Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:37 pm GMT

PDB ID	:	6EQC
EMDB ID	:	EMD-3821
Title	:	Cryo-EM reconstruction of a complex of a binding protein and human adenovirus C5 hexon
Authors	:	Schmid, M.; Ernst, P.; Honegger, A.; Suomalainen, M.; Zimmermann, M.; Braun, L.; Stauffer, S.; Thom, C.; Dreier, B.; Eibauer, M.; Kipar, A.; Vogel, V.; Greber, U.F.; Medalia, O.; Plueckthun, A.
Deposited on	:	2017-10-12
Resolution	:	7.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

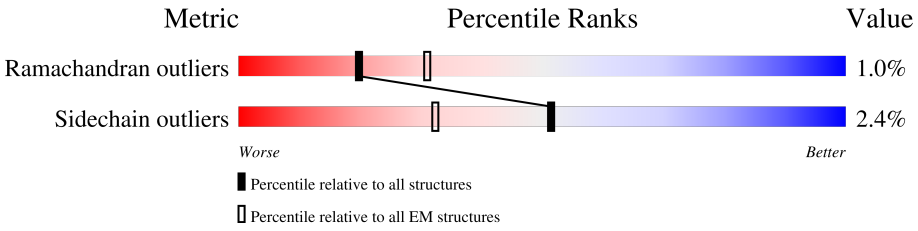
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	952	74% 20%
1	B	952	73% 21%
1	C	952	74% 19%
2	D	254	74% 14% 8%
2	E	254	71% 19% 8%
2	F	254	69% 21% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 53964 atoms, of which 26442 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 Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	B	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	C	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	THR	conflict	UNP P04133
A	420	GLY	ILE	conflict	UNP P04133
A	422	ASN	THR	conflict	UNP P04133
A	423	SER	GLU	conflict	UNP P04133
A	425	TYR	LEU	conflict	UNP P04133
B	272	ALA	THR	conflict	UNP P04133
B	420	GLY	ILE	conflict	UNP P04133
B	422	ASN	THR	conflict	UNP P04133
B	423	SER	GLU	conflict	UNP P04133
B	425	TYR	LEU	conflict	UNP P04133
C	272	ALA	THR	conflict	UNP P04133
C	420	GLY	ILE	conflict	UNP P04133
C	422	ASN	THR	conflict	UNP P04133
C	423	SER	GLU	conflict	UNP P04133
C	425	TYR	LEU	conflict	UNP P04133

- Molecule 2 is a protein called scFv of 9C12 antibody.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		
2	E	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		

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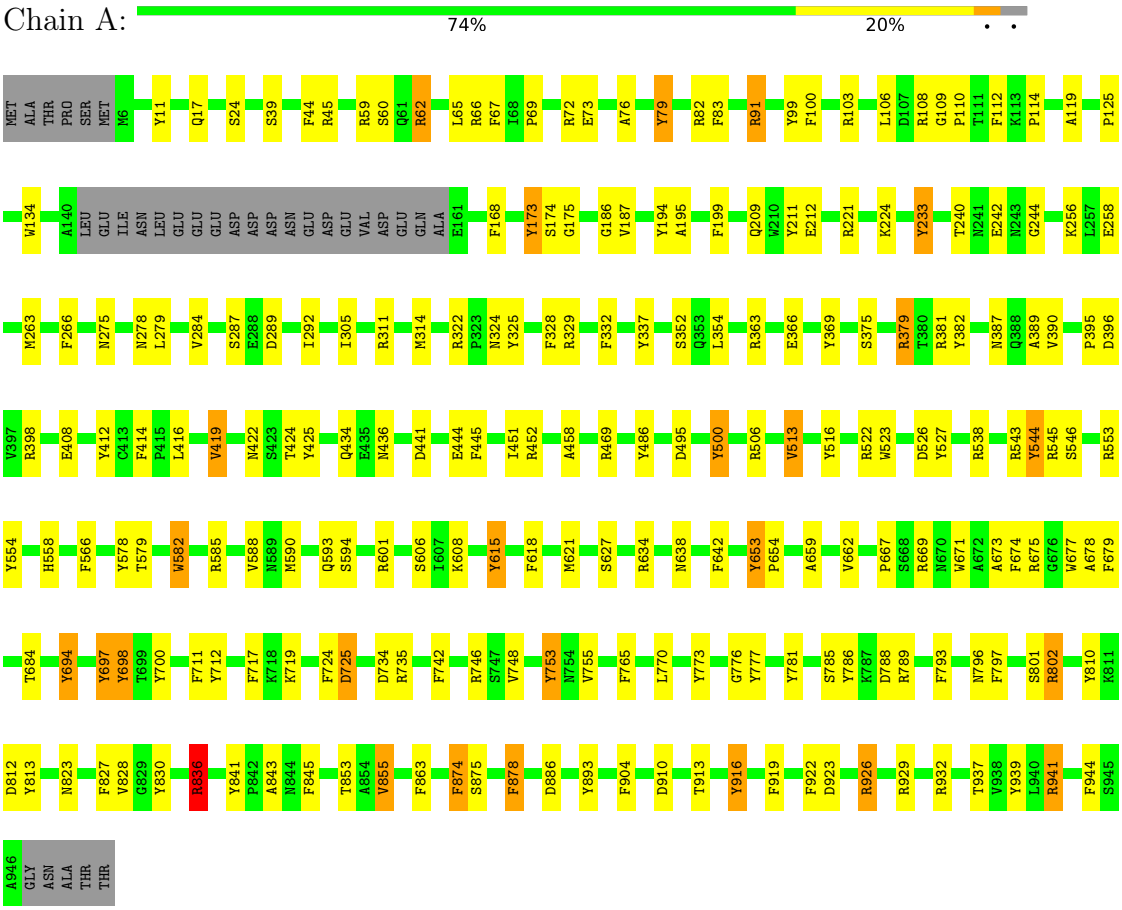
Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		

3 Residue-property plots (i)

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.

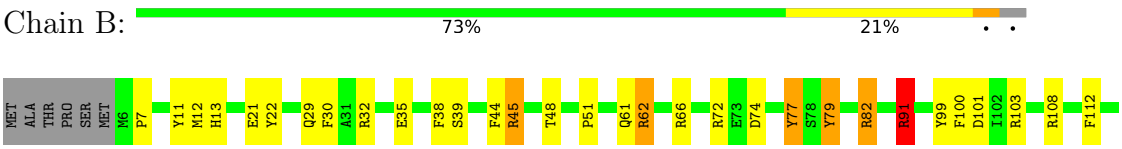
• Molecule 1: Hexon protein

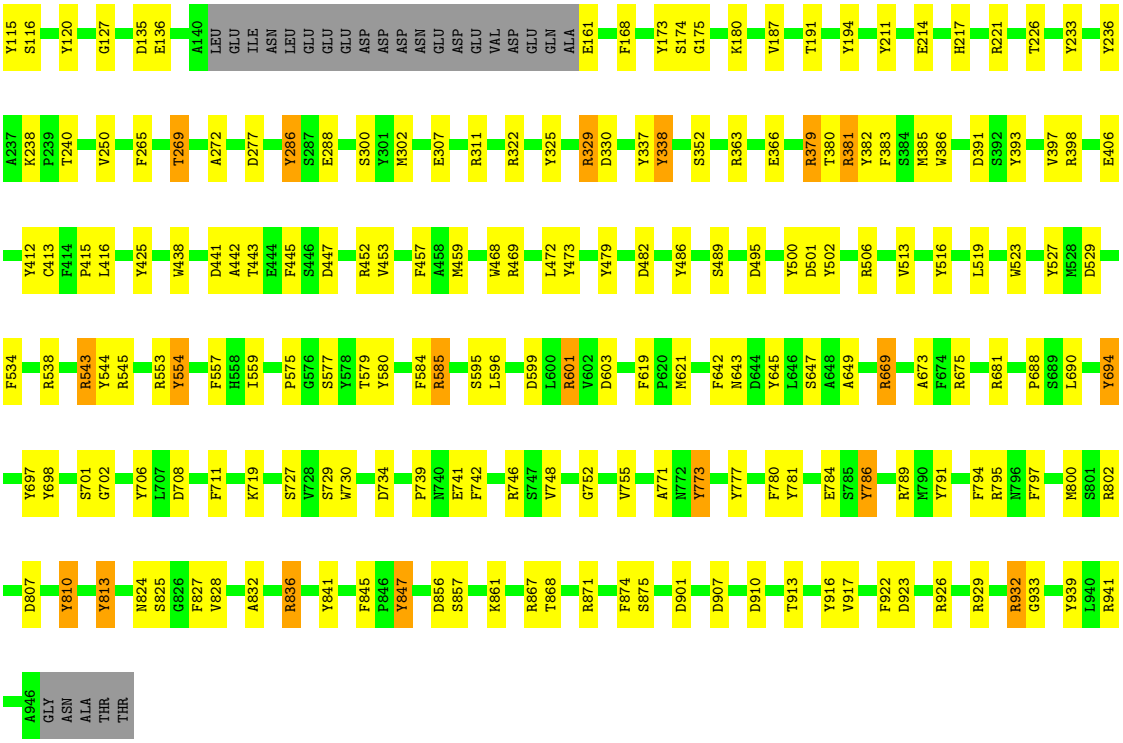
Chain A:



• Molecule 1: Hexon protein

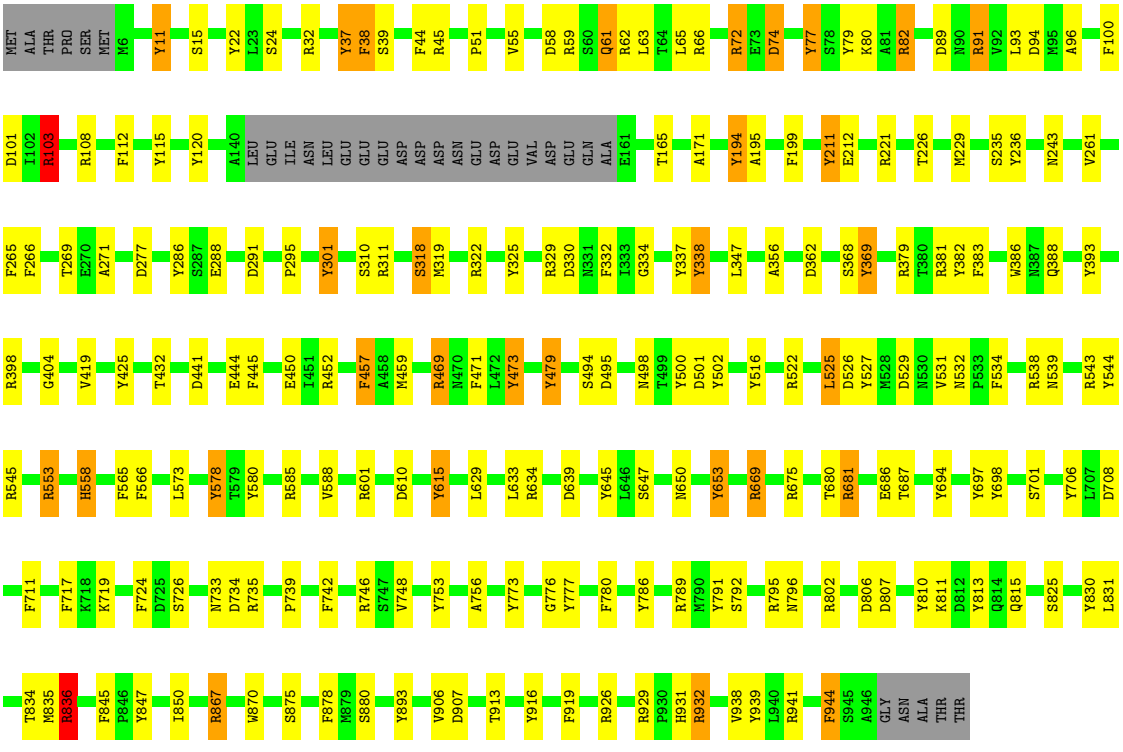
Chain B:





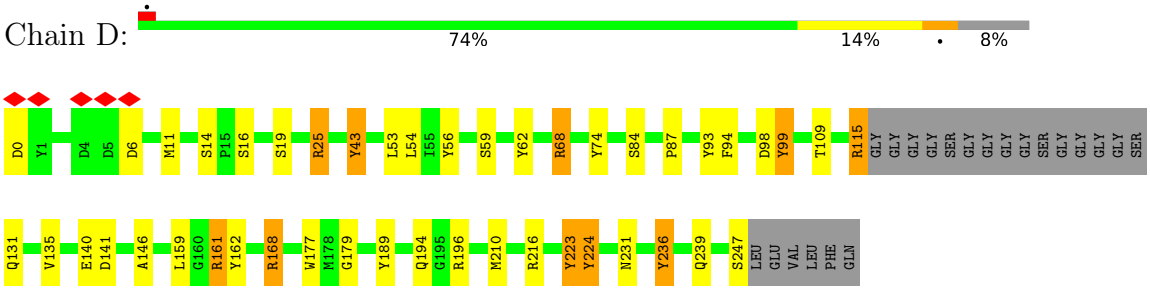
• Molecule 1: Hexon protein

Chain C:



