MET:HG3	4:D:406:LEU:CD1	2.38	0.53
3:C:224:TYR:N	3:C:225:PRO:HD2	2.23	0.53
4:D:63:LEU:O	4:D:67:GLN:HB2	2.09	0.53
4:D:202:LEU:CD2	4:D:237:MET:HE1	2.39	0.53
4:D:317:GLN:HG3	8:H:334:PHE:HB2	1.91	0.53
1:A:55:LEU:HD22	3:C:59:LEU:HD22	1.90	0.53
1:A:152:LYS:NZ	2:B:73:ASP:OD1	2.40	0.53
2:B:213:LEU:HD22	2:B:374:HIS:CD2	2.44	0.53
2:B:504:LEU:HD11	3:C:231:CYS:HB3	1.91	0.53
3:C:121:VAL:HG12	3:C:122:PRO:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:293:GLN:CD	4:D:294:SER:H	2.17	0.53
4:D:307:GLU:OE1	7:G:324:ILE:CD1	2.53	0.53
4:D:348:ILE:HD11	4:D:373:LEU:HD21	1.91	0.53
6:F:326:ARG:NH1	8:H:295:PRO:HG3	2.24	0.53
4:D:572:GLN:O	4:D:575:THR:OG1	2.26	0.52
1:A:152:LYS:CE	2:B:73:ASP:OD1	2.57	0.52
1:A:280:PRO:CA	1:A:281:SER:N	2.67	0.52
2:B:573:PHE:O	4:D:639:ARG:HD2	2.08	0.52
6:F:44:GLY:O	6:F:47:MET:CE	2.57	0.52
7:G:345:SER:O	7:G:348:ASP:HB2	2.09	0.52
1:A:48:LEU:HD22	3:C:52:LEU:HD22	1.90	0.52
3:C:285:LYS:HZ1	4:D:628:GLN:HE22	1.56	0.52
4:D:651:TRP:O	4:D:655:VAL:HG23	2.08	0.52
6:F:53:LYS:HE2	6:F:57:TYR:CZ	2.38	0.52
2:B:19:GLY:HA2	2:B:22:LEU:HD12	1.92	0.52
2:B:454:ASP:C	2:B:456:ASP:H	2.17	0.52
2:B:490:GLU:HG2	4:D:560:ARG:NH2	2.19	0.52
5:E:9:PRO:HA	6:F:197:GLN:HE22	1.74	0.52
1:A:241:LEU:CD2	1:A:248:VAL:HG13	2.39	0.52
2:B:89:VAL:O	2:B:90:PRO:C	2.49	0.52
2:B:222:PHE:HD1	2:B:241:LEU:HD13	1.55	0.52
3:C:141:LEU:CD2	3:C:147:VAL:HG21	2.38	0.52
5:E:154:THR:HG21	7:G:299:THR:HG21	1.92	0.52
7:G:327:LEU:CD1	8:H:326:PHE:CD1	2.93	0.52
1:A:214:LEU:HB2	4:D:630:VAL:HG22	1.91	0.52
2:B:83:THR:HG22	3:C:220:GLN:HG2	1.91	0.52
2:B:178:PHE:HE1	2:B:396:HIS:CE1	2.28	0.52
5:E:87:LYS:HD3	6:F:241:TRP:CD2	2.44	0.52
7:G:146:ILE:HG12	8:H:163:ILE:CG1	2.40	0.52
4:D:175:PHE:CD1	4:D:193:LEU:HD13	2.44	0.52
7:G:123:ASP:C	7:G:124:THR:O	2.53	0.52
1:A:148:LEU:HD11	2:B:80:VAL:CG2	2.28	0.52
1:A:171:LYS:CE	1:A:175:ARG:NH2	2.72	0.52
1:A:205:MET:HE1	1:A:209:LEU:C	2.34	0.52
2:B:90:PRO:O	2:B:92:ILE:N	2.43	0.52
2:B:195:SER:HA	2:B:389:TYR:HE1	1.74	0.52
2:B:289:TRP:CZ2	2:B:293:ASN:ND2	2.76	0.52
4:D:352:HIS:CD2	4:D:366:ARG:NE	2.71	0.52
6:F:28:GLY:HA2	6:F:38:LEU:CD1	2.40	0.52
8:H:241:ASP:HB2	8:H:242:PRO:HD3	1.92	0.52
2:B:454:ASP:O	2:B:456:ASP:N	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:PHE:CE1	4:D:193:LEU:HD13	2.45	0.52
6:F:168:LEU:HD11	7:G:145:CYS:SG	2.50	0.52
2:B:95:VAL:HG12	2:B:100:LEU:HG	1.93	0.51
2:B:349:ILE:CD1	4:D:316:ILE:HD12	2.40	0.51
3:C:303:GLU:OE2	3:C:303:GLU:CA	2.58	0.51
4:D:80:GLU:HA	4:D:83:GLN:OE1	2.10	0.51
6:F:335:ARG:HH22	8:H:259:HIS:HB2	0.78	0.51
1:A:145:THR:HG23	4:D:65:TRP:NE1	2.25	0.51
1:A:242:ALA:C	1:A:244:ASN:H	2.19	0.51
2:B:344:LEU:HD22	2:B:347:MET:HE1	1.92	0.51
6:F:182:LEU:CD1	8:H:177:MET:HE1	2.40	0.51
7:G:327:LEU:HD11	8:H:326:PHE:CG	2.45	0.51
2:B:349:ILE:HD13	4:D:316:ILE:HD12	1.91	0.51
4:D:203:ARG:HH12	4:D:231:HIS:HD2	1.58	0.51
6:F:240:MET:HE1	8:H:230:ASP:OD1	2.10	0.51
7:G:2:THR:HG21	7:G:37:TYR:CZ	2.44	0.51
7:G:219:GLU:O	7:G:222:VAL:HG23	2.10	0.51
2:B:7:PHE:CE1	2:B:11:LEU:HD11	2.45	0.51
2:B:482:MET:HE3	4:D:554:ARG:CG	2.41	0.51
5:E:127:TYR:CD2	7:G:275:GLY:HA3	2.45	0.51
6:F:297:MET:HE3	6:F:313:GLN:HB2	1.92	0.51
1:A:271:ASN:O	1:A:273:MET:N	2.44	0.51
6:F:51:PRO:HA	6:F:121:PRO:O	2.11	0.51
2:B:36:LEU:HD21	4:D:34:LEU:CG	2.41	0.51
2:B:358:MET:O	2:B:362:THR:HG23	2.11	0.51
6:F:156:ALA:C	6:F:170:ARG:HH22	2.18	0.51
6:F:166:LYS:CE	7:G:84:LEU:HD12	2.40	0.51
2:B:80:VAL:HG11	4:D:65:TRP:CE2	2.45	0.51
4:D:4:ARG:CG	4:D:32:GLN:HE21	2.21	0.51
3:C:63:ARG:CZ	4:D:535:ALA:HB1	2.37	0.51
4:D:296:SER:HB3	4:D:301:THR:HG21	1.75	0.51
5:E:141:PHE:N	7:G:289:PHE:HZ	2.08	0.51
1:A:24:TYR:HB3	3:C:31:VAL:HG21	1.92	0.51
1:A:152:LYS:HE3	2:B:73:ASP:OD1	2.12	0.51
2:B:259:MET:CE	2:B:346:ASN:HB3	2.41	0.51
6:F:209:GLU:OE1	8:H:210:LYS:NZ	2.36	0.51
4:D:266:LYS:HB3	4:D:270:PHE:CZ	2.45	0.50
2:B:84:PHE:CE2	4:D:65:TRP:HZ3	2.23	0.50
2:B:458:THR:C	2:B:460:LYS:N	2.69	0.50
6:F:234:ILE:HD11	8:H:222:LEU:HD21	1.93	0.50
2:B:430:LEU:O	2:B:431:SER:O	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:219:ASN:O	5:E:221:HIS:N	2.45	0.50
6:F:260:ALA:CB	8:H:258:ARG:HH11	2.13	0.50
1:A:152:LYS:CE	2:B:73:ASP:CG	2.83	0.50
2:B:37:LYS:N	2:B:38:PRO:CD	2.75	0.50
6:F:192:TYR:CD2	8:H:188:ALA:HB1	2.47	0.50
7:G:81:ILE:CG2	7:G:99:ILE:HD12	2.42	0.50
3:C:92:LEU:HD23	3:C:97:ARG:N	2.27	0.50
6:F:260:ALA:HB3	8:H:258:ARG:HH11	1.69	0.50
1:A:171:LYS:HE2	1:A:175:ARG:CZ	2.40	0.50
2:B:407:VAL:HB	4:D:459:TRP:HZ3	1.77	0.50
4:D:192:VAL:HG22	4:D:245:HIS:ND1	2.27	0.50
4:D:661:ALA:C	4:D:663:GLY:N	2.69	0.50
8:H:156:PRO:C	8:H:158:ASP:N	2.70	0.50
4:D:8:GLN:CG	4:D:28:GLU:OE1	2.44	0.49
7:G:30:LEU:HD22	7:G:35:SER:HB3	1.93	0.49
3:C:1:MET:HE1	3:C:23:GLU:HA	1.94	0.49
4:D:525:TYR:OH	4:D:536:PRO:HA	2.13	0.49
5:E:79:THR:HG21	8:H:222:LEU:CD1	2.42	0.49
6:F:251:MET:HE3	8:H:247:TYR:CD1	2.46	0.49
1:A:271:ASN:C	1:A:273:MET:N	2.69	0.49
1:A:278:PRO:CG	1:A:279:GLU:CG	2.82	0.49
2:B:243:VAL:HG12	2:B:243:VAL:O	2.12	0.49
3:C:324:PHE:O	3:C:328:VAL:HG23	2.13	0.49
7:G:62:VAL:O	7:G:66:LEU:HD12	2.12	0.49
7:G:124:THR:CG2	7:G:125:ILE:HG13	2.28	0.49
1:A:99:CYS:CB	3:C:67:MET:CE	2.89	0.49
1:A:227:GLN:HB3	3:C:307:LEU:HD11	1.93	0.49
4:D:4:ARG:HA	4:D:32:GLN:HE21	1.78	0.49
2:B:95:VAL:CG1	2:B:100:LEU:HG	2.43	0.49
2:B:264:LEU:HD13	6:F:381:TRP:CZ2	2.45	0.49
4:D:594:LEU:O	4:D:599:PRO:HD3	2.13	0.49
1:A:207:GLU:N	1:A:208:PRO:HD2	2.27	0.49
2:B:264:LEU:HD13	6:F:381:TRP:HH2	1.69	0.49
2:B:482:MET:HE3	4:D:554:ARG:HE	1.77	0.49
3:C:86:ARG:HB2	3:C:92:LEU:CD1	2.43	0.49
5:E:49:LEU:CD2	8:H:196:ASN:HD22	2.11	0.49
6:F:182:LEU:HD12	8:H:177:MET:HE1	1.95	0.49
1:A:71:ASP:CA	3:C:114:ARG:HH21	2.25	0.49
2:B:84:PHE:CE2	4:D:65:TRP:HE3	2.25	0.49
2:B:271:HIS:CE1	8:H:360:TRP:CE2	3.01	0.49
2:B:385:LEU:HD12	4:D:254:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:CYS:SG	6:F:187:LEU:CD2	3.00	0.49
5:E:190:ARG:NH1	6:F:370:ILE:CG1	2.76	0.49
2:B:221:PHE:CZ	2:B:367:ARG:HB2	2.48	0.49
2:B:587:LEU:HD23	4:D:654:ALA:CB	2.42	0.49
3:C:209:LYS:HG2	3:C:213:MET:HE2	1.95	0.49
7:G:14:TYR:HB2	7:G:36:ILE:HG21	1.94	0.49
7:G:124:THR:HG22	7:G:125:ILE:N	2.26	0.49
7:G:178:LYS:N	7:G:179:PRO:CD	2.76	0.49
7:G:294:SER:OG	8:H:305:PHE:HB2	2.13	0.49
2:B:37:LYS:N	2:B:38:PRO:HD2	2.28	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
5:E:135:LEU:CB	5:E:136:PRO:HD3	2.33	0.48
2:B:36:LEU:HD21	4:D:34:LEU:HG	1.95	0.48
5:E:190:ARG:CZ	6:F:370:ILE:CG1	2.91	0.48
3:C:218:GLU:OE1	4:D:556:GLN:HG3	2.13	0.48
6:F:335:ARG:HH22	8:H:259:HIS:CD2	2.21	0.48
8:H:156:PRO:C	8:H:158:ASP:H	2.20	0.48
1:A:281:SER:O	1:A:282:LYS:C	2.22	0.48
4:D:590:TYR:CE1	4:D:594:LEU:HD11	2.48	0.48
5:E:221:HIS:CB	5:E:222:PRO:O	2.60	0.48
1:A:189:TYR:CG	3:C:271:MET:CE	2.92	0.48
3:C:36:CYS:N	3:C:37:PRO:HD2	2.28	0.48
5:E:38:LEU:HD11	6:F:180:LYS:HD3	1.95	0.48
1:A:145:THR:OG1	4:D:65:TRP:CH2	2.63	0.48
1:A:211:HIS:O	1:A:215:VAL:HG23	2.14	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
4:D:528:VAL:HG12	4:D:546:MET:SD	2.53	0.48
5:E:121:LEU:HD23	8:H:276:LEU:HD11	1.94	0.48
6:F:227:ILE:CB	8:H:223:ARG:HH22	2.27	0.48
4:D:213:ASP:OD2	4:D:227:ARG:NH2	2.41	0.48
6:F:138:MET:HE1	8:H:169:LEU:HA	1.95	0.48
1:A:150:LEU:CD2	2:B:504:LEU:HD21	2.43	0.48
2:B:35:ASP:HB3	4:D:30:MET:SD	2.53	0.48
2:B:225:MET:O	2:B:226:SER:C	2.50	0.48
5:E:158:ILE:CD1	6:F:334:VAL:HG11	2.44	0.48
6:F:166:LYS:HE3	7:G:84:LEU:CD1	2.44	0.48
6:F:60:PHE:HE1	6:F:99:LEU:CD1	2.24	0.48
6:F:16:MET:SD	6:F:130:LEU:CD2	3.02	0.47
1:A:148:LEU:CD1	2:B:80:VAL:HG21	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:VAL:O	2:B:83:THR:OG1	2.21	0.47
2:B:263:GLN:HE21	2:B:346:ASN:ND2	2.06	0.47