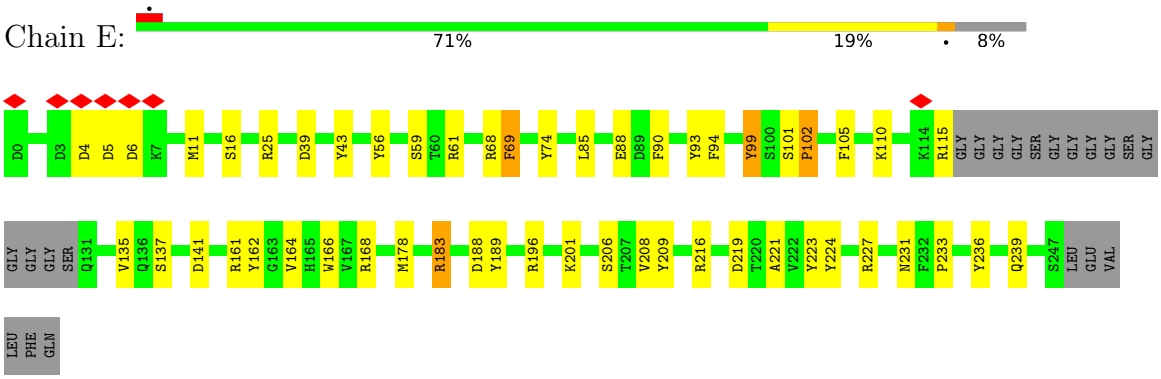
• Molecule 2: scFv of 9C12 antibody

Chain D:



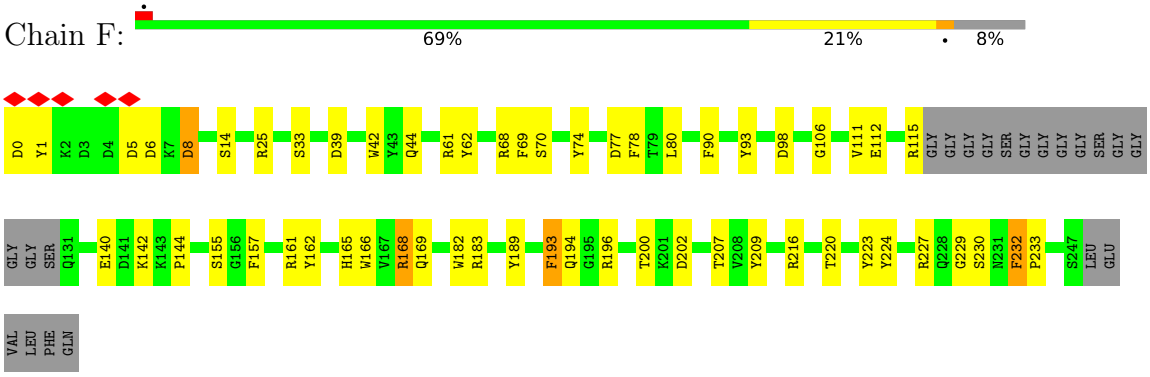
- Molecule 2: scFv of 9C12 antibody

Chain E:



- Molecule 2: scFv of 9C12 antibody

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	1568.0, 1568.0, 1568.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.96, 1.96, 1.96	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.66	46/7574 (0.6%)	2.11	221/10299 (2.1%)
1	B	1.65	51/7574 (0.7%)	2.08	228/10299 (2.2%)
1	C	1.66	44/7574 (0.6%)	2.00	218/10299 (2.1%)
2	D	1.73	14/1839 (0.8%)	1.98	50/2490 (2.0%)
2	E	1.71	19/1839 (1.0%)	2.24	53/2490 (2.1%)
2	F	1.75	22/1839 (1.2%)	2.10	55/2490 (2.2%)
All	All	1.67	196/28239 (0.7%)	2.07	825/38367 (2.2%)

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	26
1	B	0	28
1	C	0	33
2	D	0	10
2	E	0	6
2	F	0	4
All	All	0	107

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	33	SER	CA-CB	8.58	1.65	1.52
1	A	186	GLY	CA-C	8.47	1.65	1.51
2	E	224	TYR	CB-CG	-8.27	1.39	1.51
1	B	21	GLU	CG-CD	7.95	1.63	1.51
1	C	653	TYR	CE2-CZ	7.74	1.48	1.38
1	C	24	SER	CA-CB	7.68	1.64	1.52
1	B	875	SER	CA-CB	7.60	1.64	1.52
2	D	131	GLN	N-CA	7.52	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	43	TYR	CG-CD1	7.52	1.49	1.39
1	C	15	SER	CA-CB	7.48	1.64	1.52
2	E	189	TYR	CB-CG	-7.44	1.40	1.51
1	B	382	TYR	CG-CD1	7.42	1.48	1.39
1	A	801	SER	CA-CB	7.42	1.64	1.52
2	F	223	TYR	CE2-CZ	7.27	1.48	1.38
2	D	93	TYR	CG-CD1	7.27	1.48	1.39
1	A	39	SER	CA-CB	7.24	1.63	1.52
2	F	70	SER	CA-CB	7.24	1.63	1.52
1	C	791	TYR	CE1-CZ	7.21	1.48	1.38
1	C	368	SER	CB-OG	7.18	1.51	1.42
1	C	585	ARG	CD-NE	7.07	1.58	1.46
1	C	880	SER	CA-CB	7.05	1.63	1.52
1	A	916	TYR	CG-CD1	7.03	1.48	1.39
2	F	93	TYR	CZ-OH	6.97	1.49	1.37
1	A	841	TYR	CE1-CZ	6.82	1.47	1.38
1	C	51	PRO	N-CD	6.81	1.57	1.47
2	E	88	GLU	CD-OE2	-6.79	1.18	1.25
1	B	647	SER	CB-OG	6.77	1.51	1.42
2	F	162	TYR	CE2-CZ	6.72	1.47	1.38
1	C	777	TYR	CB-CG	-6.62	1.41	1.51
1	B	825	SER	CB-OG	6.62	1.50	1.42
1	B	777	TYR	CE1-CZ	6.60	1.47	1.38
1	B	527	TYR	CZ-OH	6.59	1.49	1.37
1	A	566	PHE	CG-CD2	6.58	1.48	1.38
1	B	580	TYR	CG-CD1	6.57	1.47	1.39
1	A	242	GLU	CG-CD	6.55	1.61	1.51
1	C	701	SER	CB-OG	6.54	1.50	1.42
1	C	753	TYR	CG-CD1	6.53	1.47	1.39
2	E	99	TYR	CG-CD2	6.51	1.47	1.39
2	E	94	PHE	CG-CD2	6.51	1.48	1.38
1	B	79	TYR	CE1-CZ	6.47	1.47	1.38
1	B	847	TYR	CG-CD2	6.46	1.47	1.39
1	C	338	TYR	CZ-OH	6.45	1.48	1.37
1	C	334	GLY	N-CA	6.45	1.55	1.46
1	C	310	SER	CA-CB	6.43	1.62	1.52
2	F	69	PHE	CG-CD1	6.37	1.48	1.38
1	C	66	ARG	CD-NE	6.32	1.57	1.46
1	B	780	PHE	CE2-CZ	6.30	1.49	1.37
1	B	730	TRP	NE1-CE2	-6.27	1.29	1.37
2	E	101	SER	CA-CB	6.25	1.62	1.52
1	A	786	TYR	CE1-CZ	6.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	310	SER	CB-OG	6.22	1.50	1.42
1	B	706	TYR	CG-CD1	6.20	1.47	1.39
1	C	615	TYR	CG-CD2	6.19	1.47	1.39
1	B	702	GLY	N-CA	6.11	1.55	1.46
1	B	473	TYR	CD1-CE1	6.10	1.48	1.39
1	A	875	SER	CB-OG	6.09	1.50	1.42
2	E	11	MET	CA-CB	6.06	1.67	1.53
1	B	791	TYR	CE1-CZ	6.06	1.46	1.38
1	C	825	SER	CA-CB	6.05	1.62	1.52
1	A	875	SER	CA-CB	6.02	1.61	1.52
2	D	140	GLU	CB-CG	6.02	1.63	1.52
1	B	174	SER	CA-CB	6.00	1.61	1.52
2	D	247	SER	CB-OG	6.00	1.50	1.42
1	A	578	TYR	CE2-CZ	5.87	1.46	1.38
2	E	25	ARG	CD-NE	5.87	1.56	1.46
1	A	366	GLU	CG-CD	5.87	1.60	1.51
2	F	62	TYR	CE1-CZ	5.85	1.46	1.38
1	B	489	SER	CA-CB	5.84	1.61	1.52
1	A	173	TYR	CE1-CZ	5.82	1.46	1.38
1	A	444	GLU	CD-OE2	5.80	1.32	1.25
1	B	127	GLY	CA-C	-5.80	1.42	1.51
1	A	893	TYR	CE2-CZ	5.80	1.46	1.38
1	B	807	ASP	CB-CG	5.78	1.63	1.51
2	D	62	TYR	CE1-CZ	5.77	1.46	1.38
2	F	229	GLY	CA-C	-5.76	1.42	1.51
1	B	706	TYR	CZ-OH	5.73	1.47	1.37
1	C	748	VAL	CB-CG1	5.73	1.64	1.52
2	F	106	GLY	CA-C	-5.73	1.42	1.51
1	A	777	TYR	CG-CD2	5.73	1.46	1.39
1	B	516	TYR	CG-CD1	5.72	1.46	1.39
1	A	785	SER	CA-CB	5.71	1.61	1.52
1	A	606	SER	CA-CB	5.71	1.61	1.52
1	B	932	ARG	NE-CZ	-5.69	1.25	1.33
1	B	781	TYR	CZ-OH	5.69	1.47	1.37
1	C	686	GLU	CG-CD	5.68	1.60	1.51
1	C	445	PHE	CG-CD2	5.67	1.47	1.38
1	C	786	TYR	CE2-CZ	5.66	1.46	1.38
1	C	450	GLU	CB-CG	5.66	1.62	1.52
2	D	223	TYR	CG-CD1	5.66	1.46	1.39
1	A	944	PHE	CG-CD2	5.65	1.47	1.38
1	B	752	GLY	N-CA	5.65	1.54	1.46
1	C	338	TYR	CB-CG	-5.65	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	168	ARG	CD-NE	5.65	1.56	1.46
1	B	77	TYR	CZ-OH	5.65	1.47	1.37
1	B	519	LEU	C-N	5.64	1.43	1.33
1	A	444	GLU	CB-CG	5.64	1.62	1.52
1	A	212	GLU	CG-CD	5.63	1.60	1.51
1	B	338	TYR	CD1-CE1	5.62	1.47	1.39
2	E	189	TYR	CZ-OH	5.62	1.47	1.37
1	B	502	TYR	CZ-OH	5.61	1.47	1.37
1	B	708	ASP	C-N	5.61	1.43	1.33
1	C	79	TYR	CD1-CE1	5.61	1.47	1.39
1	A	452	ARG	CZ-NH2	-5.58	1.25	1.33
2	D	19	SER	CA-CB	5.58	1.61	1.52
2	F	14	SER	CB-OG	5.57	1.49	1.42
2	F	182	TRP	CE3-CZ3	5.57	1.48	1.38
2	D	99	TYR	CE1-CZ	5.56	1.45	1.38
1	A	24	SER	CA-CB	5.55	1.61	1.52
2	D	194	GLN	CA-CB	5.54	1.66	1.53
1	A	109	GLY	N-CA	5.54	1.54	1.46
2	E	206	SER	CA-CB	5.54	1.61	1.52
2	D	161	ARG	CD-NE	5.54	1.55	1.46
2	D	99	TYR	CE2-CZ	5.54	1.45	1.38
1	B	99	TYR	CG-CD1	-5.53	1.31	1.39
1	C	926	ARG	CZ-NH2	-5.51	1.25	1.33
1	B	577	SER	CB-OG	5.49	1.49	1.42
2	E	16	SER	CA-CB	5.49	1.61	1.52
1	B	554	TYR	CD1-CE1	5.48	1.47	1.39
2	F	155	SER	CA-CB	5.47	1.61	1.52
1	A	753	TYR	CE2-CZ	5.47	1.45	1.38
1	C	120	TYR	CB-CG	5.47	1.59	1.51
1	B	554	TYR	CG-CD2	5.44	1.46	1.39
1	A	100	PHE	CD1-CE1	5.44	1.50	1.39
1	A	416	LEU	C-N	5.42	1.42	1.33
1	C	502	TYR	CE1-CZ	5.42	1.45	1.38
1	C	494	SER	CA-CB	5.42	1.61	1.52
1	C	680	THR	CA-C	5.42	1.67	1.52
1	A	546	SER	CA-CB	5.41	1.61	1.52
1	A	375	SER	CA-CB	5.41	1.61	1.52
1	C	211	TYR	CD2-CE2	5.41	1.47	1.39
1	B	300	SER	CA-CB	5.38	1.61	1.52
1	A	44	PHE	CG-CD2	5.37	1.46	1.38
1	C	337	TYR	CZ-OH	5.36	1.47	1.37
1	B	645	TYR	CE1-CZ	5.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	393	TYR	CB-CG	-5.34	1.43	1.51
1	C	32	ARG	CD-NE	5.34	1.55	1.46
1	A	194	TYR	CG-CD2	5.33	1.46	1.39
2	E	162	TYR	CE1-CZ	5.33	1.45	1.38
1	B	45	ARG	CD-NE	5.31	1.55	1.46
1	A	594	SER	CA-CB	5.31	1.60	1.52
1	C	61	GLN	CA-CB	5.30	1.65	1.53
2	F	1	TYR	CE2-CZ	5.30	1.45	1.38
2	E	61	ARG	CD-NE	5.30	1.55	1.46
2	F	230	SER	CB-OG	5.29	1.49	1.42
1	B	30	PHE	CG-CD1	5.29	1.46	1.38
1	B	797	PHE	CE2-CZ	5.28	1.47	1.37
1	C	875	SER	CA-CB	5.28	1.60	1.52
2	E	208	VAL	CB-CG2	5.28	1.64	1.52
1	B	288	GLU	CB-CG	5.28	1.62	1.52
2	D	54	LEU	CA-CB	-5.27	1.41	1.53
2	F	8	ASP	CA-CB	5.26	1.65	1.53
1	B	917	VAL	CB-CG2	5.25	1.63	1.52
1	B	933	GLY	CA-C	-5.25	1.43	1.51
1	C	634	ARG	CD-NE	5.24	1.55	1.46
1	A	106	LEU	CA-CB	5.24	1.65	1.53
1	C	318	SER	CA-CB	5.23	1.60	1.52
1	B	425	TYR	CG-CD1	5.21	1.46	1.39
1	A	642	PHE	CE2-CZ	5.21	1.47	1.37
1	B	773	TYR	CB-CG	5.21	1.59	1.51
1	B	51	PRO	N-CD	5.21	1.55	1.47
2	D	99	TYR	CZ-OH	5.19	1.46	1.37
2	E	201	LYS	CA-CB	5.19	1.65	1.53
1	A	653	TYR	CZ-OH	5.17	1.46	1.37
2	E	166	TRP	NE1-CE2	-5.17	1.30	1.37
1	A	770	LEU	CA-CB	5.17	1.65	1.53
1	B	175	GLY	C-O	-5.17	1.15	1.23
2	F	162	TYR	CG-CD2	5.17	1.45	1.39
1	A	785	SER	CB-OG	5.16	1.49	1.42
2	E	43	TYR	CE1-CZ	5.16	1.45	1.38
1	A	73	GLU	CA-CB	5.15	1.65	1.53
1	C	311	ARG	CA-CB	5.15	1.65	1.53
1	A	244	GLY	N-CA	-5.14	1.38	1.46
1	C	398	ARG	CD-NE	5.14	1.55	1.46
1	A	287	SER	CB-OG	5.14	1.49	1.42
1	B	35	GLU	CD-OE2	5.13	1.31	1.25
1	C	419	VAL	C-N	5.12	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	207	THR	N-CA	5.11	1.56	1.46
1	B	916	TYR	CE1-CZ	5.10	1.45	1.38
2	F	74	TYR	CZ-OH	5.10	1.46	1.37
1	A	486	TYR	CG-CD1	5.10	1.45	1.39
1	B	922	PHE	CB-CG	5.10	1.60	1.51
2	F	112	GLU	CB-CG	5.10	1.61	1.52
1	B	366	GLU	CD-OE1	5.09	1.31	1.25
1	A	735	ARG	CD-NE	5.09	1.55	1.46
1	C	789	ARG	CZ-NH2	-5.09	1.26	1.33
1	C	919	PHE	CG-CD2	5.09	1.46	1.38
2	F	74	TYR	CD2-CE2	5.07	1.47	1.39
1	A	175	GLY	CA-C	-5.04	1.43	1.51
2	D	179	GLY	N-CA	-5.04	1.38	1.46
2	E	183	ARG	CZ-NH1	-5.04	1.26	1.33
2	F	194	GLN	CA-CB	5.04	1.65	1.53
1	A	516	TYR	CD1-CE1	5.04	1.47	1.39
1	B	115	TYR	CE2-CZ	5.04	1.45	1.38
1	A	211	TYR	CE2-CZ	5.03	1.45	1.38
1	A	422	ASN	CB-CG	5.02	1.62	1.51
1	C	717	PHE	CB-CG	5.01	1.59	1.51

All (825) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	ARG	NE-CZ-NH2	-27.23	106.68	120.30
2	E	196	ARG	NE-CZ-NH1	26.14	133.37	120.30
2	E	183	ARG	NE-CZ-NH2	-25.28	107.66	120.30
1	B	746	ARG	NE-CZ-NH1	23.92	132.26	120.30
2	F	168	ARG	NE-CZ-NH2	-23.38	108.61	120.30
1	A	836	ARG	NE-CZ-NH1	-22.82	108.89	120.30
1	B	746	ARG	NE-CZ-NH2	-22.74	108.93	120.30
2	E	68	ARG	NE-CZ-NH1	20.64	130.62	120.30
1	C	82	ARG	NE-CZ-NH2	19.62	130.11	120.30
1	C	543	ARG	NE-CZ-NH1	19.47	130.04	120.30
1	A	601	ARG	NE-CZ-NH1	19.24	129.92	120.30
2	D	115	ARG	NE-CZ-NH1	18.92	129.76	120.30
1	A	836	ARG	NE-CZ-NH2	18.71	129.66	120.30
1	A	601	ARG	NE-CZ-NH2	-18.25	111.17	120.30
1	A	311	ARG	NE-CZ-NH2	-17.98	111.31	120.30
1	B	311	ARG	NE-CZ-NH2	-17.93	111.33	120.30
1	B	681	ARG	NE-CZ-NH1	17.88	129.24	120.30
1	C	553	ARG	NE-CZ-NH1	-17.32	111.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	ARG	NE-CZ-NH1	-17.28	111.66	120.30
1	C	746	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	A	62	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	A	675	ARG	NE-CZ-NH1	16.87	128.74	120.30
1	A	62	ARG	NE-CZ-NH1	16.56	128.58	120.30
2	F	61	ARG	NE-CZ-NH1	16.37	128.49	120.30
1	A	221	ARG	NE-CZ-NH1	16.15	128.38	120.30
1	A	91	ARG	NE-CZ-NH1	16.14	128.37	120.30
1	C	543	ARG	NE-CZ-NH2	-16.04	112.28	120.30
1	A	694	TYR	CB-CG-CD2	-16.00	111.40	121.00
2	E	168	ARG	NE-CZ-NH1	15.82	128.21	120.30
2	E	68	ARG	NE-CZ-NH2	-15.82	112.39	120.30
1	B	836	ARG	NE-CZ-NH2	15.79	128.20	120.30
1	B	77	TYR	CB-CG-CD1	-15.58	111.65	121.00
1	B	363	ARG	NE-CZ-NH1	15.37	127.98	120.30
2	E	216	ARG	NE-CZ-NH1	-15.23	112.69	120.30
2	D	115	ARG	NE-CZ-NH2	-14.99	112.80	120.30
1	B	810	TYR	CB-CG-CD1	14.89	129.93	121.00
1	B	681	ARG	NE-CZ-NH2	-14.72	112.94	120.30
1	B	32	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	B	810	TYR	CB-CG-CD2	-14.59	112.24	121.00
1	A	545	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	C	836	ARG	NE-CZ-NH2	14.39	127.50	120.30
1	A	469	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	A	506	ARG	NE-CZ-NH2	-14.25	113.17	120.30
1	A	746	ARG	NE-CZ-NH1	14.23	127.42	120.30
1	A	941	ARG	NE-CZ-NH2	14.22	127.41	120.30
1	B	108	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	B	554	TYR	CB-CG-CD2	-14.12	112.53	121.00
1	B	82	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	A	789	ARG	NE-CZ-NH1	13.94	127.27	120.30
1	A	506	ARG	NE-CZ-NH1	13.89	127.24	120.30
1	B	932	ARG	NE-CZ-NH1	13.87	127.23	120.30
1	A	103	ARG	NE-CZ-NH2	13.72	127.16	120.30
1	C	382	TYR	CB-CG-CD1	13.59	129.16	121.00
1	B	452	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	B	554	TYR	CB-CG-CD1	13.48	129.09	121.00
1	B	82	ARG	NE-CZ-NH2	-13.44	113.58	120.30
2	D	141	ASP	CB-CG-OD1	13.35	130.32	118.30
1	A	379	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	735	ARG	NE-CZ-NH2	-13.16	113.72	120.30
2	D	43	TYR	CB-CG-CD2	-13.13	113.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH1	13.11	126.86	120.30
1	A	382	TYR	CB-CG-CD2	-13.10	113.14	121.00
2	E	216	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	C	452	ARG	NE-CZ-NH1	12.96	126.78	120.30
2	F	115	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	C	753	TYR	CB-CG-CD1	12.79	128.68	121.00
2	F	183	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	C	545	ARG	NE-CZ-NH2	12.60	126.60	120.30
1	C	103	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	B	469	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	C	94	ASP	CB-CG-OD1	12.45	129.50	118.30
1	B	473	TYR	CB-CG-CD2	-12.42	113.55	121.00
1	B	553	ARG	NE-CZ-NH1	-12.39	114.11	120.30
1	A	332	PHE	CB-CG-CD2	-12.35	112.16	120.80
1	A	108	ARG	NE-CZ-NH2	-12.31	114.14	120.30
1	B	221	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	B	221	ARG	NE-CZ-NH2	-12.27	114.16	120.30
2	D	68	ARG	NE-CZ-NH1	12.24	126.42	120.30
2	F	168	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	A	697	TYR	CB-CG-CD2	-12.21	113.67	121.00
1	C	742	PHE	CB-CG-CD1	-12.16	112.29	120.80
1	C	522	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	A	91	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	C	669	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	A	929	ARG	NE-CZ-NH2	11.96	126.28	120.30
1	B	452	ARG	NE-CZ-NH2	-11.77	114.41	120.30
2	F	189	TYR	CB-CG-CD1	-11.59	114.05	121.00
1	B	506	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	A	941	ARG	NE-CZ-NH1	-11.45	114.57	120.30
1	A	926	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	C	62	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	A	634	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	B	506	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	311	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	A	735	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	E	105	PHE	CB-CG-CD2	-10.95	113.14	120.80
1	A	697	TYR	CB-CG-CD1	10.83	127.50	121.00
1	C	601	ARG	NE-CZ-NH1	10.79	125.70	120.30
2	F	196	ARG	NE-CZ-NH2	10.78	125.69	120.30
1	C	845	PHE	CB-CG-CD2	-10.76	113.27	120.80
1	C	382	TYR	CB-CG-CD2	-10.73	114.56	121.00
1	C	697	TYR	CB-CG-CD1	-10.68	114.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	618	PHE	CB-CG-CD1	10.66	128.26	120.80
1	A	66	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	469	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	B	337	TYR	CB-CG-CD2	10.61	127.37	121.00
1	B	553	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	C	645	TYR	CB-CG-CD1	-10.59	114.64	121.00
1	A	329	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	C	545	ARG	NH1-CZ-NH2	-10.47	107.88	119.40
1	C	932	ARG	NE-CZ-NH2	10.47	125.54	120.30
1	A	789	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	221	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	B	62	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	289	ASP	CB-CG-OD2	10.42	127.68	118.30
1	B	32	ARG	NE-CZ-NH2	-10.33	115.14	120.30
2	E	6	ASP	CB-CG-OD1	10.30	127.57	118.30
1	A	734	ASP	CB-CG-OD2	10.30	127.57	118.30
1	C	545	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	B	311	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	59	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	694	TYR	CB-CG-CD1	10.14	127.08	121.00
2	F	93	TYR	CB-CG-CD1	10.12	127.07	121.00
2	F	90	PHE	CB-CG-CD1	-10.11	113.73	120.80
2	F	227	ARG	NE-CZ-NH1	10.06	125.33	120.30
2	E	93	TYR	CB-CG-CD2	-10.05	114.97	121.00
2	E	61	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	B	867	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	939	TYR	CB-CG-CD2	-10.02	114.99	121.00
1	A	923	ASP	CB-CG-OD2	-9.97	109.33	118.30
1	A	543	ARG	NE-CZ-NH1	9.93	125.27	120.30
2	E	196	ARG	NH1-CZ-NH2	-9.92	108.49	119.40
1	B	585	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	B	797	PHE	CB-CG-CD1	9.90	127.73	120.80
1	B	115	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	B	786	TYR	CB-CG-CD1	-9.83	115.10	121.00
2	E	161	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	618	PHE	CB-CG-CD2	-9.76	113.97	120.80
1	C	810	TYR	CB-CG-CD2	-9.76	115.15	121.00
1	C	381	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	B	871	ARG	NE-CZ-NH1	9.70	125.15	120.30
2	D	196	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	479	TYR	CB-CG-CD1	-9.65	115.21	121.00
1	B	236	TYR	CG-CD1-CE1	-9.64	113.59	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	286	TYR	CB-CG-CD2	-9.59	115.25	121.00
2	F	5	ASP	CB-CG-OD1	9.54	126.88	118.30
1	C	753	TYR	CB-CG-CD2	-9.53	115.28	121.00
1	B	585	ARG	NE-CZ-NH2	9.51	125.06	120.30
1	A	452	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	100	PHE	CB-CG-CD1	9.44	127.41	120.80
1	C	325	TYR	CB-CG-CD1	-9.43	115.34	121.00
1	B	771	ALA	N-CA-CB	-9.33	97.04	110.10
1	A	910	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	679	PHE	CB-CG-CD2	-9.29	114.30	120.80
1	A	675	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	C	786	TYR	CB-CG-CD1	9.26	126.56	121.00
2	E	93	TYR	CB-CG-CD1	9.25	126.55	121.00
1	A	923	ASP	CB-CG-OD1	9.14	126.53	118.30
2	F	224	TYR	CB-CG-CD2	-9.14	115.52	121.00
1	B	734	ASP	CB-CG-OD1	9.13	126.52	118.30
2	D	223	TYR	CB-CG-CD2	9.10	126.46	121.00
1	B	398	ARG	NE-CZ-NH1	9.08	124.84	120.30
2	F	93	TYR	CB-CG-CD2	-9.08	115.55	121.00
2	D	168	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	D	162	TYR	CB-CG-CD1	9.02	126.41	121.00
1	C	369	TYR	CB-CG-CD2	-9.01	115.60	121.00
2	F	78	PHE	CB-CG-CD1	-8.95	114.53	120.80
2	F	216	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	A	381	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	679	PHE	CB-CG-CD1	8.92	127.04	120.80
1	A	545	ARG	NH1-CZ-NH2	-8.91	109.60	119.40
1	A	588	VAL	CA-CB-CG2	8.86	124.20	110.90
1	C	944	PHE	CB-CG-CD2	8.83	126.98	120.80
1	B	337	TYR	CB-CG-CD1	-8.81	115.72	121.00
1	A	929	ARG	NE-CZ-NH1	-8.79	115.90	120.30
1	C	929	ARG	NE-CZ-NH1	8.79	124.69	120.30
2	D	25	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	325	TYR	CB-CG-CD1	-8.78	115.73	121.00
1	A	363	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	B	529	ASP	CB-CG-OD1	8.75	126.18	118.30
2	F	227	ARG	NE-CZ-NH2	-8.75	115.92	120.30
2	D	74	TYR	CB-CG-CD2	-8.74	115.76	121.00
1	C	329	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	C	82	ARG	NH1-CZ-NH2	-8.73	109.80	119.40
2	E	5	ASP	CB-CG-OD1	8.72	126.15	118.30
1	C	100	PHE	CB-CG-CD2	8.71	126.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	565	PHE	CB-CG-CD2	8.67	126.87	120.80
1	B	827	PHE	CB-CG-CD2	-8.64	114.75	120.80
1	C	516	TYR	CB-CG-CD1	-8.56	115.86	121.00
1	B	781	TYR	CB-CG-CD1	8.54	126.12	121.00
1	C	277	ASP	CB-CG-OD2	-8.53	110.62	118.30
2	D	43	TYR	CG-CD2-CE2	-8.52	114.48	121.30
1	B	322	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	694	TYR	CB-CG-CD2	-8.49	115.91	121.00
1	A	328	PHE	CB-CG-CD1	-8.48	114.86	120.80
2	D	43	TYR	CZ-CE2-CD2	8.47	127.42	119.80
1	A	671	TRP	CB-CG-CD2	8.46	137.60	126.60
1	C	580	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	B	473	TYR	CB-CG-CD1	8.44	126.07	121.00
2	D	216	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	C	634	ARG	CD-NE-CZ	8.41	135.37	123.60
2	F	202	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	B	479	TYR	CB-CG-CD2	8.39	126.03	121.00
1	A	45	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	B	802	ARG	NE-CZ-NH1	-8.35	116.12	120.30
2	F	25	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	923	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	325	TYR	CB-CG-CD2	8.33	126.00	121.00
1	B	621	MET	CG-SD-CE	-8.32	86.88	100.20
1	A	698	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	A	83	PHE	CB-CG-CD1	-8.24	115.03	120.80
1	A	263	MET	CG-SD-CE	-8.23	87.03	100.20
1	B	926	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	322	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	379	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	566	PHE	CB-CG-CD2	-8.18	115.07	120.80
1	A	802	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	C	806	ASP	CB-CG-OD1	8.15	125.63	118.30
2	E	43	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	C	615	TYR	CB-CG-CD1	8.11	125.87	121.00
1	C	398	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	38	PHE	CB-CG-CD2	8.10	126.47	120.80
1	C	383	PHE	CB-CG-CD1	-8.10	115.13	120.80
1	C	236	TYR	CB-CG-CD1	-8.10	116.14	121.00
1	C	271	ALA	N-CA-CB	-8.09	98.77	110.10
1	A	67	PHE	CB-CG-CD1	-8.08	115.14	120.80
1	A	698	TYR	CG-CD2-CE2	-8.07	114.84	121.30
1	B	791	TYR	CB-CG-CD1	-8.05	116.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	615	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	A	753	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	C	11	TYR	CB-CG-CD1	-8.00	116.20	121.00
1	A	932	ARG	NE-CZ-NH2	8.00	124.30	120.30
2	E	90	PHE	CB-CG-CD2	-7.99	115.20	120.80
1	B	441	ASP	CB-CG-OD1	7.96	125.46	118.30
1	B	797	PHE	CB-CG-CD2	-7.95	115.24	120.80
1	B	381	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	412	TYR	CB-CG-CD1	-7.94	116.24	121.00
1	B	383	PHE	CB-CG-CD2	-7.94	115.25	120.80
1	B	544	TYR	CB-CG-CD2	-7.93	116.24	121.00
2	E	5	ASP	CB-CG-OD2	-7.92	111.17	118.30
2	E	183	ARG	NH1-CZ-NH2	7.91	128.10	119.40
1	B	385	MET	CG-SD-CE	-7.90	87.57	100.20
2	E	69	PHE	CB-CG-CD2	7.89	126.32	120.80
1	A	82	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	C	194	TYR	CZ-CE2-CD2	-7.87	112.72	119.80
1	A	746	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	325	TYR	CB-CG-CD2	7.84	125.71	121.00
2	F	209	TYR	CG-CD2-CE2	-7.84	115.02	121.30
1	C	538	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	59	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	565	PHE	CB-CG-CD1	-7.80	115.34	120.80
1	A	266	PHE	CB-CG-CD2	-7.79	115.34	120.80
1	C	445	PHE	CB-CG-CD2	-7.78	115.35	120.80
1	B	386	TRP	CB-CG-CD2	7.77	136.71	126.60
1	C	44	PHE	CB-CG-CD2	-7.75	115.38	120.80
1	A	734	ASP	CB-CG-OD1	-7.74	111.33	118.30
2	F	25	ARG	NE-CZ-NH2	-7.73	116.44	120.30
2	E	223	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	C	445	PHE	CB-CG-CD1	7.68	126.18	120.80
1	B	211	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	C	708	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	A	414	PHE	CB-CG-CD1	-7.65	115.45	120.80
1	A	425	TYR	CG-CD2-CE2	7.65	127.42	121.30
1	B	101	ASP	CB-CG-OD1	7.65	125.18	118.30
1	B	907	ASP	CB-CG-OD1	7.64	125.18	118.30
1	B	599	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	834	THR	CA-CB-CG2	-7.62	101.73	112.40
1	A	724	PHE	CB-CG-CD2	-7.61	115.48	120.80
1	C	553	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	B	742	PHE	CB-CG-CD1	-7.59	115.49	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	801	SER	N-CA-CB	7.58	121.88	110.50
1	C	653	TYR	CB-CG-CD1	7.54	125.52	121.00
1	C	926	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	332	PHE	CB-CG-CD1	7.52	126.06	120.80
2	E	39	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	307	GLU	OE1-CD-OE2	-7.51	114.29	123.30