5:E:28:LEU:HD11	6:F:179:LEU:HD21	1.96	0.47
7:G:239:ARG:HG3	8:H:232:VAL:CG2	2.39	0.47
1:A:40:TRP:CH2	3:C:43:GLY:HA3	2.48	0.47
7:G:274:MET:SD	8:H:280:GLN:CB	2.99	0.47
2:B:51:ASN:HD22	4:D:18:MET:HE1	1.79	0.47
2:B:95:VAL:HA	2:B:99:LYS:HD2	1.96	0.47
2:B:266:TYR:CD2	2:B:345:LEU:HD11	2.49	0.47
2:B:493:HIS:CE1	2:B:497:LEU:HD11	2.49	0.47
4:D:257:LEU:HA	4:D:260:ASN:ND2	2.29	0.47
1:A:211:HIS:HB3	4:D:629:PRO:HG2	1.96	0.47
3:C:118:ALA:O	3:C:119:ASP:C	2.48	0.47
1:A:124:VAL:HG21	2:B:110:GLN:HE22	1.78	0.47
1:A:137:LEU:HD21	3:C:217:LEU:N	2.29	0.47
2:B:376:MET:HE3	4:D:211:HIS:HB2	1.95	0.47
2:B:457:ASN:O	2:B:459:GLN:N	2.48	0.47
5:E:19:LEU:HD21	6:F:182:LEU:HD23	1.96	0.47
6:F:138:MET:HE1	8:H:169:LEU:HD23	1.96	0.47
6:F:277:THR:HA	6:F:301:TYR:OH	2.14	0.47
6:F:283:LEU:CD2	6:F:321:LEU:HD13	2.44	0.47
6:F:389:LEU:HD11	8:H:362:PHE:CE2	2.49	0.47
7:G:137:SER:C	7:G:139:GLU:H	2.22	0.47
3:C:99:PHE:CE1	3:C:157:GLN:OE1	2.67	0.47
3:C:146:LEU:O	3:C:150:VAL:HG23	2.15	0.47
3:C:227:VAL:HG22	3:C:230:ARG:NH2	2.20	0.47
3:C:280:CYS:HB2	4:D:625:TRP:CD1	2.48	0.47
4:D:355:LEU:O	4:D:362:SER:HB3	2.15	0.47
6:F:9:LEU:HD22	6:F:124:PRO:CA	2.45	0.47
6:F:47:MET:HG3	6:F:48:PHE:CD2	2.50	0.47
6:F:309:ILE:HG23	8:H:282:HIS:CD2	2.49	0.47
6:F:359:ARG:HG2	8:H:328:GLN:OE1	2.05	0.47
3:C:12:LEU:HD13	3:C:15:LEU:CD1	2.45	0.47
5:E:189:TRP:CE3	8:H:340:ILE:HD11	2.50	0.47
2:B:86:ILE:HG22	2:B:86:ILE:O	2.14	0.47
2:B:97:ILE:CD1	4:D:82:GLN:HG2	2.42	0.47
2:B:577:GLU:OE1	4:D:640:GLY:HA2	2.15	0.47
5:E:94:MET:HE1	6:F:251:MET:HE2	1.96	0.47
5:E:121:LEU:HD23	8:H:276:LEU:HD21	1.97	0.47
1:A:123:LEU:O	1:A:126:ILE:HG22	2.15	0.47
4:D:46:ILE:CG2	4:D:50:ILE:HD12	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:261:VAL:HG22	8:H:258:ARG:HD2	1.96	0.47
7:G:13:LEU:HD22	7:G:116:LEU:HD12	1.97	0.47
7:G:13:LEU:HD11	7:G:109:ILE:HG23	1.96	0.47
2:B:89:VAL:C	2:B:90:PRO:O	2.58	0.46
4:D:595:ASP:O	4:D:599:PRO:HG2	2.15	0.46
5:E:181:GLU:HG2	7:G:335:ARG:HH12	1.77	0.46
1:A:192:LYS:HD2	3:C:271:MET:SD	2.55	0.46
2:B:199:LEU:H	2:B:199:LEU:HG	1.43	0.46
2:B:273:LEU:HD13	4:D:330:LEU:HA	1.98	0.46
4:D:307:GLU:HB3	7:G:318:LYS:HE3	1.97	0.46
4:D:509:ARG:CD	4:D:521:PHE:CZ	2.98	0.46
5:E:21:LYS:HZ2	7:G:159:SER:HA	1.80	0.46
5:E:155:ILE:N	5:E:156:PRO:CD	2.78	0.46
6:F:5:SER:O	6:F:7:PRO:HD3	2.15	0.46
7:G:139:GLU:HG3	8:H:155:VAL:CG2	2.40	0.46
2:B:383:GLU:OE2	4:D:203:ARG:CZ	2.62	0.46
2:B:521:THR:HG23	3:C:247:GLN:CG	2.44	0.46
6:F:288:ILE:CD1	6:F:314:LEU:CD2	2.93	0.46
5:E:69:LEU:HB3	7:G:217:LEU:CD2	2.46	0.46
6:F:170:ARG:NH2	7:G:89:MET:SD	2.82	0.46
1:A:121:SER:HB3	4:D:104:GLN:HE22	1.81	0.46
4:D:486:LEU:HB2	4:D:487:PRO:HD3	1.96	0.46
5:E:137:LEU:CD2	7:G:285:LEU:HD23	2.44	0.46
6:F:359:ARG:NE	8:H:321:GLU:OE1	2.47	0.46
3:C:67:MET:O	3:C:71:VAL:HG23	2.16	0.46
6:F:6:ARG:HD3	6:F:8:HIS:HD2	1.81	0.46
6:F:166:LYS:HE2	7:G:84:LEU:HD12	1.98	0.46
6:F:251:MET:HE1	8:H:243:PHE:CE1	2.50	0.46
2:B:74:GLU:OE1	4:D:54:ARG:CG	2.56	0.46
3:C:86:ARG:HB3	3:C:92:LEU:HD12	1.97	0.46
4:D:459:TRP:N	4:D:460:PRO:CD	2.78	0.46
7:G:14:TYR:HB2	7:G:36:ILE:HG23	1.98	0.46
2:B:134:LYS:CD	3:C:85:VAL:CG1	2.84	0.46
3:C:170:LEU:HD22	3:C:189:VAL:HG23	1.97	0.46
2:B:85:SER:C	2:B:87:SER:N	2.73	0.46
2:B:357:GLN:O	2:B:361:GLN:HG3	2.16	0.46
3:C:180:GLU:CD	3:C:184:LEU:HD23	2.40	0.46
6:F:377:ARG:HH22	8:H:343:GLN:NE2	2.12	0.46
6:F:170:ARG:NE	7:G:89:MET:SD	2.81	0.46
6:F:301:TYR:CE1	6:F:306:VAL:HG22	2.51	0.46
2:B:330:SER:O	2:B:335:PRO:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ARG:CZ	8:H:363:ASP:O	2.64	0.45
2:B:430:LEU:C	2:B:431:SER:O	2.58	0.45
4:D:352:HIS:CB	4:D:366:ARG:NH2	2.37	0.45
6:F:330:ASP:OD1	6:F:334:VAL:HG23	2.16	0.45
7:G:93:PHE:CD2	7:G:94:ASP:OD1	2.68	0.45
1:A:40:TRP:CH2	3:C:43:GLY:CA	2.99	0.45
1:A:71:ASP:CA	3:C:114:ARG:NH2	2.78	0.45
2:B:407:VAL:HG23	4:D:459:TRP:CZ3	2.50	0.45
3:C:28:PHE:CE1	3:C:32:LEU:HD11	2.52	0.45
7:G:2:THR:CG2	7:G:37:TYR:CZ	2.99	0.45
7:G:235:ILE:HD11	8:H:225:LEU:CD2	2.44	0.45
2:B:132:CYS:N	4:D:119:LEU:HD11	2.32	0.45
2:B:465:TYR:HB3	4:D:520:ILE:HG21	1.99	0.45
3:C:129:ILE:HD11	4:D:489:LEU:CD1	2.46	0.45
3:C:140:LEU:HD11	4:D:136:ALA:HB2	1.98	0.45
4:D:46:ILE:HA	4:D:50:ILE:HD12	1.98	0.45
5:E:121:LEU:HD22	8:H:276:LEU:HD21	1.94	0.45
7:G:146:ILE:CG1	8:H:163:ILE:HG13	2.47	0.45
1:A:33:ILE:CG2	3:C:15:LEU:HD22	2.43	0.45
1:A:238:TYR:OH	3:C:325:GLU:OE1	2.33	0.45
2:B:97:ILE:CD1	4:D:82:GLN:OE1	2.63	0.45
4:D:272:GLN:O	4:D:276:LEU:HG	2.16	0.45
5:E:207:CYS:O	5:E:208:ILE:C	2.58	0.45
7:G:132:GLU:HB3	7:G:133:SER:H	1.44	0.45
2:B:43:PHE:CZ	4:D:46:ILE:CD1	2.97	0.45
2:B:449:LEU:HD23	2:B:468:LEU:HD21	1.97	0.45
4:D:355:LEU:HD22	4:D:365:THR:HB	1.98	0.45
5:E:88:HIS:HB2	7:G:238:LEU:HD12	1.98	0.45
6:F:173:LEU:HD11	7:G:118:VAL:HG21	1.87	0.45
7:G:139:GLU:O	7:G:143:VAL:HG23	2.16	0.45
7:G:162:PHE:O	7:G:165:THR:OG1	2.35	0.45
7:G:178:LYS:HB3	7:G:179:PRO:HD3	1.99	0.45
2:B:229:VAL:O	2:B:230:GLU:C	2.60	0.45
2:B:521:THR:CG2	3:C:247:GLN:HE21	2.30	0.45
4:D:117:GLN:O	4:D:118:ASP:C	2.54	0.45
4:D:171:ARG:O	4:D:249:HIS:NE2	2.46	0.45
5:E:148:TYR:HB3	7:G:292:LEU:HD13	1.98	0.45
7:G:47:ARG:CZ	7:G:101:GLY:HA2	2.46	0.45
6:F:377:ARG:NH1	8:H:343:GLN:N	2.63	0.45
1:A:65:GLU:OE2	4:D:507:ILE:HD12	2.17	0.45
2:B:95:VAL:HG13	2:B:99:LYS:CB	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:ASN:C	4:D:122:GLU:H	2.25	0.45
6:F:170:ARG:HE	7:G:89:MET:CE	2.30	0.45
2:B:407:VAL:CG2	4:D:459:TRP:CE3	2.90	0.45
3:C:8:VAL:HG13	3:C:12:LEU:HD12	1.99	0.45
8:H:294:MET:SD	8:H:298:ALA:CB	3.05	0.45
2:B:453:LEU:HB3	2:B:471:VAL:CG1	2.47	0.45
7:G:340:ALA:O	7:G:344:SER:OG	2.34	0.45
7:G:41:CYS:CA	7:G:108:GLN:OE1	2.62	0.44
1:A:215:VAL:CG2	4:D:629:PRO:HB2	2.47	0.44
2:B:199:LEU:HD11	2:B:389:TYR:OH	2.17	0.44
2:B:271:HIS:CE1	8:H:360:TRP:NE1	2.85	0.44
7:G:127:SER:C	7:G:129:VAL:N	2.75	0.44
1:A:206:GLU:C	1:A:208:PRO:HD2	2.43	0.44
2:B:536:LEU:HD11	3:C:262:SER:HB2	1.98	0.44
6:F:261:VAL:CG2	8:H:254:LEU:HD23	2.45	0.44
2:B:93:GLU:C	2:B:94:GLU:O	2.58	0.44
2:B:406:ILE:CD1	4:D:155:ILE:HD11	2.47	0.44
4:D:248:ASN:OD1	4:D:248:ASN:C	2.60	0.44
4:D:266:LYS:HA	4:D:269:GLN:CD	2.43	0.44
6:F:64:PHE:CD1	6:F:98:TRP:CE3	3.05	0.44
6:F:170:ARG:NE	7:G:89:MET:CG	2.81	0.44
7:G:188:GLN:O	7:G:192:THR:OG1	2.35	0.44
2:B:370:LEU:HD23	2:B:371:VAL:HG23	1.99	0.44
1:A:207:GLU:HB3	1:A:208:PRO:HD3	2.00	0.44
2:B:263:GLN:NE2	2:B:343:GLN:HA	2.32	0.44
4:D:352:HIS:HB3	4:D:366:ARG:CZ	2.40	0.44
4:D:590:TYR:CE1	4:D:594:LEU:CD1	3.01	0.44
5:E:97:HIS:ND1	6:F:255:VAL:HG13	2.32	0.44
6:F:84:ASP:OD1	6:F:87:ARG:HD2	2.17	0.44
1:A:145:THR:HG23	4:D:65:TRP:HE1	1.82	0.44
2:B:319:THR:HG23	4:D:378:LEU:CD1	2.46	0.44
3:C:129:ILE:HD11	4:D:489:LEU:HD13	1.96	0.44
5:E:149:ILE:HG23	6:F:325:GLU:HG3	1.99	0.44
7:G:235:ILE:CD1	8:H:225:LEU:CD2	2.95	0.44
7:G:298:PHE:HB2	8:H:308:ILE:HD13	2.00	0.44
1:A:211:HIS:CG	4:D:629:PRO:HD2	2.53	0.44
5:E:21:LYS:HZ3	7:G:159:SER:HA	1.82	0.44
7:G:135:SER:O	7:G:136:HIS:C	2.52	0.44
2:B:120:LYS:HZ3	3:C:171:SER:C	2.24	0.44
4:D:572:GLN:HA	4:D:575:THR:OG1	2.18	0.44
5:E:94:MET:HG2	7:G:245:PHE:HE2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:330:ASP:OD1	6:F:334:VAL:N	2.50	0.44
1:A:95:ILE:HG13	3:C:166:CYS:SG	2.58	0.43
1:A:175:ARG:NH1	3:C:254:ASN:OD1	2.44	0.43
2:B:190:GLN:OE1	4:D:169:SER:C	2.61	0.43
1:A:133:MET:SD	3:C:217:LEU:CD2	3.05	0.43
2:B:447:HIS:ND1	2:B:463:ARG:HD2	2.33	0.43
2:B:456:ASP:O	2:B:458:THR:N	2.51	0.43
3:C:266:PHE:CD2	4:D:611:HIS:CD2	3.06	0.43
5:E:179:MET:CG	8:H:329:ILE:HD12	2.48	0.43
7:G:124:THR:CG2	7:G:125:ILE:H	2.20	0.43
3:C:4:THR:HG23	3:C:33:ILE:CD1	2.35	0.43
3:C:270:ARG:HD2	4:D:614:TYR:CZ	2.53	0.43