1	A	414	PHE	CB-CG-CD2	7.50	126.05	120.80
1	C	500	TYR	CB-CG-CD1	-7.49	116.51	121.00
1	C	742	PHE	CB-CG-CD2	7.45	126.02	120.80
1	B	941	ARG	NE-CZ-NH2	7.45	124.02	120.30
2	E	6	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	379	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	C	742	PHE	CZ-CE2-CD2	-7.41	111.21	120.10
2	E	183	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	D	236	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	A	863	PHE	CB-CG-CD2	-7.38	115.64	120.80
1	B	393	TYR	CB-CG-CD2	7.37	125.42	121.00
1	C	580	TYR	CB-CG-CD1	7.37	125.42	121.00
1	B	922	PHE	CB-CG-CD2	-7.37	115.64	120.80
1	C	939	TYR	CB-CG-CD1	-7.37	116.58	121.00
2	F	68	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	E	69	PHE	CB-CG-CD1	-7.35	115.66	120.80
1	A	919	PHE	CB-CG-CD1	-7.34	115.66	120.80
1	B	112	PHE	CB-CG-CD2	7.34	125.94	120.80
1	C	944	PHE	CB-CG-CD1	-7.33	115.67	120.80
1	C	45	ARG	NE-CZ-NH2	7.32	123.96	120.30
2	E	141	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	B	781	TYR	CB-CG-CD2	-7.31	116.61	121.00
1	A	886	ASP	CB-CG-OD2	7.31	124.88	118.30
1	C	669	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
1	A	79	TYR	CG-CD2-CE2	-7.30	115.46	121.30
1	C	531	VAL	CA-CB-CG2	-7.28	99.98	110.90
2	E	115	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	76	ALA	N-CA-CB	-7.28	99.91	110.10
1	B	867	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	311	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	D	161	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	328	PHE	CB-CG-CD2	7.26	125.88	120.80
1	B	302	MET	CA-CB-CG	7.23	125.59	113.30
1	B	453	VAL	CA-CB-CG1	7.23	121.74	110.90
2	D	161	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	932	ARG	NH1-CZ-NH2	-7.21	111.47	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	671	TRP	CB-CG-CD1	-7.21	117.63	127.00
1	A	389	ALA	N-CA-CB	-7.15	100.09	110.10
1	C	735	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	11	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	B	44	PHE	CB-CG-CD1	7.11	125.77	120.80
1	B	173	TYR	CB-CG-CD1	7.10	125.26	121.00
1	C	301	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	B	827	PHE	CB-CG-CD1	7.09	125.77	120.80
1	B	711	PHE	CB-CG-CD1	-7.09	115.84	120.80
2	F	8	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	910	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	266	PHE	CB-CG-CD1	7.07	125.75	120.80
1	B	603	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	425	TYR	CZ-CE2-CD2	-7.05	113.45	119.80
2	E	99	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	C	807	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	711	PHE	CB-CG-CD1	7.00	125.70	120.80
1	C	338	TYR	CB-CG-CD1	-6.99	116.81	121.00
2	D	216	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	C	108	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	527	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	B	910	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	A	878	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	B	173	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	A	932	ARG	NH1-CZ-NH2	-6.92	111.78	119.40
1	C	471	PHE	CB-CG-CD2	-6.92	115.96	120.80
1	C	634	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	639	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	473	TYR	CB-CG-CD2	6.90	125.14	121.00
1	A	289	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	845	PHE	CB-CG-CD1	6.88	125.61	120.80
1	B	383	PHE	CB-CG-CD1	6.87	125.61	120.80
2	D	87	PRO	N-CA-CB	6.86	111.53	103.30
1	C	382	TYR	CG-CD2-CE2	6.84	126.77	121.30
1	A	674	PHE	CB-CG-CD1	-6.83	116.02	120.80
2	E	236	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C	319	MET	CG-SD-CE	-6.82	89.28	100.20
1	C	746	ARG	NH1-CZ-NH2	-6.82	111.89	119.40
1	C	558	HIS	CA-CB-CG	6.82	125.19	113.60
1	A	662	VAL	CG1-CB-CG2	-6.79	100.04	110.90
1	B	382	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	B	698	TYR	CG-CD2-CE2	-6.78	115.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	845	PHE	CB-CG-CD1	6.77	125.54	120.80
1	A	119	ALA	CB-CA-C	6.76	120.24	110.10
1	A	855	VAL	CG1-CB-CG2	6.75	121.71	110.90
2	F	224	TYR	CB-CG-CD1	6.75	125.05	121.00
1	A	634	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	797	PHE	CB-CG-CD2	6.75	125.52	120.80
2	F	157	PHE	CB-CG-CD1	-6.74	116.08	120.80
1	A	932	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	66	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	D	94	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	A	195	ALA	O-C-N	-6.69	111.99	122.70
1	B	856	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	A	452	ARG	NH1-CZ-NH2	-6.69	112.04	119.40
1	B	77	TYR	CB-CG-CD2	6.68	125.01	121.00
1	C	425	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	C	261	VAL	CA-CB-CG2	-6.68	100.88	110.90
1	A	240	THR	CA-CB-CG2	-6.68	103.05	112.40
1	B	447	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	412	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	67	PHE	CB-CG-CD2	6.66	125.47	120.80
1	A	168	PHE	CB-CG-CD2	6.66	125.47	120.80
1	C	59	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	E	74	TYR	CZ-CE2-CD2	-6.66	113.81	119.80
1	C	795	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	580	TYR	CB-CG-CD1	6.64	124.98	121.00
1	A	174	SER	N-CA-CB	6.63	120.45	110.50
1	B	425	TYR	CB-CG-CD1	6.62	124.97	121.00
1	C	74	ASP	CB-CG-OD2	-6.62	112.34	118.30
2	F	33	SER	N-CA-CB	6.62	120.44	110.50
2	F	115	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	B	856	ASP	CB-CG-OD2	6.59	124.23	118.30
1	C	266	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	A	103	ARG	NH1-CZ-NH2	-6.58	112.17	119.40
2	F	62	TYR	CB-CG-CD1	6.58	124.95	121.00
1	B	39	SER	N-CA-CB	6.57	120.36	110.50
1	B	468	TRP	CG-CD1-NE1	-6.57	103.53	110.10
2	F	223	TYR	N-CA-CB	6.56	122.41	110.60
2	D	84	SER	N-CA-CB	6.56	120.34	110.50
1	A	419	VAL	CA-CB-CG2	-6.56	101.07	110.90
1	B	495	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	39	SER	N-CA-CB	6.53	120.30	110.50
1	B	619	PHE	CG-CD2-CE2	6.53	127.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	878	PHE	CB-CG-CD2	-6.52	116.23	120.80
2	D	11	MET	CG-SD-CE	-6.52	89.77	100.20
1	A	412	TYR	CB-CG-CD2	6.52	124.91	121.00
1	B	557	PHE	CB-CG-CD1	-6.51	116.24	120.80
1	B	690	LEU	CB-CG-CD2	6.51	122.07	111.00
1	B	789	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	38	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	A	314	MET	CG-SD-CE	6.50	110.59	100.20
1	A	495	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	22	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	C	332	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	C	653	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	A	582	TRP	CE3-CZ3-CH2	6.46	128.31	121.20
1	C	101	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	527	TYR	CG-CD1-CE1	-6.46	116.13	121.30
1	B	836	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
1	B	329	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	265	PHE	CB-CG-CD2	6.46	125.32	120.80
1	B	447	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	38	PHE	CB-CG-CD1	-6.45	116.28	120.80
1	C	432	THR	CA-CB-CG2	-6.45	103.37	112.40
1	C	697	TYR	CG-CD2-CE2	-6.43	116.15	121.30
1	B	789	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	681	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	393	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	B	108	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	B	706	TYR	CG-CD1-CE1	-6.39	116.19	121.30
2	E	4	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	93	LEU	O-C-N	-6.36	112.53	122.70
1	B	601	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	134	TRP	CB-CG-CD1	-6.35	118.74	127.00
1	C	329	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	396	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	910	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	C	878	PHE	CG-CD1-CE1	-6.31	113.86	120.80
1	B	513	VAL	CG1-CB-CG2	-6.30	100.82	110.90
1	B	795	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	500	TYR	CD1-CE1-CZ	-6.29	114.14	119.80
2	E	219	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	F	61	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
2	F	42	TRP	CB-CG-CD1	6.29	135.18	127.00
1	A	922	PHE	CB-CG-CD2	-6.29	116.40	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	907	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	916	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	599	ASP	CB-CG-OD1	6.28	123.95	118.30
2	E	74	TYR	CG-CD2-CE2	6.28	126.32	121.30
1	B	649	ALA	CB-CA-C	6.28	119.51	110.10
1	C	112	PHE	CB-CG-CD2	6.28	125.19	120.80
1	C	469	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	A	828	VAL	CG1-CB-CG2	-6.27	100.87	110.90
1	B	580	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	C	780	PHE	CB-CG-CD2	-6.26	116.41	120.80
1	C	382	TYR	CZ-CE2-CD2	-6.26	114.17	119.80
2	F	98	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	649	ALA	N-CA-CB	-6.25	101.34	110.10
1	C	72	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	C	398	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	916	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	B	386	TRP	CB-CG-CD1	-6.24	118.89	127.00
1	B	236	TYR	CD1-CE1-CZ	6.24	125.41	119.80
1	C	532	ASN	CB-CG-OD1	6.22	134.05	121.60
2	F	193	PHE	CB-CG-CD1	6.21	125.15	120.80
2	F	189	TYR	CB-CG-CD2	6.21	124.73	121.00
1	C	288	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	C	381	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	436	ASN	O-C-N	-6.18	112.69	123.20
1	B	380	THR	CA-CB-CG2	-6.18	103.74	112.40
1	C	37	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	C	867	ARG	N-CA-C	6.16	127.63	111.00
1	B	45	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	C	362	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	286	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	E	168	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
1	A	544	TYR	CB-CG-CD2	6.12	124.67	121.00
1	C	502	TYR	CG-CD1-CE1	6.12	126.20	121.30
1	B	501	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	815	GLN	CA-CB-CG	6.11	126.84	113.40
2	D	98	ASP	CB-CG-OD1	6.10	123.79	118.30
2	D	141	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	99	TYR	CG-CD2-CE2	-6.10	116.42	121.30
2	F	142	LYS	O-C-N	-6.10	112.94	122.70
2	D	115	ARG	CD-NE-CZ	-6.09	115.08	123.60
2	F	161	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	E	99	TYR	CZ-CE2-CD2	-6.07	114.33	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	678	ALA	CB-CA-C	6.07	119.21	110.10
2	E	188	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	538	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	645	TYR	CB-CG-CD2	6.06	124.64	121.00
1	B	72	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	C	893	TYR	CA-CB-CG	-6.05	101.90	113.40
2	E	25	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	C	332	PHE	N-CA-CB	6.05	121.49	110.60
1	C	724	PHE	CB-CG-CD2	-6.05	116.57	120.80
2	E	178	MET	CG-SD-CE	-6.04	90.53	100.20
1	B	79	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	B	939	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	C	780	PHE	CD1-CE1-CZ	6.02	127.32	120.10
1	C	522	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	441	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	195	ALA	N-CA-CB	-6.00	101.71	110.10
1	B	841	TYR	CG-CD2-CE2	5.99	126.09	121.30
1	C	694	TYR	CB-CG-CD1	5.99	124.59	121.00
1	B	22	TYR	CG-CD1-CE1	-5.98	116.52	121.30
1	C	527	TYR	CB-CG-CD2	-5.98	117.41	121.00
2	D	135	VAL	CA-CB-CG1	-5.98	101.93	110.90
1	A	527	TYR	CB-CG-CD2	5.98	124.59	121.00
1	C	526	ASP	N-CA-CB	-5.97	99.84	110.60
2	F	232	PHE	CB-CG-CD2	-5.97	116.62	120.80
1	A	712	TYR	CB-CG-CD2	5.97	124.58	121.00
1	B	269	THR	CA-CB-CG2	-5.97	104.04	112.40
1	B	698	TYR	CD1-CG-CD2	5.97	124.47	117.90
1	A	863	PHE	CB-CG-CD1	5.97	124.98	120.80
1	C	386	TRP	CZ3-CH2-CZ2	-5.95	114.46	121.60
1	C	444	GLU	OE1-CD-OE2	-5.95	116.17	123.30
2	F	0	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	F	166	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	C	687	THR	CA-CB-CG2	5.94	120.71	112.40
1	B	932	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
1	C	501	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	C	243	ASN	N-CA-CB	5.93	121.27	110.60
1	B	813	TYR	CB-CG-CD2	5.93	124.56	121.00
2	F	111	VAL	CA-CB-CG2	5.93	119.79	110.90
2	E	221	ALA	N-CA-CB	5.92	118.39	110.10
1	C	473	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	A	659	ALA	N-CA-CB	5.90	118.36	110.10
1	C	578	TYR	CG-CD1-CE1	-5.89	116.58	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	529	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	579	THR	N-CA-CB	5.89	121.49	110.30
1	A	60	SER	N-CA-CB	5.88	119.33	110.50
2	D	146	ALA	CB-CA-C	5.88	118.92	110.10
1	B	66	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	B	136	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	A	516	TYR	CG-CD2-CE2	-5.87	116.61	121.30
1	A	526	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	843	ALA	N-CA-CB	-5.85	101.91	110.10
1	C	100	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	C	502	TYR	CD1-CE1-CZ	-5.83	114.55	119.80
1	C	836	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	A	390	VAL	O-C-N	-5.82	113.39	122.70
1	C	211	TYR	CG-CD2-CE2	-5.82	116.65	121.30
1	A	939	TYR	CG-CD1-CE1	-5.81	116.65	121.30
1	A	904	PHE	CB-CG-CD1	-5.81	116.73	120.80
1	C	578	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	C	338	TYR	CG-CD2-CE2	-5.80	116.66	121.30
2	F	78	PHE	CD1-CG-CD2	5.80	125.84	118.30
2	E	141	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	938	VAL	CA-CB-CG1	-5.80	102.20	110.90
1	B	115	TYR	CB-CG-CD2	5.80	124.48	121.00
2	D	43	TYR	CB-CG-CD1	5.79	124.47	121.00
2	F	220	THR	N-CA-CB	5.79	121.30	110.30
1	B	233	TYR	CB-CG-CD2	5.78	124.47	121.00
2	E	135	VAL	CG1-CB-CG2	-5.78	101.66	110.90
1	B	688	PRO	N-CA-CB	5.77	110.22	103.30
1	C	479	TYR	CD1-CE1-CZ	-5.77	114.61	119.80
2	D	224	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	A	753	TYR	CB-CG-CD1	5.76	124.46	121.00
1	B	412	TYR	CB-CG-CD1	5.76	124.46	121.00
1	B	486	TYR	CG-CD1-CE1	-5.75	116.70	121.30
1	C	516	TYR	CB-CG-CD2	5.75	124.45	121.00
1	B	391	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	701	SER	N-CA-CB	5.74	119.12	110.50
1	A	845	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	C	235	SER	N-CA-CB	5.74	119.10	110.50
1	C	459	MET	CG-SD-CE	-5.73	91.03	100.20
1	B	675	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	277	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	445	PHE	CG-CD2-CE2	-5.72	114.50	120.80
1	A	788	ASP	CB-CG-OD1	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	12	MET	CG-SD-CE	-5.72	91.05	100.20
1	B	77	TYR	CG-CD1-CE1	-5.71	116.73	121.30
2	D	0	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	553	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	445	PHE	CB-CG-CD1	5.70	124.79	120.80
2	E	208	VAL	CG1-CB-CG2	-5.70	101.78	110.90
2	D	189	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	538	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	379	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	B	406	GLU	OE1-CD-OE2	-5.67	116.49	123.30
1	A	615	TYR	CG-CD2-CE2	-5.67	116.77	121.30
1	B	901	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	698	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	C	585	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	C	931	HIS	CA-CB-CG	5.66	123.22	113.60
2	D	93	TYR	CG-CD1-CE1	-5.65	116.78	121.30
1	B	286	TYR	CG-CD1-CE1	-5.65	116.78	121.30
1	C	756	ALA	N-CA-CB	-5.65	102.19	110.10
1	A	802	ARG	NH1-CZ-NH2	-5.65	113.19	119.40
1	B	48	THR	CA-CB-CG2	-5.64	104.50	112.40
1	B	694	TYR	O-C-N	-5.64	113.67	122.70
1	A	773	TYR	CB-CG-CD2	5.64	124.38	121.00
1	B	791	TYR	O-C-N	-5.64	113.68	122.70
1	A	677	TRP	CZ3-CH2-CZ2	-5.63	114.84	121.60
2	D	43	TYR	CB-CA-C	-5.63	99.14	110.40
1	C	330	ASP	CB-CA-C	5.63	121.66	110.40
2	F	77	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	543	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	588	VAL	CA-CB-CG1	-5.62	102.47	110.90
1	C	457	PHE	CB-CG-CD2	-5.62	116.87	120.80
1	A	590	MET	CG-SD-CE	-5.61	91.22	100.20
1	B	706	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	C	62	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	194	TYR	CG-CD2-CE2	5.61	125.79	121.30
1	A	781	TYR	CD1-CE1-CZ	-5.61	114.75	119.80
2	E	105	PHE	CG-CD1-CE1	-5.61	114.63	120.80
1	C	171	ALA	N-CA-CB	-5.60	102.25	110.10
1	A	199	PHE	CB-CG-CD2	5.60	124.72	120.80
1	B	845	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	B	322	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	120	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	A	578	TYR	CB-CG-CD1	5.59	124.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	813	TYR	CG-CD1-CE1	-5.58	116.83	121.30
1	A	700	TYR	CG-CD2-CE2	-5.58	116.83	121.30
1	C	531	VAL	CA-CB-CG1	5.57	119.25	110.90
1	C	645	TYR	CG-CD1-CE1	-5.57	116.84	121.30
2	E	221	ALA	CB-CA-C	-5.57	101.75	110.10
1	A	836	ARG	CD-NE-CZ	5.56	131.39	123.60
1	C	495	ASP	CB-CG-OD1	5.55	123.30	118.30
2	E	43	TYR	CG-CD2-CE2	-5.55	116.86	121.30
1	A	553	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	72	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	717	PHE	CB-CG-CD1	-5.54	116.92	120.80
2	D	109	THR	CA-CB-CG2	-5.54	104.65	112.40
1	A	66	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	B	579	THR	CA-CB-CG2	-5.53	104.66	112.40
1	A	724	PHE	CB-CG-CD1	5.52	124.67	120.80
1	C	269	THR	CA-CB-CG2	-5.52	104.68	112.40
2	F	189	TYR	CG-CD1-CE1	-5.52	116.89	121.30
1	B	13	HIS	O-C-N	-5.51	113.88	122.70
1	C	610	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	390	VAL	CA-CB-CG1	5.50	119.15	110.90
1	C	629	LEU	O-C-N	-5.50	113.90	122.70
1	A	381	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	C	610	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	459	MET	CG-SD-CE	-5.49	91.42	100.20
1	C	698	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	793	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	B	694	TYR	CA-CB-CG	5.48	123.81	113.40
1	B	596	LEU	CB-CG-CD2	5.48	120.31	111.00
1	B	807	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	711	PHE	CB-CG-CD2	-5.46	116.98	120.80
2	F	209	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	B	272	ALA	N-CA-CB	-5.46	102.46	110.10
2	D	231	ASN	N-CA-CB	5.46	120.42	110.60
2	E	196	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	135	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	531	VAL	CG1-CB-CG2	-5.46	102.17	110.90
1	B	495	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	513	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	A	279	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	B	832	ALA	CB-CA-C	5.44	118.26	110.10
1	C	525	LEU	CB-CA-C	5.43	120.53	110.20
1	B	194	TYR	CB-CG-CD1	5.43	124.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	638	ASN	O-C-N	-5.43	114.01	122.70
1	A	516	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	278	ASN	CB-CG-OD1	5.42	132.45	121.60
1	B	168	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	C	199	PHE	CB-CG-CD1	5.42	124.59	120.80
2	D	6	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	874	PHE	CB-CG-CD1	-5.41	117.01	120.80
2	F	68	ARG	CD-NE-CZ	5.40	131.17	123.60
1	A	458	ALA	N-CA-CB	5.40	117.66	110.10
2	D	223	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	486	TYR	CD1-CE1-CZ	5.40	124.66	119.80
2	E	236	TYR	CB-CG-CD1	5.39	124.24	121.00
1	B	325	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
2	F	193	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	A	673	ALA	CB-CA-C	5.39	118.19	110.10
1	A	812	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	C	291	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	125	PRO	O-C-N	5.38	131.31	122.70
1	A	823	ASN	N-CA-C	-5.38	96.49	111.00
1	A	369	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	E	88	GLU	CB-CA-C	5.37	121.14	110.40
1	A	810	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	E	223	TYR	CA-CB-CG	-5.37	103.20	113.40
1	C	115	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	830	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	134	TRP	CB-CG-CD2	5.36	133.56	126.60
1	B	669	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	673	ALA	CB-CA-C	5.36	118.13	110.10
1	A	168	PHE	CB-CG-CD1	-5.35	117.05	120.80
1	B	240	THR	CA-CB-CG2	-5.35	104.91	112.40
1	B	217	HIS	CA-CB-CG	-5.35	104.50	113.60
2	F	39	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	725	ASP	CB-CG-OD1	-5.34	113.49	118.30
2	D	196	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	E	164	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	B	777	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	C	558	HIS	N-CA-CB	5.33	120.19	110.60
1	A	593	GLN	CA-CB-CG	5.32	125.11	113.40
1	B	698	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	C	534	PHE	CG-CD1-CE1	5.32	126.66	120.80
1	A	684	THR	CA-CB-CG2	-5.32	104.95	112.40
1	B	397	VAL	CA-CB-CG1	5.32	118.88	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	GLU	OE1-CD-OE2	-5.32	116.92	123.30
2	E	137	SER	C-N-CA	5.31	133.45	122.30
1	A	451	ILE	CB-CA-C	-5.30	101.00	111.60
1	B	116	SER	N-CA-CB	5.29	118.44	110.50
1	C	796	ASN	N-CA-CB	-5.29	101.07	110.60
2	D	68	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	65	LEU	CB-CG-CD2	5.29	120.00	111.00
1	A	937	THR	O-C-N	-5.29	114.23	122.70
2	D	74	TYR	CG-CD1-CE1	-5.29	117.07	121.30
1	A	585	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	381	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	B	413	CYS	CA-CB-SG	5.28	123.51	114.00
1	A	836	ARG	CB-CG-CD	5.28	125.33	111.60
1	C	79	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	712	TYR	CD1-CG-CD2	-5.28	112.10	117.90
1	A	69	PRO	C-N-CA	5.27	134.87	121.70
1	A	324	ASN	CB-CA-C	5.26	120.93	110.40
1	A	233	TYR	N-CA-CB	-5.26	101.14	110.60
2	D	210	MET	CA-CB-CG	5.26	122.24	113.30
1	B	11	TYR	CB-CG-CD2	5.25	124.15	121.00
1	B	482	ASP	CB-CG-OD2	-5.25	113.57	118.30
2	F	140	GLU	OE1-CD-OE2	-5.25	117.00	123.30
2	F	196	ARG	CD-NE-CZ	5.25	130.95	123.60
1	A	434	GLN	O-C-N	-5.25	114.30	122.70
2	F	74	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	C	221	ARG	CD-NE-CZ	5.24	130.94	123.60
1	C	780	PHE	CG-CD1-CE1	-5.24	115.04	120.80
1	A	796	ASN	CB-CG-OD1	-5.24	111.13	121.60
1	A	112	PHE	CB-CG-CD2	-5.24	117.14	120.80
1	A	697	TYR	CG-CD2-CE2	-5.23	117.11	121.30
1	C	63	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	784	GLU	O-C-N	-5.22	114.35	122.70
1	C	347	LEU	O-C-N	-5.22	114.35	122.70
1	A	452	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	791	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	B	523	TRP	CZ3-CH2-CZ2	-5.21	115.35	121.60
1	B	545	ARG	N-CA-CB	5.21	119.98	110.60
1	B	916	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	A	621	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	457	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	C	756	ALA	N-CA-C	5.20	125.05	111.00
1	A	523	TRP	CD1-CG-CD2	-5.19	102.15	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	742	PHE	CB-CG-CD2	5.19	124.43	120.80
1	C	441	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	452	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	D	14	SER	CB-CA-C	5.18	119.95	110.10
1	B	236	TYR	CD1-CG-CD2	5.18	123.60	117.90
1	C	907	ASP	CB-CG-OD1	5.18	122.96	118.30
2	F	200	THR	N-CA-CB	5.18	120.14	110.30
1	B	559	ILE	O-C-N	-5.17	114.42	122.70
2	F	44	GLN	N-CA-CB	5.17	119.91	110.60
1	B	214	GLU	CG-CD-OE1	5.17	128.63	118.30
1	B	706	TYR	CB-CG-CD2	5.17	124.10	121.00
1	B	442	ALA	CB-CA-C	5.16	117.84	110.10
1	B	473	TYR	CG-CD2-CE2	-5.16	117.17	121.30
1	C	500	TYR	CB-CG-CD2	5.16	124.09	121.00
2	D	168	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	53	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	C	229	MET	CG-SD-CE	-5.15	91.96	100.20
1	A	275	ASN	CA-C-N	5.15	126.50	116.20
2	F	77	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	C	265	PHE	CB-CG-CD2	-5.14	117.20	120.80
2	F	80	LEU	CB-CG-CD2	5.14	119.75	111.00
2	E	102	PRO	N-CA-CB	5.14	109.47	103.30
1	A	830	TYR	CG-CD1-CE1	5.14	125.41	121.30
1	B	584	PHE	CG-CD1-CE1	-5.14	115.15	120.80
1	B	941	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	91	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	D	162	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	919	PHE	CB-CG-CD2	5.12	124.39	120.80
1	B	39	SER	O-C-N	-5.12	114.50	122.70
1	B	363	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	C	115	TYR	CE1-CZ-CE2	-5.12	111.61	119.80
1	B	874	PHE	CB-CG-CD1	-5.12	117.22	120.80
2	D	16	SER	N-CA-CB	5.12	118.18	110.50
1	C	265	PHE	CB-CG-CD1	5.12	124.38	120.80
1	C	277	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	675	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	114	PRO	N-CA-CB	-5.11	96.98	102.60
1	B	538	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	356	ALA	O-C-N	-5.11	114.52	122.70
1	A	134	TRP	CE3-CZ3-CH2	5.11	126.82	121.20
1	C	634	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	578	TYR	O-C-N	-5.10	114.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	200	THR	CA-CB-CG2	-5.10	105.26	112.40
1	B	534	PHE	CB-CG-CD2	5.10	124.37	120.80
1	C	498	ASN	CB-CG-OD1	-5.09	111.41	121.60
1	B	694	TYR	CG-CD1-CE1	-5.09	117.22	121.30
1	B	786	TYR	CB-CG-CD2	5.09	124.05	121.00
1	C	708	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	209	GLN	O-C-N	-5.08	114.56	122.70
1	A	904	PHE	CB-CG-CD2	5.08	124.36	120.80
1	C	941	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	408	GLU	N-CA-C	5.08	124.72	111.00
1	B	250	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	C	65	LEU	N-CA-CB	5.08	120.55	110.40
1	C	573	LEU	CB-CG-CD1	5.07	119.62	111.00
1	C	870	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	C	639	ASP	O-C-N	-5.07	114.59	122.70
1	B	44	PHE	O-C-N	-5.06	114.60	122.70
1	B	438	TRP	CE2-CD2-CG	-5.06	103.25	107.30
1	B	472	LEU	CB-CG-CD2	5.06	119.59	111.00
1	C	831	LEU	CB-CG-CD1	5.06	119.60	111.00
1	B	416	LEU	C-N-CA	5.05	132.92	122.30
1	C	55	VAL	CA-CB-CG1	-5.05	103.32	110.90
1	A	187	VAL	CA-CB-CG2	5.05	118.48	110.90
1	B	642	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	B	807	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	C	386	TRP	CH2-CZ2-CE2	5.05	122.45	117.40
2	D	236	TYR	CG-CD2-CE2	-5.05	117.26	121.30
1	A	112	PHE	CB-CG-CD1	5.04	124.33	120.80
1	C	82	ARG	CG-CD-NE	-5.04	101.21	111.80
1	B	603	ASP	CA-C-N	5.04	126.28	116.20
1	B	338	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	554	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	B	601	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	781	TYR	CG-CD2-CE2	5.04	125.33	121.30
1	C	115	TYR	CG-CD2-CE2	5.03	125.33	121.30
1	C	633	LEU	CB-CG-CD2	5.03	119.54	111.00
1	C	58	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	77	TYR	CB-CG-CD1	-5.02	117.98	121.00
1	C	386	TRP	CA-CB-CG	5.02	123.25	113.70
1	B	727	SER	N-CA-CB	5.02	118.03	110.50
1	C	96	ALA	CB-CA-C	-5.02	102.56	110.10
2	D	159	LEU	O-C-N	-5.02	114.66	123.20
1	A	627	SER	N-CA-CB	5.02	118.03	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	558	HIS	N-CA-CB	5.01	119.62	110.60
2	E	110	LYS	O-C-N	-5.01	114.67	122.70
1	A	284	VAL	CA-CB-CG2	-5.01	103.38	110.90
1	B	516	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	B	800	MET	CA-CB-CG	5.01	121.82	113.30
1	B	187	VAL	C-N-CA	5.01	134.22	121.70
2	D	56	TYR	CB-CG-CD1	-5.00	118.00	121.00
1	B	649	ALA	O-C-N	-5.00	114.69	122.70
2	D	177	TRP	CB-CG-CD2	5.00	133.10	126.60