4:D:423:LYS:O	4:D:427:ILE:HG13	2.19	0.43
6:F:288:ILE:HD11	6:F:314:LEU:HD23	1.97	0.43
2:B:197:LEU:HD11	4:D:247:PRO:C	2.44	0.43
2:B:220:HIS:CE1	4:D:272:GLN:HB3	2.53	0.43
2:B:388:GLY:HA3	4:D:242:TRP:CZ2	2.53	0.43
6:F:166:LYS:HE3	7:G:84:LEU:HD12	2.01	0.43
6:F:241:TRP:HZ2	7:G:238:LEU:CD2	2.25	0.43
6:F:335:ARG:HH21	8:H:259:HIS:HA	1.58	0.43
1:A:145:THR:CB	4:D:69:LEU:HD11	2.47	0.43
2:B:80:VAL:HG11	4:D:65:TRP:CD2	2.54	0.43
2:B:431:SER:O	2:B:433:SER:N	2.51	0.43
2:B:540:ASN:O	2:B:544:VAL:HG23	2.18	0.43
3:C:12:LEU:CB	3:C:15:LEU:HD12	2.47	0.43
4:D:296:SER:CB	4:D:301:THR:HG21	2.37	0.43
4:D:663:GLY:O	4:D:665:ARG:N	2.48	0.43
6:F:335:ARG:NH1	8:H:259:HIS:HB2	2.23	0.43
1:A:78:GLY:O	1:A:81:TYR:CD1	2.68	0.43
2:B:81:LEU:HA	2:B:84:PHE:HD2	1.83	0.43
2:B:90:PRO:O	2:B:91:ALA:C	2.61	0.43
4:D:17:GLU:OE2	4:D:17:GLU:HA	2.18	0.43
4:D:352:HIS:CG	4:D:366:ARG:CZ	3.01	0.43
6:F:297:MET:HE1	6:F:314:LEU:CG	2.45	0.43
1:A:158:LEU:HD13	3:C:238:ALA:HB2	2.00	0.43
2:B:30:LEU:HD23	4:D:34:LEU:HD23	1.96	0.43
5:E:9:PRO:HB3	6:F:197:GLN:CD	2.44	0.43
6:F:170:ARG:HE	7:G:89:MET:CG	2.31	0.43
6:F:224:ASP:CG	8:H:216:LEU:HD21	2.39	0.43
1:A:13:LYS:HG3	1:A:21:LEU:HD11	2.00	0.43
2:B:193:PHE:HB2	2:B:196:GLN:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:663:GLY:C	4:D:665:ARG:N	2.76	0.43
1:A:189:TYR:CA	3:C:271:MET:CE	2.92	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	2.61	0.42
2:B:322:ILE:HD13	4:D:379:ARG:HG3	2.00	0.42
2:B:571:VAL:HG13	3:C:288:VAL:HG21	2.01	0.42
3:C:36:CYS:N	3:C:37:PRO:CD	2.82	0.42
4:D:10:LEU:HD11	4:D:43:TRP:CE3	2.54	0.42
4:D:206:PHE:HD2	4:D:230:SER:OG	2.00	0.42
4:D:298:ASN:O	4:D:299:GLU:CB	2.49	0.42
4:D:457:LEU:O	4:D:460:PRO:HD2	2.19	0.42
5:E:137:LEU:HD23	7:G:285:LEU:HB3	2.01	0.42
6:F:176:GLN:NE2	7:G:117:ASP:HB3	2.34	0.42
6:F:341:LEU:HD21	7:G:298:PHE:HE2	1.83	0.42
6:F:377:ARG:HH11	8:H:343:GLN:N	2.17	0.42
7:G:9:ALA:HB3	7:G:109:ILE:HD13	2.01	0.42
5:E:166:ASP:OD1	6:F:344:LYS:HE3	2.18	0.42
6:F:6:ARG:HA	6:F:7:PRO:HD2	1.50	0.42
6:F:165:GLN:NE2	7:G:60:PRO:HD2	2.34	0.42
6:F:192:TYR:CE1	7:G:172:PRO:HD3	2.55	0.42
7:G:60:PRO:N	7:G:61:PRO:CD	2.82	0.42
7:G:173:TRP:HA	7:G:174:PRO:HD3	1.83	0.42
2:B:432:ALA:C	2:B:433:SER:O	2.57	0.42
3:C:280:CYS:CB	4:D:625:TRP:HD1	2.31	0.42
4:D:76:ARG:HA	4:D:79:GLU:OE2	2.19	0.42
5:E:145:LEU:HD22	6:F:284:LEU:HD13	2.01	0.42
7:G:280:PHE:CE1	8:H:287:LYS:CG	2.82	0.42
4:D:46:ILE:HG23	4:D:50:ILE:CD1	2.40	0.42
4:D:248:ASN:OD1	4:D:248:ASN:O	2.36	0.42
4:D:285:LYS:HD3	4:D:287:PHE:CZ	2.54	0.42
4:D:289:GLU:HA	4:D:290:PRO:HD3	1.58	0.42
4:D:659:GLN:O	4:D:664:SER:O	2.37	0.42
6:F:157:LEU:HG	6:F:170:ARG:HH21	1.84	0.42
8:H:358:ARG:HH21	8:H:366:LEU:HD13	1.82	0.42
1:A:8:ILE:HD12	1:A:31:MET:CE	2.50	0.42
2:B:196:GLN:HG3	2:B:196:GLN:H	1.66	0.42
2:B:500:LEU:CD2	4:D:571:LEU:CD1	2.85	0.42
4:D:419:LEU:HD23	4:D:420:LEU:HG	2.01	0.42
4:D:525:TYR:CZ	4:D:539:VAL:CG2	3.03	0.42
6:F:244:ILE:HD12	8:H:233:LEU:HD22	2.01	0.42
6:F:261:VAL:CG2	8:H:258:ARG:HD2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:HG21	3:C:250:ILE:HG23	2.01	0.42
2:B:213:LEU:HD22	2:B:374:HIS:NE2	2.35	0.42
2:B:570:TYR:HA	4:D:644:LEU:HD11	2.02	0.42
3:C:75:LEU:CD1	3:C:162:LEU:HD23	2.45	0.42
4:D:75:GLN:O	4:D:79:GLU:HG3	2.20	0.42
4:D:263:GLN:HB3	4:D:267:LYS:NZ	2.34	0.42
2:B:183:THR:C	2:B:185:CYS:N	2.77	0.42
4:D:237:MET:O	4:D:241:VAL:HG23	2.19	0.42
4:D:268:LEU:HB3	4:D:272:GLN:NE2	2.32	0.42
5:E:58:GLU:HG2	7:G:207:LEU:HD11	2.02	0.42
2:B:35:ASP:HB2	4:D:30:MET:HE3	2.00	0.42
2:B:247:GLY:C	2:B:249:ASP:N	2.77	0.42
2:B:587:LEU:HD23	4:D:654:ALA:HB3	2.02	0.42
2:B:588:GLU:OE1	4:D:650:ARG:NE	2.48	0.42
3:C:70:GLU:OE2	3:C:70:GLU:HA	2.20	0.42
4:D:601:MET:HE1	4:D:604:LEU:CD1	2.50	0.42
7:G:139:GLU:CG	8:H:155:VAL:HG22	2.41	0.42
7:G:178:LYS:N	7:G:179:PRO:HD2	2.34	0.42
1:A:193:ILE:HG23	3:C:274:LEU:HD12	2.02	0.42
1:A:266:LEU:HD21	3:C:344:MET:CE	2.49	0.42
2:B:97:ILE:O	2:B:101:GLU:HG3	2.19	0.42
2:B:347:MET:HB3	2:B:348:PRO:CD	2.47	0.42
3:C:185:ARG:O	3:C:189:VAL:HG23	2.20	0.42
3:C:285:LYS:NZ	4:D:628:GLN:NE2	2.67	0.42
1:A:104:LEU:O	3:C:63:ARG:NH2	2.47	0.42
2:B:274:ILE:CD1	4:D:392:LEU:HD11	2.50	0.42
7:G:176:ASP:OD1	7:G:176:ASP:N	2.50	0.42
7:G:183:ALA:HB1	7:G:187:LEU:HD12	2.02	0.42
2:B:450:TYR:HB3	2:B:463:ARG:NH1	2.35	0.41
4:D:6:LEU:HD11	4:D:44:LYS:HE3	2.01	0.41
5:E:78:ILE:HG13	5:E:79:THR:HG23	2.01	0.41
5:E:182:VAL:HG23	7:G:335:ARG:NH2	2.34	0.41
6:F:173:LEU:HD12	7:G:118:VAL:HG22	1.91	0.41
2:B:97:ILE:CD1	4:D:82:GLN:CB	2.66	0.41
2:B:132:CYS:HA	4:D:119:LEU:HD22	1.88	0.41
6:F:251:MET:CE	8:H:247:TYR:CD1	3.03	0.41
2:B:55:ASP:OD2	4:D:49:HIS:CE1	2.71	0.41
2:B:570:TYR:CD1	4:D:631:GLN:HG2	2.55	0.41
6:F:84:ASP:OD1	6:F:87:ARG:CG	2.68	0.41
7:G:40:LEU:O	7:G:47:ARG:NH1	2.53	0.41
7:G:143:VAL:HG23	8:H:159:MET:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LEU:HD11	4:D:39:CYS:SG	2.60	0.41
3:C:4:THR:O	3:C:8:VAL:HG23	2.20	0.41
3:C:36:CYS:O	3:C:39:LEU:O	2.38	0.41
4:D:67:GLN:O	4:D:71:HIS:HB2	2.20	0.41
5:E:179:MET:HG3	8:H:329:ILE:CD1	2.50	0.41
7:G:150:GLU:HG2	8:H:166:GLN:HE21	1.84	0.41
2:B:79:GLU:OE2	3:C:230:ARG:NH2	2.38	0.41
3:C:12:LEU:HD13	3:C:15:LEU:HD12	2.02	0.41
4:D:183:SER:HG	4:D:184:SER:H	1.63	0.41
6:F:168:LEU:HD12	7:G:145:CYS:SG	2.60	0.41
4:D:215:ILE:HA	4:D:422:LYS:CE	2.51	0.41
6:F:166:LYS:HE2	7:G:87:ASP:HB2	2.02	0.41
2:B:160:LEU:HB2	4:D:145:CYS:SG	2.61	0.41
3:C:142:PRO:CB	3:C:146:LEU:HD23	2.50	0.41
4:D:259:LEU:O	4:D:263:GLN:HG3	2.20	0.41
5:E:181:GLU:HG2	7:G:335:ARG:NH1	2.35	0.41
6:F:168:LEU:HD11	7:G:145:CYS:CB	2.51	0.41
2:B:454:ASP:C	2:B:456:ASP:N	2.78	0.41
2:B:543:THR:OG1	3:C:269:LEU:HD12	2.20	0.41
4:D:215:ILE:HA	4:D:422:LYS:HE2	2.01	0.41
4:D:260:ASN:HA	4:D:263:GLN:OE1	2.21	0.41
4:D:525:TYR:CE2	4:D:539:VAL:HG21	2.55	0.41
6:F:173:LEU:HD11	7:G:118:VAL:CG2	2.45	0.41
1:A:236:ASN:HA	1:A:239:LEU:HD12	2.02	0.41
2:B:51:ASN:ND2	4:D:18:MET:HE1	2.36	0.41
2:B:301:ALA:O	4:D:361:VAL:HG11	2.21	0.41
4:D:34:LEU:O	4:D:39:CYS:HB3	2.21	0.41
4:D:269:GLN:HG3	4:D:269:GLN:H	1.75	0.41
5:E:134:LEU:HD22	7:G:278:PHE:HD1	1.85	0.41
5:E:179:MET:HG3	8:H:329:ILE:HD12	2.03	0.41
6:F:247:MET:HE2	8:H:243:PHE:CD1	2.51	0.41
3:C:285:LYS:NZ	4:D:628:GLN:HE22	2.18	0.41
5:E:189:TRP:CZ3	8:H:336:VAL:HG12	2.50	0.41
1:A:211:HIS:ND1	4:D:630:VAL:HG23	2.36	0.40
2:B:521:THR:HG23	3:C:247:GLN:HE21	1.86	0.40
6:F:84:ASP:OD1	6:F:87:ARG:HG3	2.21	0.40
7:G:166:LEU:O	8:H:180:ASN:ND2	2.38	0.40
3:C:5:LEU:HD13	3:C:22:LEU:HD12	2.00	0.40
4:D:413:ILE:O	4:D:417:CYS:N	2.50	0.40
5:E:19:LEU:CD2	6:F:182:LEU:HD23	2.51	0.40
5:E:78:ILE:HD13	6:F:234:ILE:HG23	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:VAL:HG13	6:F:278:LEU:HD12	2.02	0.40
6:F:227:ILE:O	6:F:227:ILE:CG2	2.68	0.40
1:A:144:LEU:HD13	3:C:224:TYR:HA	2.04	0.40
1:A:145:THR:CG2	4:D:69:LEU:HD13	2.28	0.40
3:C:236:ARG:NH1	4:D:574:ASN:O	2.54	0.40
1:A:270:VAL:CA	1:A:273:MET:HE3	2.47	0.40
6:F:377:ARG:CZ	8:H:343:GLN:CG	2.94	0.40
7:G:318:LYS:HG3	7:G:324:ILE:HG12	2.02	0.40
1:A:41:ASN:ND2	3:C:39:LEU:CD2	2.85	0.40
2:B:78:ASP:O	2:B:82:LYS:HG3	2.22	0.40
2:B:368:GLN:OE1	4:D:423:LYS:HB2	2.21	0.40
2:B:521:THR:HG23	3:C:247:GLN:NE2	2.37	0.40
7:G:146:ILE:CG1	8:H:163:ILE:CG1	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/286 (99%)	273 (96%)	4 (1%)	7 (2%)	4	26
2	B	595/597 (100%)	545 (92%)	18 (3%)	32 (5%)	1	15
3	C	351/353 (99%)	338 (96%)	7 (2%)	6 (2%)	7	36
4	D	664/666 (100%)	626 (94%)	16 (2%)	22 (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%)	310 (92%)	10 (3%)	15 (4%)	2	17
8	H	199/367 (54%)	197 (99%)	1 (0%)	1 (0%)	24	63
All	All	3024/3817 (79%)	2857 (94%)	70 (2%)	97 (3%)	5	21