There are no chirality outliers.

All (107) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	337	TYR	Sidechain
1	A	379	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	500	TYR	Sidechain
1	A	544	TYR	Sidechain
1	A	615	TYR	Sidechain
1	A	62	ARG	Sidechain
1	A	653	TYR	Sidechain
1	A	669	ARG	Sidechain
1	A	694	TYR	Sidechain
1	A	697	TYR	Sidechain
1	A	698	TYR	Sidechain
1	A	753	TYR	Sidechain
1	A	765	PHE	Sidechain
1	A	79	TYR	Sidechain
1	A	802	ARG	Sidechain
1	A	813	TYR	Sidechain
1	A	827	PHE	Sidechain
1	A	874	PHE	Sidechain
1	A	878	PHE	Sidechain
1	A	91	ARG	Sidechain
1	A	916	TYR	Sidechain
1	A	926	ARG	Sidechain
1	A	941	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	120	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	286	TYR	Sidechain
1	B	329	ARG	Sidechain
1	B	338	TYR	Sidechain
1	B	379	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	500	TYR	Sidechain
1	B	543	ARG	Sidechain
1	B	554	TYR	Sidechain
1	B	585	ARG	Sidechain
1	B	601	ARG	Sidechain
1	B	62	ARG	Sidechain
1	B	669	ARG	Sidechain
1	B	697	TYR	Sidechain
1	B	77	TYR	Sidechain
1	B	773	TYR	Sidechain
1	B	786	TYR	Sidechain
1	B	79	TYR	Sidechain
1	B	794	PHE	Sidechain
1	B	810	TYR	Sidechain
1	B	813	TYR	Sidechain
1	B	82	ARG	Sidechain
1	B	847	TYR	Sidechain
1	B	91	ARG	Sidechain
1	B	929	ARG	Sidechain
1	B	932	ARG	Sidechain
1	C	103	ARG	Sidechain
1	C	11	TYR	Sidechain
1	C	194	TYR	Sidechain
1	C	211	TYR	Sidechain
1	C	22	TYR	Sidechain
1	C	301	TYR	Sidechain
1	C	322	ARG	Sidechain
1	C	338	TYR	Sidechain
1	C	369	TYR	Sidechain
1	C	38	PHE	Sidechain
1	C	457	PHE	Sidechain
1	C	469	ARG	Sidechain
1	C	473	TYR	Sidechain
1	C	479	TYR	Sidechain
1	C	544	TYR	Sidechain
1	C	553	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	578	TYR	Sidechain
1	C	615	TYR	Sidechain
1	C	653	TYR	Sidechain
1	C	669	ARG	Sidechain
1	C	681	ARG	Sidechain
1	C	706	TYR	Sidechain
1	C	72	ARG	Sidechain
1	C	77	TYR	Sidechain
1	C	773	TYR	Sidechain
1	C	802	ARG	Sidechain
1	C	82	ARG	Sidechain
1	C	830	TYR	Sidechain
1	C	836	ARG	Sidechain
1	C	847	TYR	Sidechain
1	C	91	ARG	Sidechain
1	C	932	ARG	Sidechain
1	C	944	PHE	Sidechain
2	D	115	ARG	Sidechain
2	D	161	ARG	Sidechain
2	D	168	ARG	Sidechain
2	D	223	TYR	Sidechain
2	D	224	TYR	Sidechain
2	D	236	TYR	Sidechain
2	D	25	ARG	Sidechain
2	D	43	TYR	Sidechain
2	D	68	ARG	Sidechain
2	D	99	TYR	Sidechain
2	E	183	ARG	Sidechain
2	E	209	TYR	Sidechain
2	E	227	ARG	Sidechain
2	E	56	TYR	Sidechain
2	E	69	PHE	Sidechain
2	E	99	TYR	Sidechain
2	F	165	HIS	Sidechain
2	F	168	ARG	Sidechain
2	F	193	PHE	Sidechain
2	F	232	PHE	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7375	7070	7068	0	0
1	B	7375	7070	7068	0	0
1	C	7375	7070	7068	0	0
2	D	1799	1744	1743	0	0
2	E	1799	1744	1743	0	0
2	F	1799	1744	1743	0	0
All	All	27522	26442	26433	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	917/952 (96%)	866 (94%)	43 (5%)	8 (1%)	17 57
1	B	917/952 (96%)	863 (94%)	47 (5%)	7 (1%)	19 60
1	C	917/952 (96%)	853 (93%)	51 (6%)	13 (1%)	11 46
2	D	229/254 (90%)	213 (93%)	15 (7%)	1 (0%)	34 72
2	E	229/254 (90%)	207 (90%)	18 (8%)	4 (2%)	9 42
2	F	229/254 (90%)	211 (92%)	16 (7%)	2 (1%)	17 57
All	All	3438/3618 (95%)	3213 (94%)	190 (6%)	35 (1%)	20 54