All (97) 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	234	GLU
2	B	236	PHE
2	B	238	LEU
2	B	240	GLN
2	B	241	LEU
2	B	243	VAL
2	B	250	GLY
2	B	431	SER
2	B	432	ALA
2	B	457	ASN
2	B	459	GLN
2	B	594	GLY
3	C	118	ALA
3	C	119	ASP
3	C	122	PRO
3	C	124	SER
3	C	352	LEU
4	D	118	ASP
4	D	178	VAL
4	D	183	SER
4	D	186	THR
4	D	217	SER
4	D	219	VAL
4	D	284	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	286	GLU
4	D	299	GLU
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
4	D	221	PRO
4	D	292	THR
6	F	228	SER
6	F	337	ASP
7	G	2	THR
2	B	233	ASP
4	D	222	GLY
4	D	288	SER
7	G	122	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	125	ILE
4	D	290	PRO
5	E	5	ASN
6	F	148	ALA
6	F	333	GLY
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%)	501 (93%)	40 (7%)	13	33
3	C	326/326 (100%)	310 (95%)	16 (5%)	22	43
4	D	605/605 (100%)	561 (93%)	44 (7%)	13	34
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%)	2601 (94%)	169 (6%)	19	38

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	28	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	194	LEU
2	B	196	GLN
2	B	198	LEU
2	B	199	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	364	CYS
2	B	370	LEU
2	B	372	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	174	MET
4	D	179	ASP
4	D	182	LEU
4	D	186	THR
4	D	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	202	LEU
4	D	214	SER
4	D	224	GLU
4	D	226	LEU
4	D	229	LEU
4	D	230	SER
4	D	235	MET
4	D	259	LEU
4	D	262	THR
4	D	265	LEU
4	D	293	GLN
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	419	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 (49)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
2	B	114	HIS
2	B	220	HIS
2	B	263	GLN
2	B	346	ASN
2	B	386	GLN
2	B	493	HIS
3	C	155	GLN
3	C	174	GLN
3	C	220	GLN
3	C	247	GLN
3	C	291	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
4	D	152	ASN
4	D	161	GLN
4	D	231	HIS
4	D	272	GLN
4	D	343	HIS
4	D	352	HIS
4	D	426	HIS
4	D	440	GLN
4	D	542	HIS
4	D	549	GLN
4	D	628	GLN
4	D	631	GLN
5	E	45	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	102	HIS
7	G	161	HIS
8	H	166	GLN
8	H	196	ASN
8	H	207	HIS
8	H	282	HIS
8	H	297	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	17
6	F	17
1	A	13
2	B	10
4	D	9

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
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	B	223:GLU	C	224:GLY	N	1.81
1	A	277:VAL	C	278:PRO	N	1.79
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	C	213:MET	C	214:ARG	N	1.20
1	D	638:GLU	C	639:ARG	N	1.20
1	D	650:ARG	C	651:TRP	N	1.20
1	D	661:ALA	C	662:THR	N	1.20
1	E	51:ARG	C	52:ILE	N	1.20
1	E	72:GLU	C	73:LYS	N	1.20
1	E	95:ASN	C	96:SER	N	1.20
1	E	128:HIS	C	129:ARG	N	1.20
1	E	136:PRO	C	137:LEU	N	1.20
1	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	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	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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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	D	221:PRO	C	222:GLY	N	1.18
1	E	78:ILE	C	79:THR	N	1.18
1	E	93:ALA	C	94:MET	N	1.18
1	F	44:GLY	C	45:VAL	N	1.18
1	F	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	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	F	209:GLU	C	210:HIS	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	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	146:ALA	C	147:ASP	N	1.15

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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	262:VAL	C	263:ARG	N	1.14
1	D	227:ARG	C	228:SER	N	1.13
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	A	272:MET	C	273:MET	N	0.96

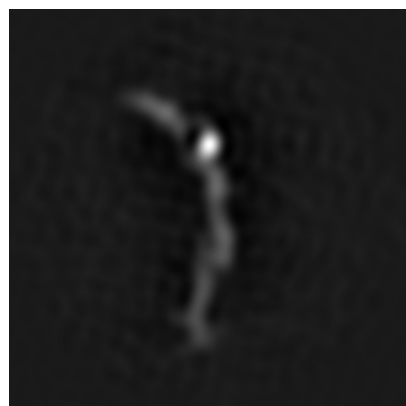
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15633. 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](#)