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	295	PRO

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Mol	Chain	Res	Type
1	C	539	ASN
2	E	231	ASN
1	C	61	GLN
1	C	734	ASP
1	C	776	GLY
1	C	836	ARG
2	D	59	SER
1	A	725	ASP
1	A	836	ARG
1	B	443	THR
1	C	647	SER
1	C	726	SER
1	C	867	ARG
2	E	59	SER
2	F	233	PRO
1	A	354	LEU
1	A	419	VAL
1	B	748	VAL
1	B	824	ASN
1	A	224	LYS
1	A	748	VAL
1	B	739	PRO
1	C	733	ASN
2	F	6	ASP
1	A	352	SER
1	B	61	GLN
1	C	212	GLU
2	E	233	PRO
1	B	7	PRO
1	A	776	GLY
1	B	575	PRO
1	C	404	GLY
1	C	739	PRO
2	E	102	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	800/827 (97%)	780 (98%)	20 (2%)	47	68
1	B	800/827 (97%)	775 (97%)	25 (3%)	40	62
1	C	800/827 (97%)	778 (97%)	22 (3%)	43	65
2	D	197/206 (96%)	196 (100%)	1 (0%)	88	93
2	E	197/206 (96%)	195 (99%)	2 (1%)	76	86
2	F	197/206 (96%)	194 (98%)	3 (2%)	65	80
All	All	2991/3099 (96%)	2918 (98%)	73 (2%)	51	69

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	110	PRO
1	A	256	LYS
1	A	292	ILE
1	A	305	ILE
1	A	387	ASN
1	A	395	PRO
1	A	424	THR
1	A	513	VAL
1	A	522	ARG
1	A	582	TRP
1	A	608	LYS
1	A	654	PRO
1	A	667	PRO
1	A	719	LYS
1	A	755	VAL
1	A	836	ARG
1	A	853	THR
1	A	855	VAL
1	A	913	THR
1	B	29	GLN
1	B	74	ASP
1	B	91	ARG
1	B	161	GLU
1	B	180	LYS
1	B	191	THR
1	B	226	THR
1	B	238	LYS
1	B	269	THR
1	B	330	ASP

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Mol	Chain	Res	Type
1	B	352	SER
1	B	415	PRO
1	B	595	SER
1	B	643	ASN
1	B	694	TYR
1	B	719	LYS
1	B	729	SER
1	B	741	GLU
1	B	755	VAL
1	B	828	VAL
1	B	836	ARG
1	B	857	SER
1	B	861	LYS
1	B	868	THR
1	B	913	THR
1	C	37	TYR
1	C	74	ASP
1	C	80	LYS
1	C	89	ASP
1	C	91	ARG
1	C	103	ARG
1	C	165	THR
1	C	226	THR
1	C	318	SER
1	C	388	GLN
1	C	525	LEU
1	C	558	HIS
1	C	650	ASN
1	C	711	PHE
1	C	719	LYS
1	C	792	SER
1	C	811	LYS
1	C	835	MET
1	C	836	ARG
1	C	850	ILE
1	C	906	VAL
1	C	913	THR
2	D	239	GLN
2	E	85	LEU
2	E	239	GLN
2	F	8	ASP
2	F	144	PRO

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Mol	Chain	Res	Type
2	F	169	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

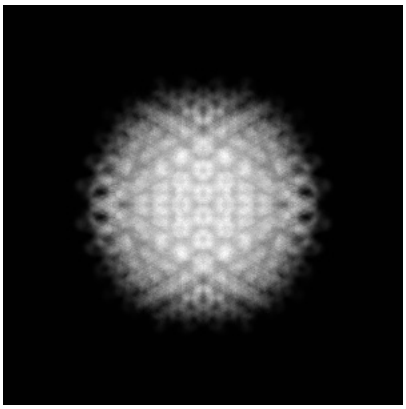
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3821. These allow visual inspection of the internal detail of the map and identification of artifacts.

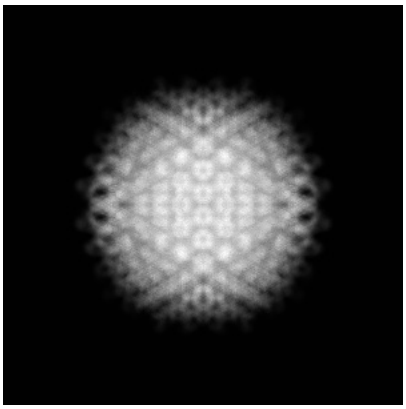
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

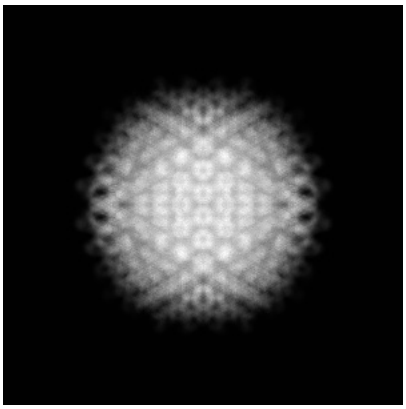
6.1.1 Primary map



X

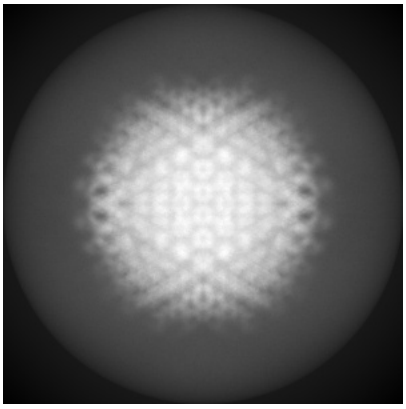


Y



Z

6.1.2 Raw map



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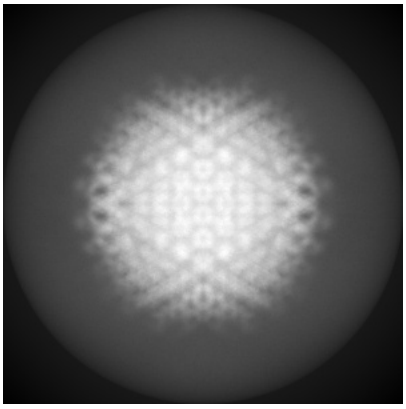

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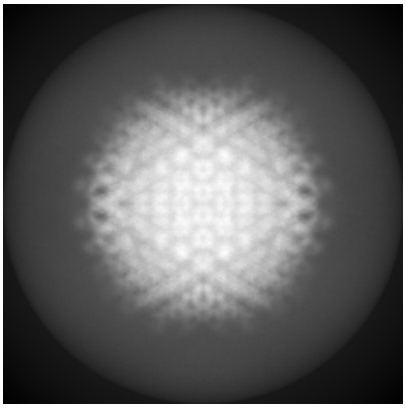
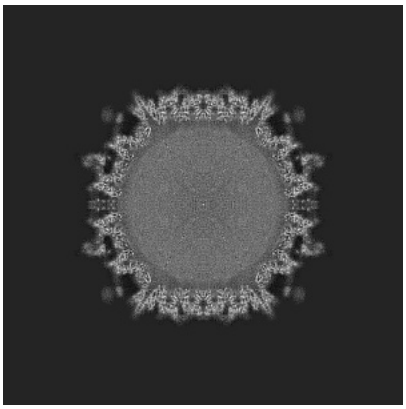


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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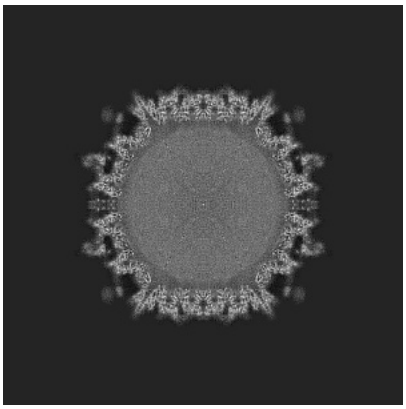

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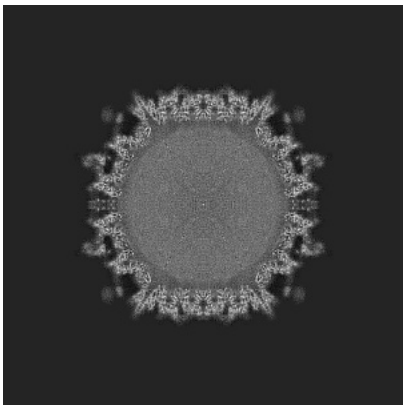

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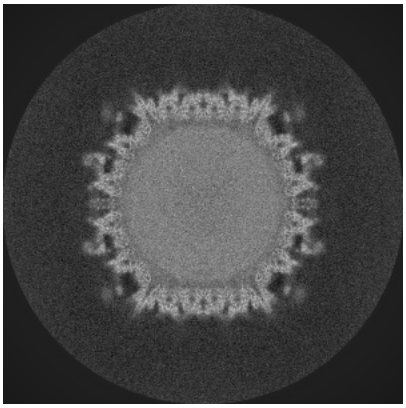
6.2.2 Raw map



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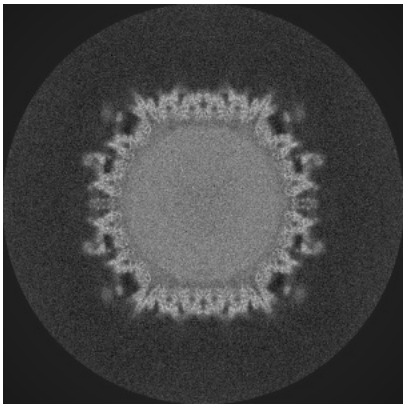

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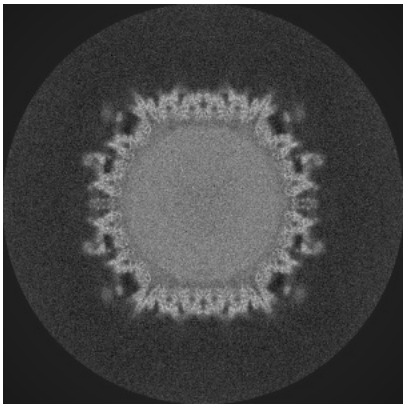
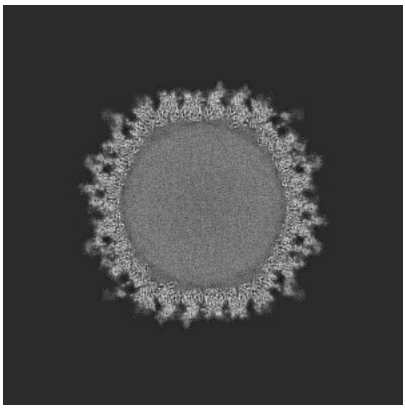