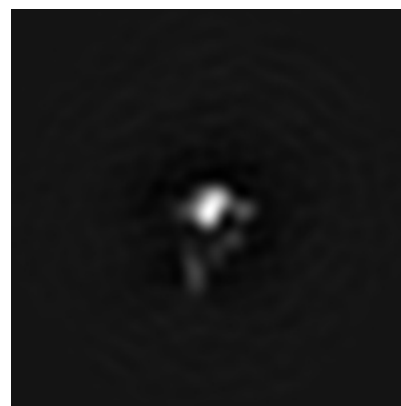
6.1.1 Primary map



X

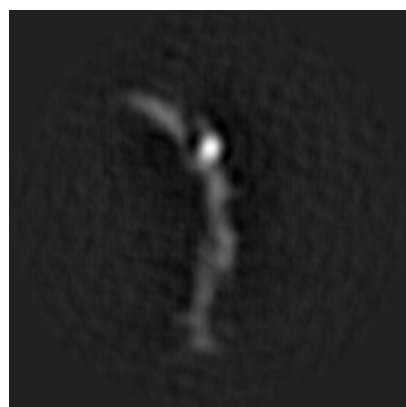


Y

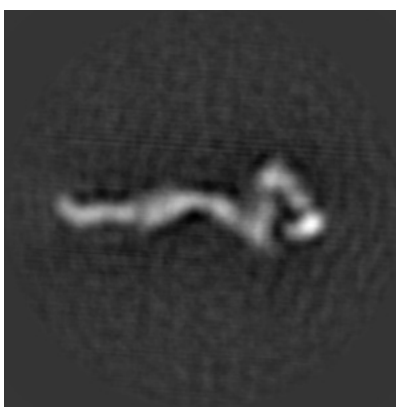


Z

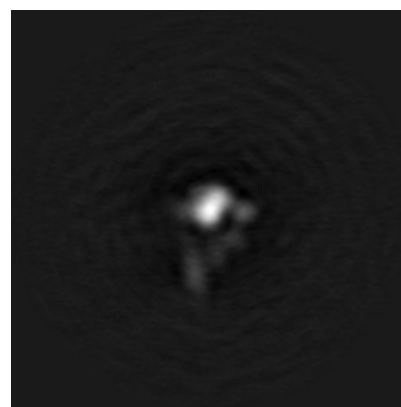
6.1.2 Raw map



X



Y

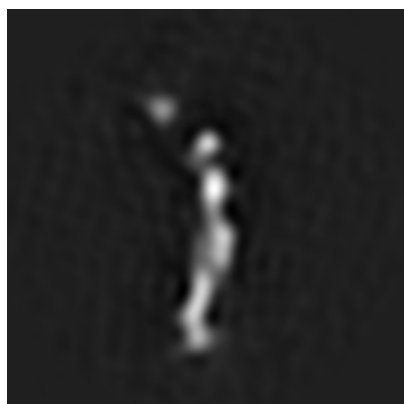


Z

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

6.2 Central slices [i](#)

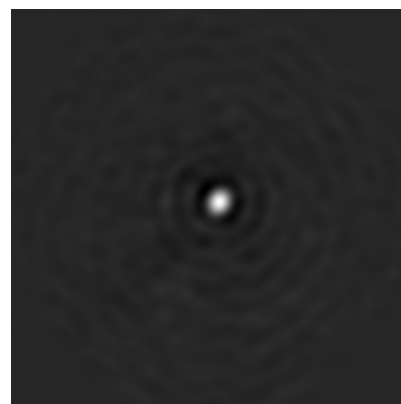
6.2.1 Primary map



X Index: 128

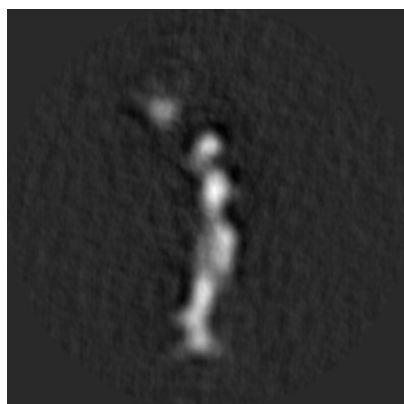


Y Index: 128

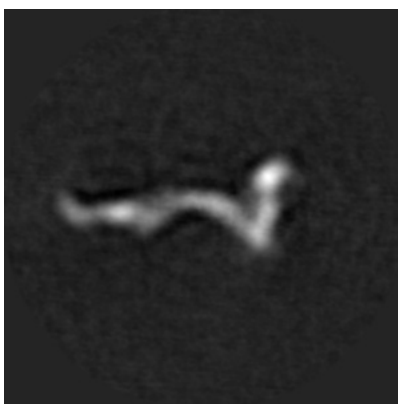


Z Index: 128

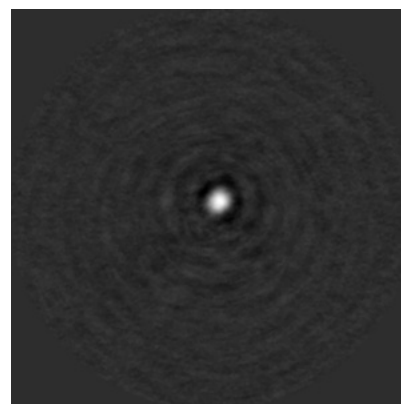
6.2.2 Raw map



X Index: 128



Y Index: 128

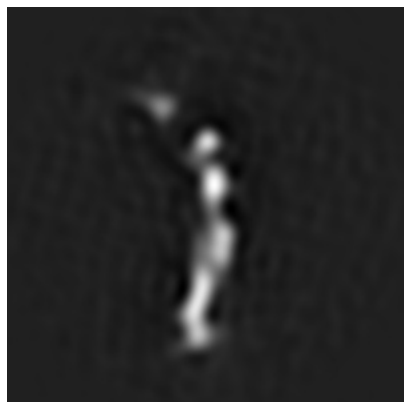


Z Index: 128

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

6.3 Largest variance slices [i](#)

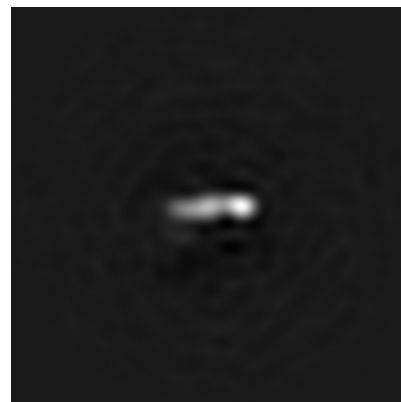
6.3.1 Primary map



X Index: 127

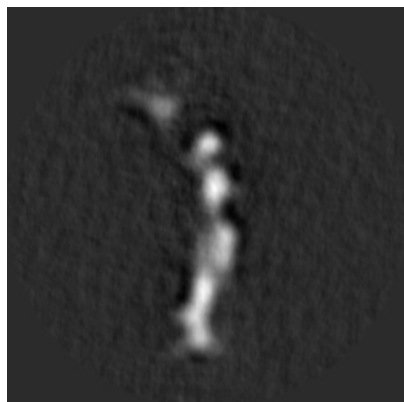


Y Index: 128

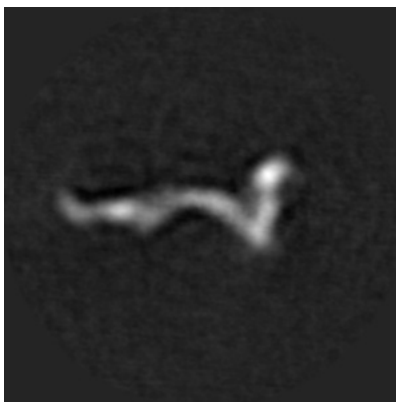


Z Index: 169

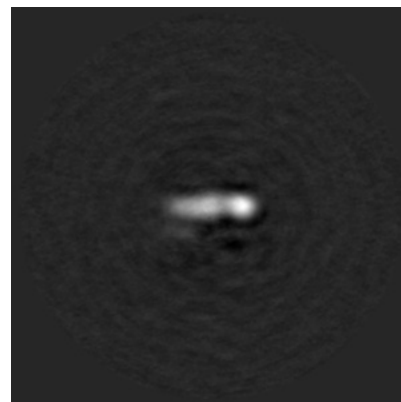
6.3.2 Raw map



X Index: 127



Y Index: 128

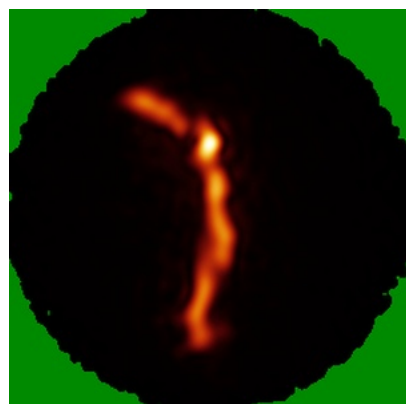


Z Index: 167

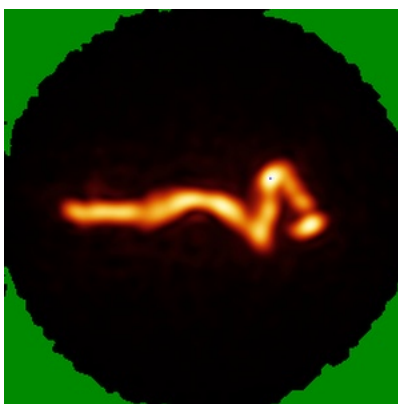
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

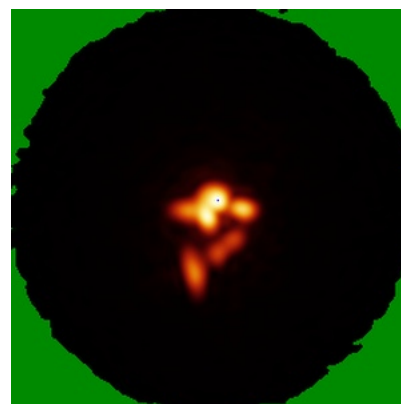
6.4.1 Primary map



X

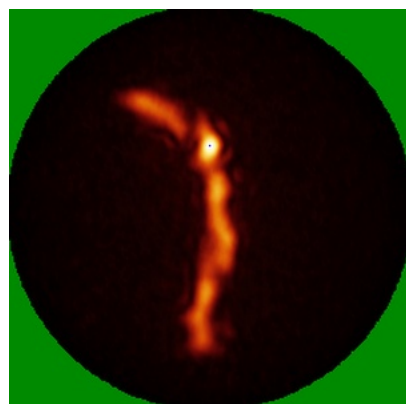


Y

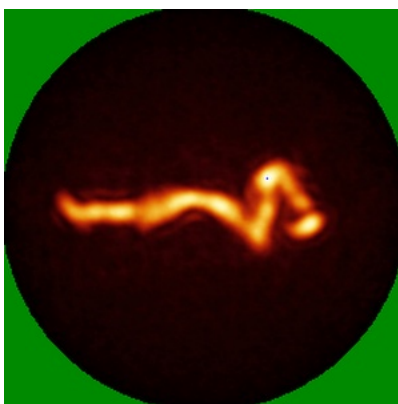


Z

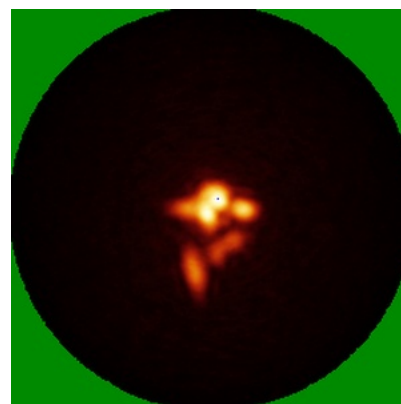
6.4.2 Raw map



X



Y

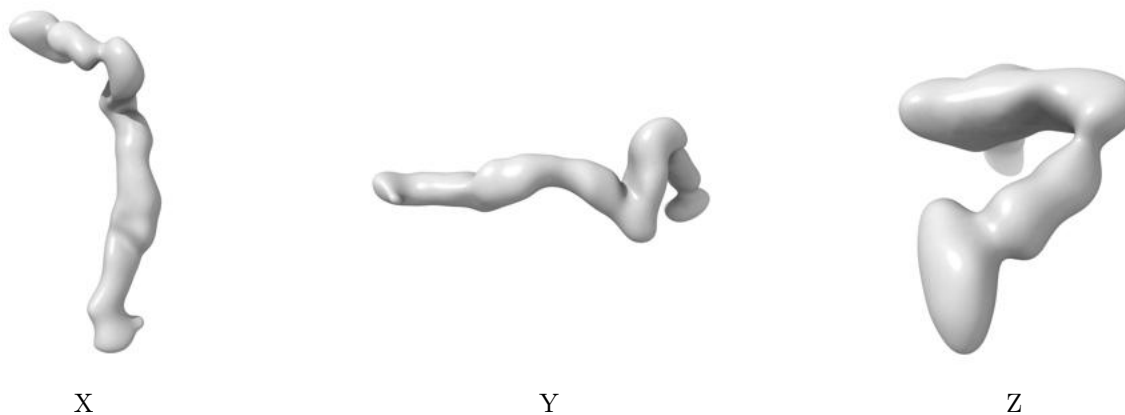


Z

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.

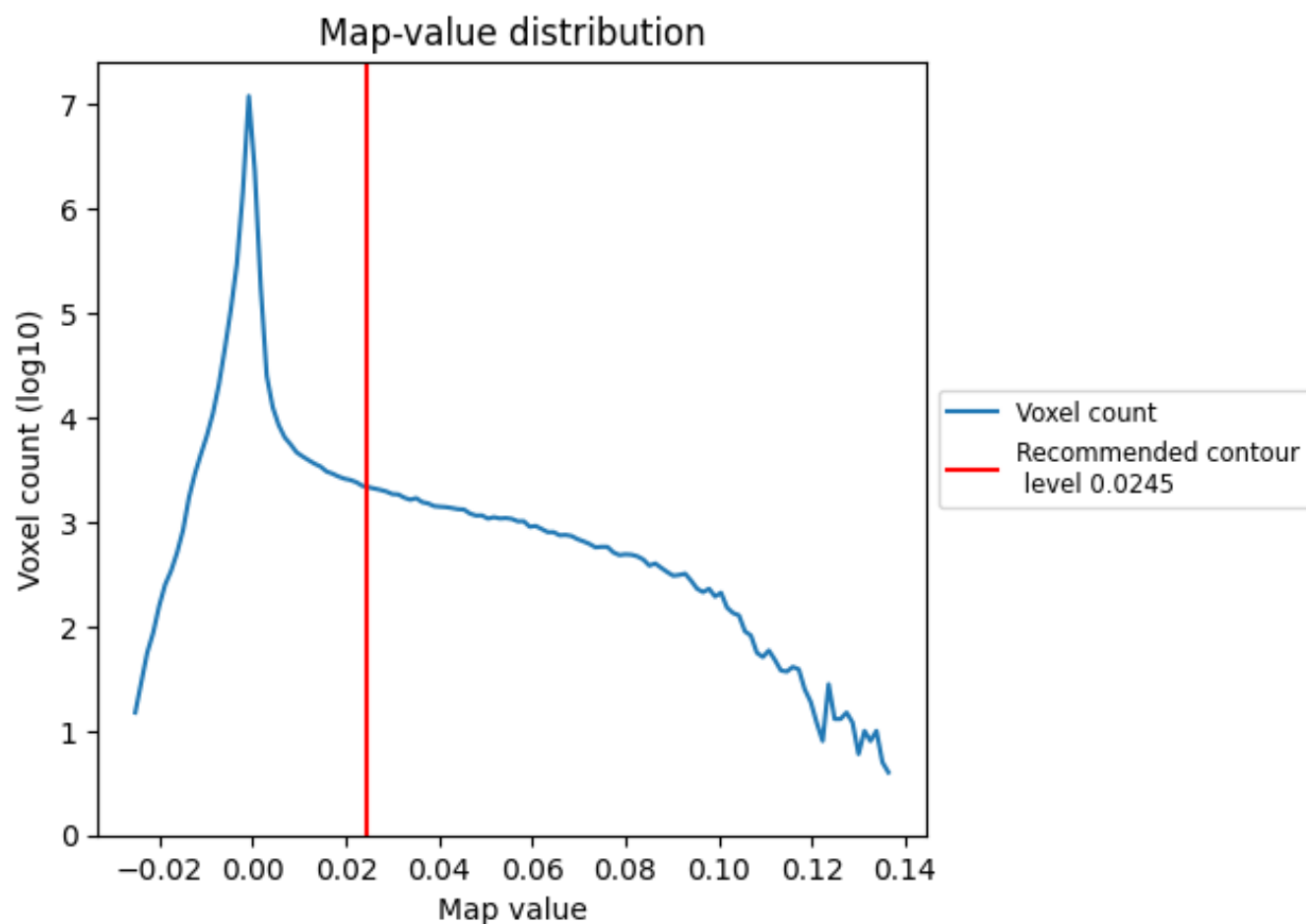
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

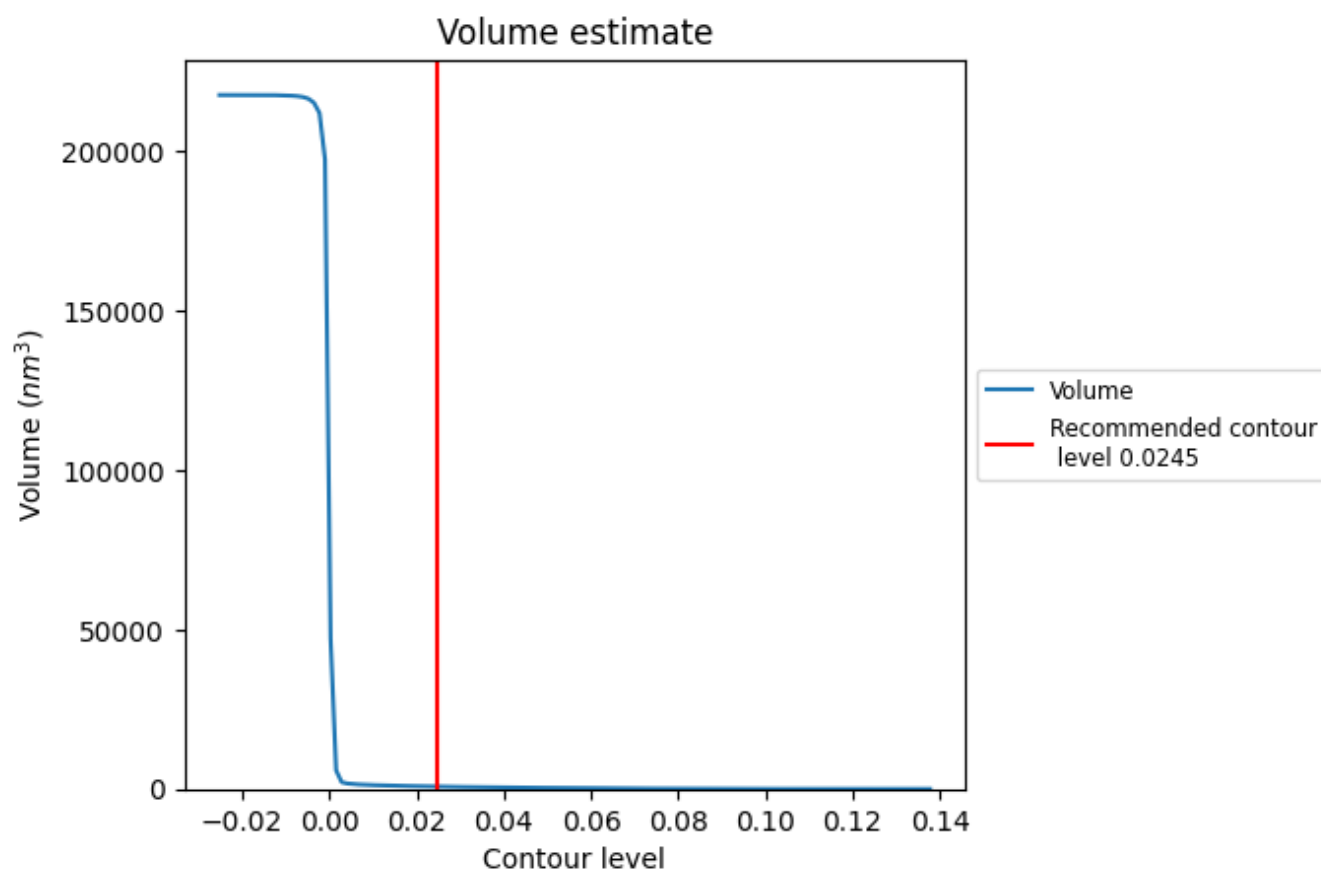
This section contains the results of statistical analysis of the map.

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.

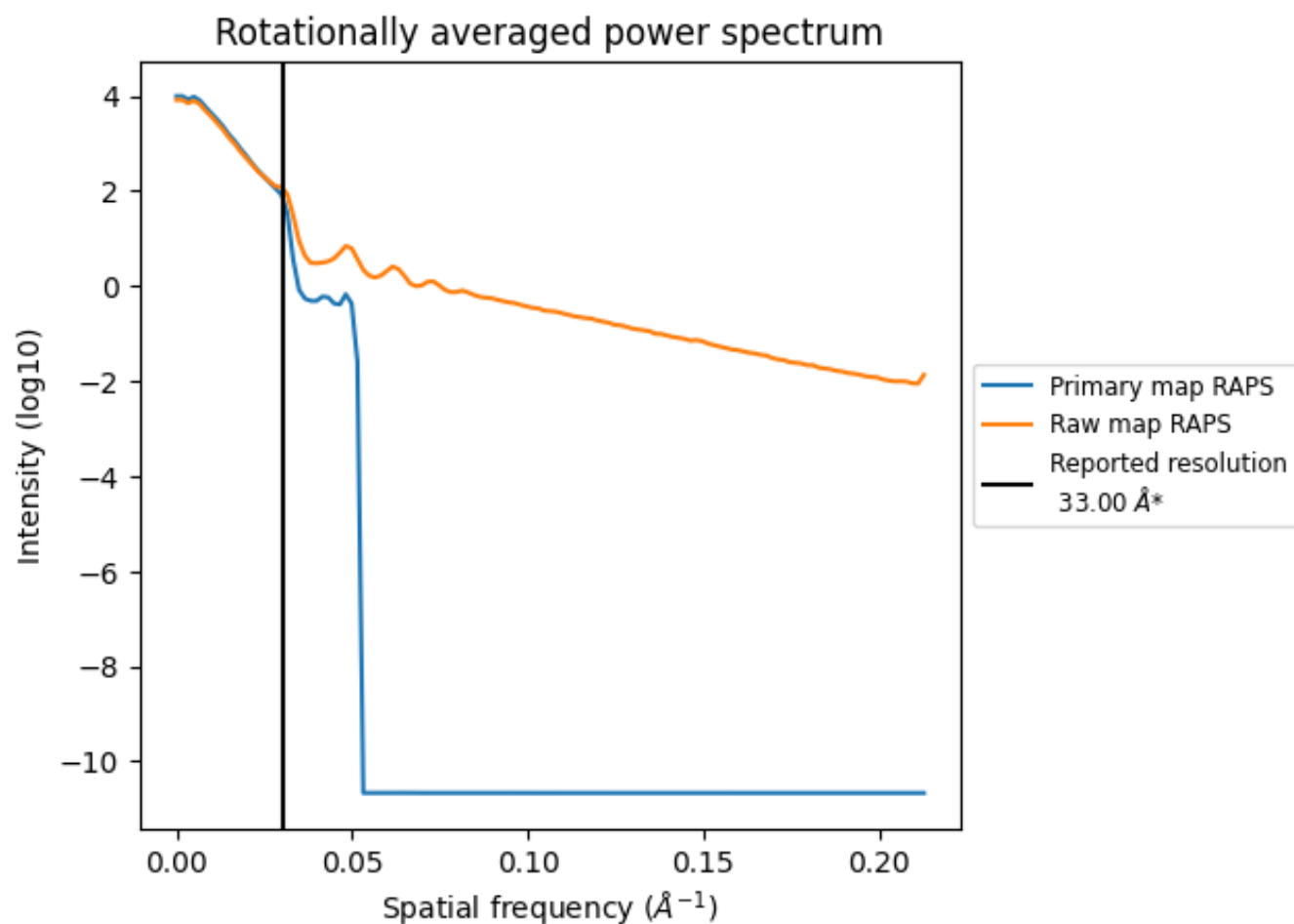
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 ⓘ

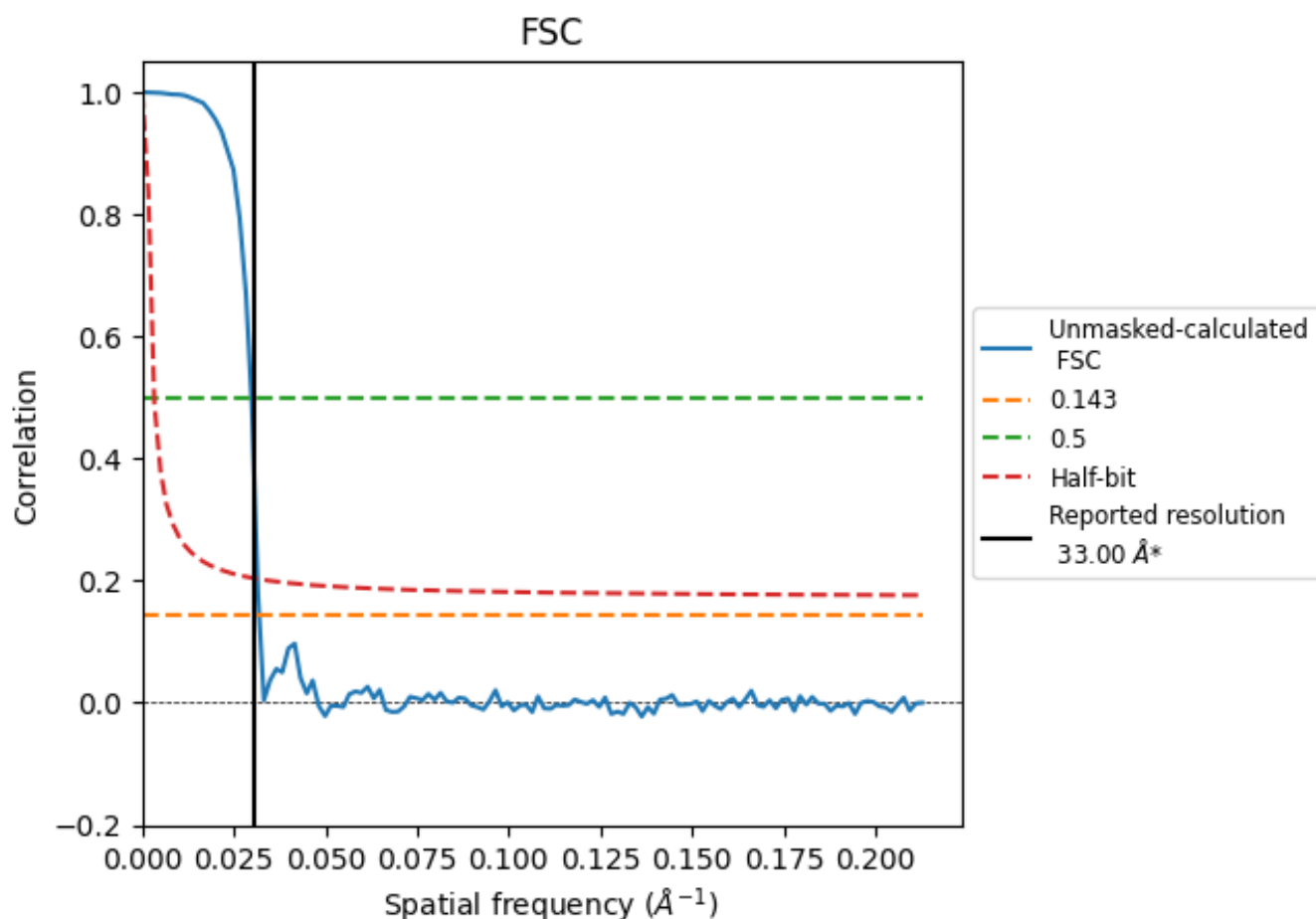


*Reported resolution corresponds to spatial frequency of 0.030 Å⁻¹

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](#)

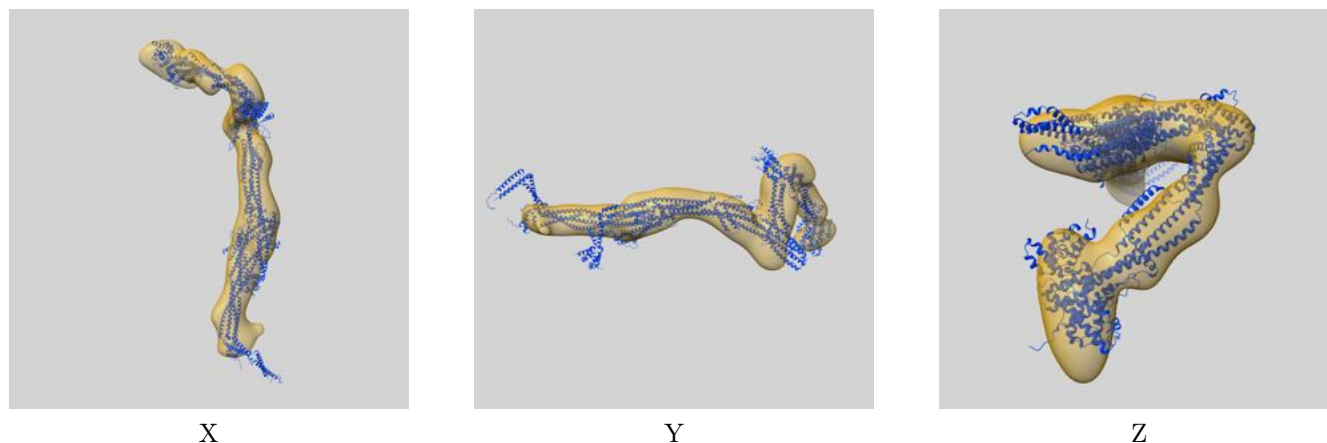
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	33.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	31.35	33.56	31.75

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

9 Map-model fit [i](#)

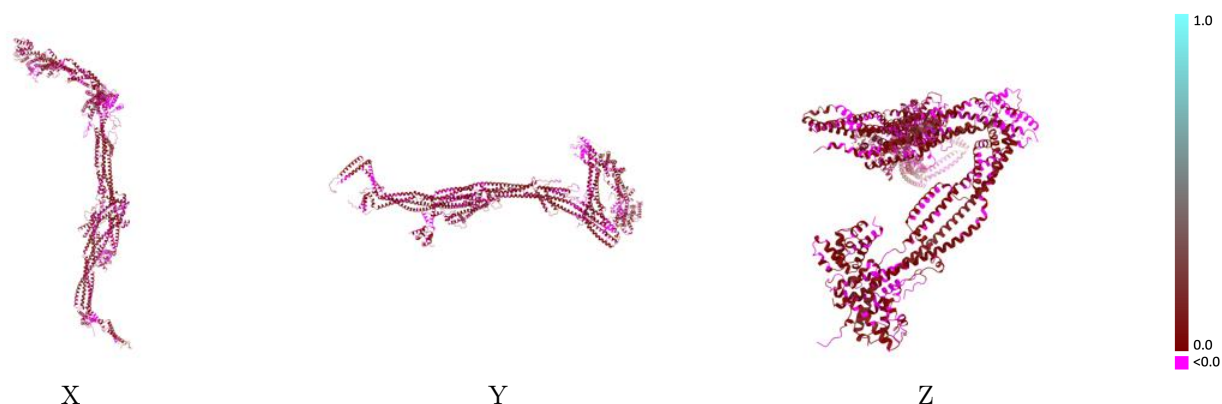
This section contains information regarding the fit between EMDB map EMD-15633 and PDB model 8AT4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



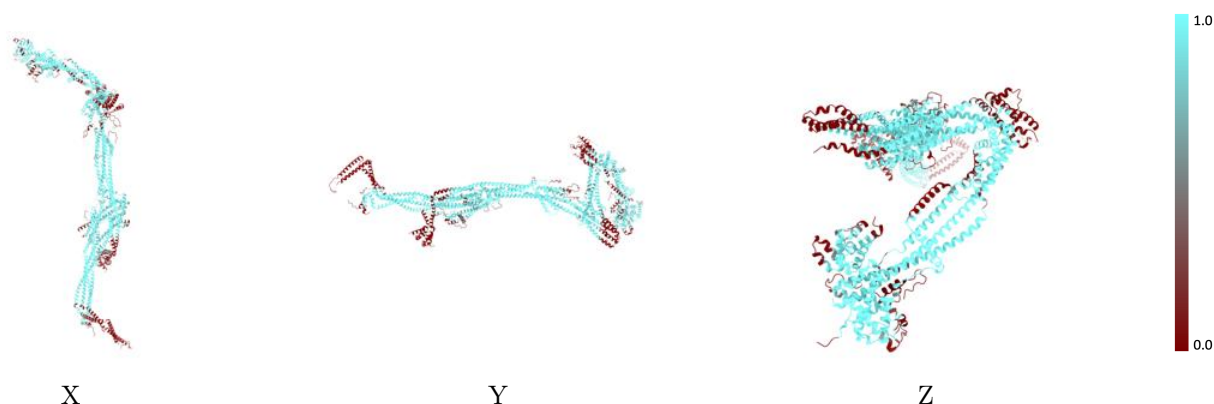
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



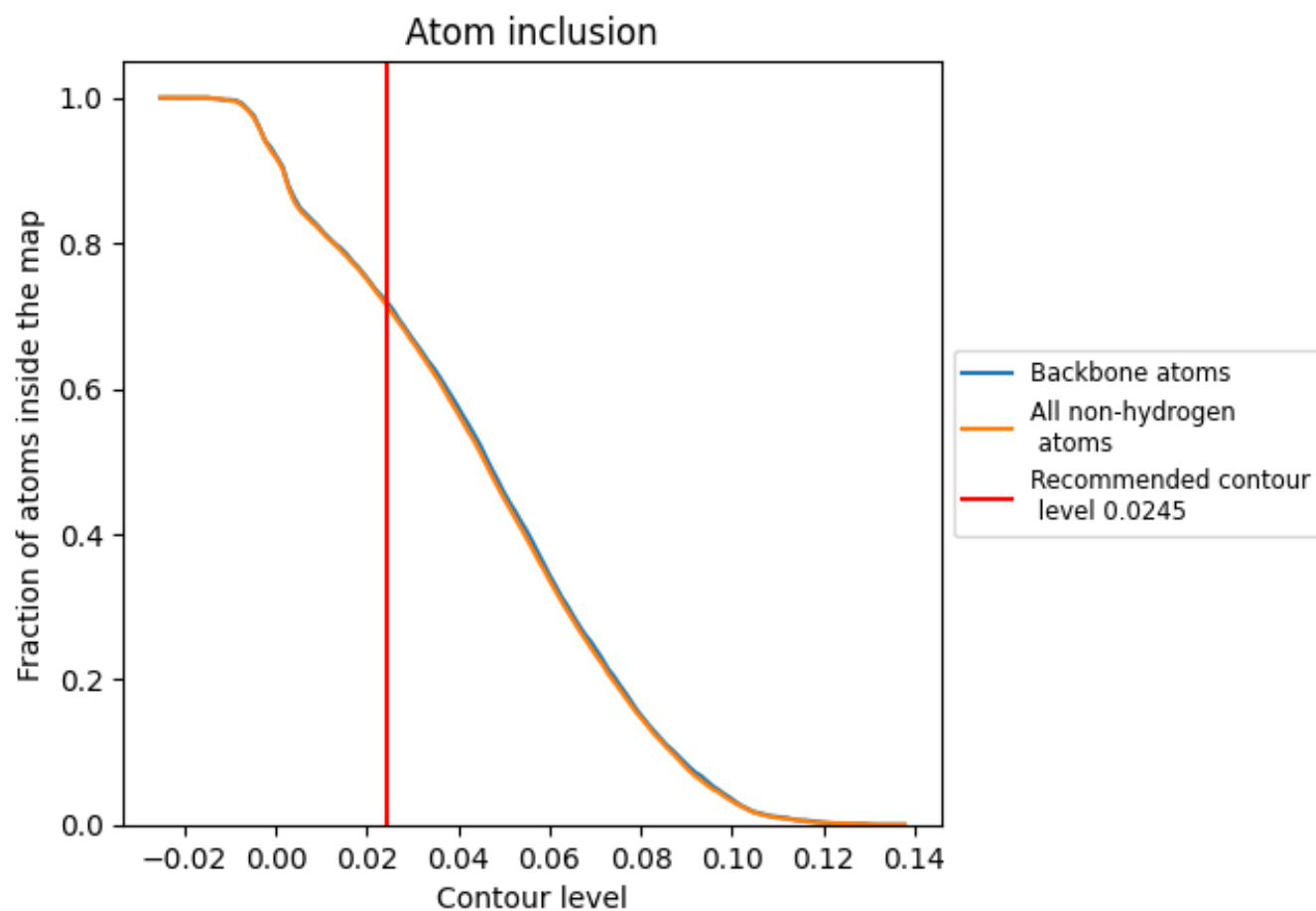
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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	0.7130	0.0400
A	0.6230	0.0480
B	0.7180	0.0410
C	0.7250	0.0530
D	0.6990	0.0330
E	0.5390	0.0190
F	0.7650	0.0340
G	0.7350	0.0310
H	0.9010	0.0710

1.0

0.0

<0.0