Z Index: 400

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

6.3 Largest variance slices (i)

6.3.1 Primary map



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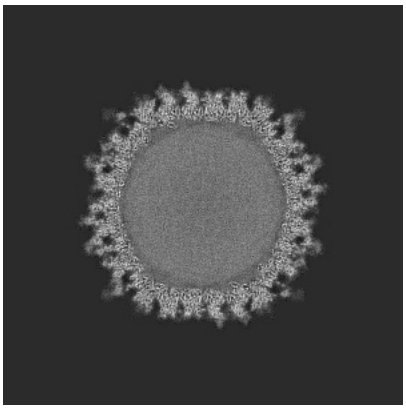

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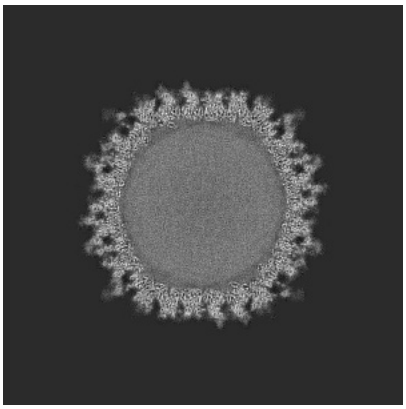
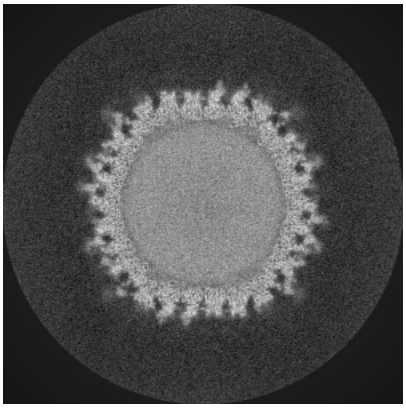
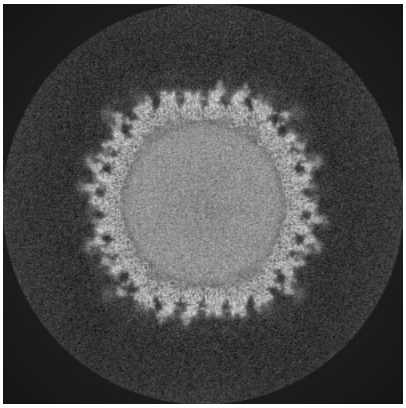


Z Index: 409

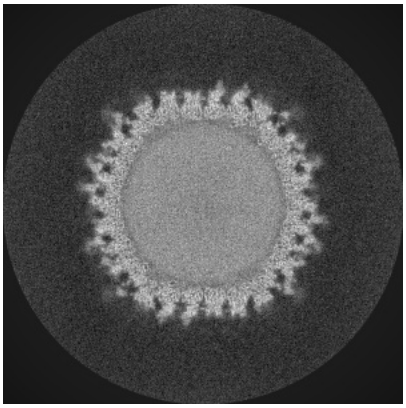
6.3.2 Raw map



X Index: 390



Y Index: 390

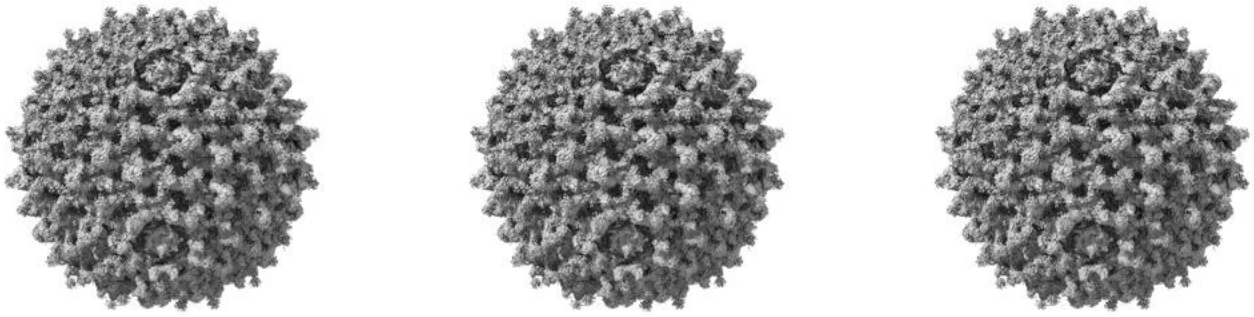


Z Index: 390

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

6.4 Orthogonal surface views (i)

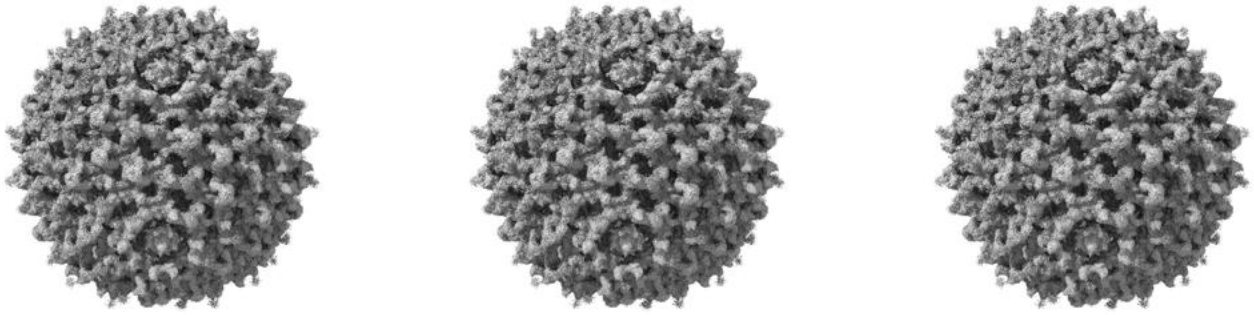
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

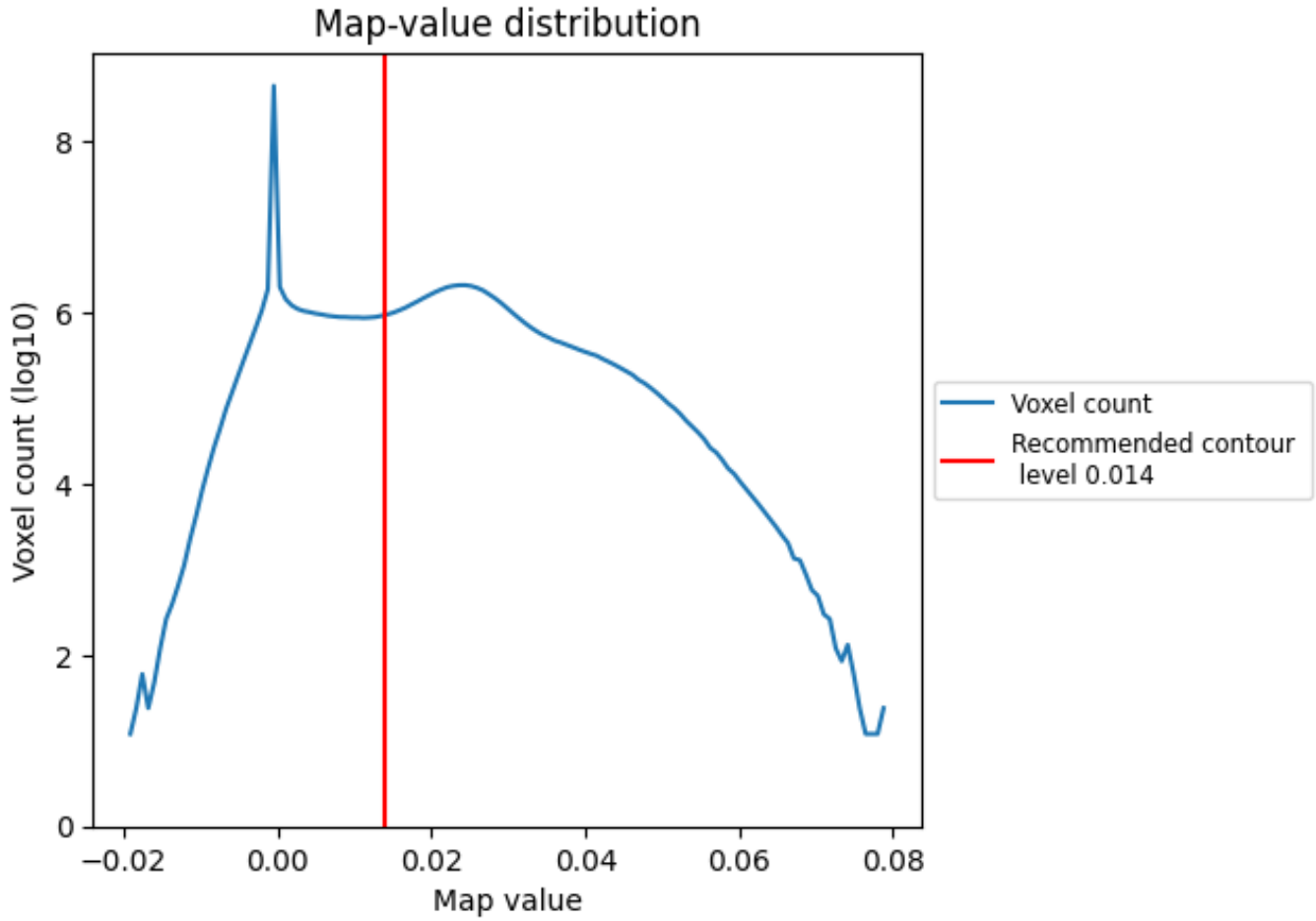
6.5 Mask visualisation (i)

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

7 Map analysis

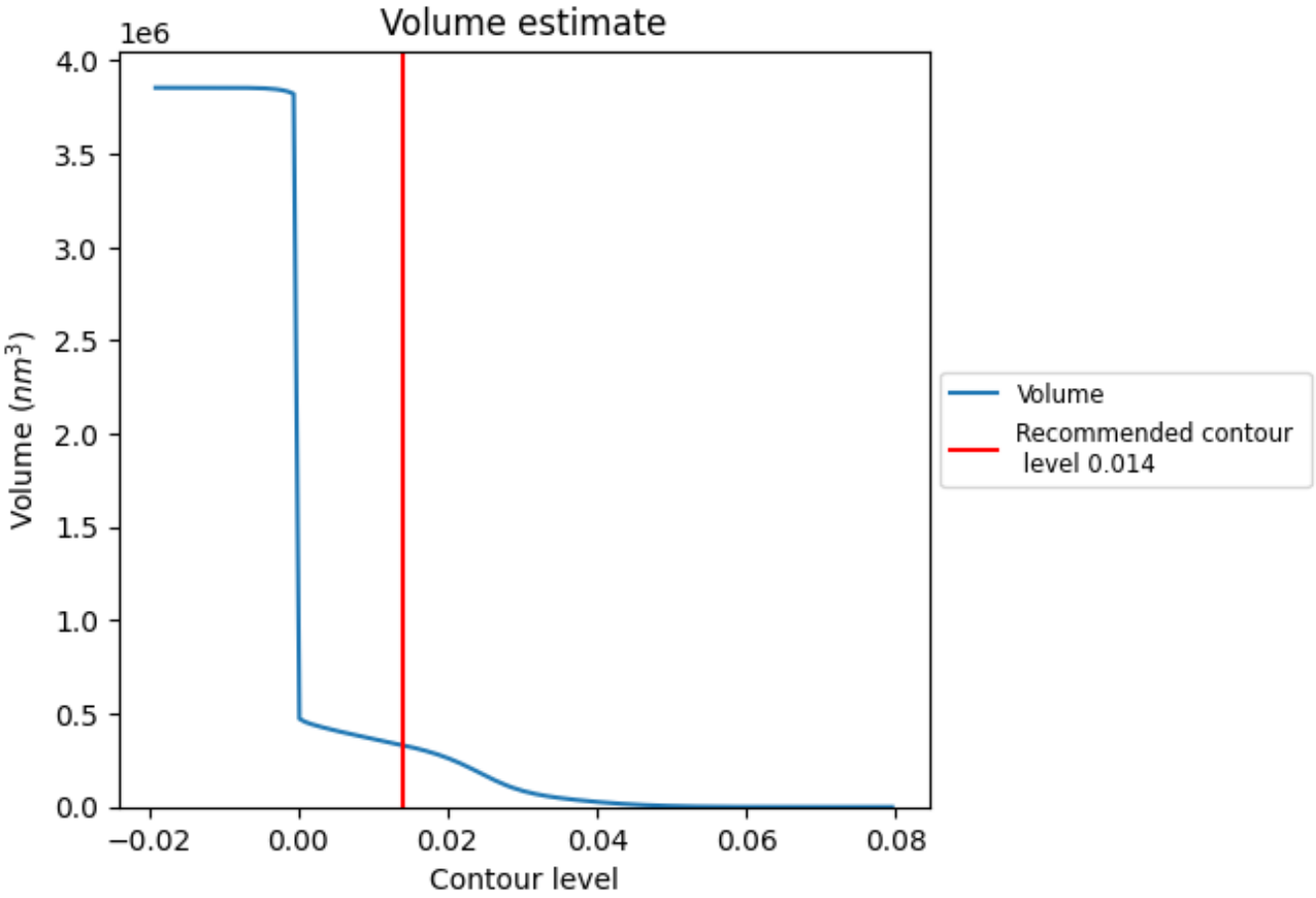
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

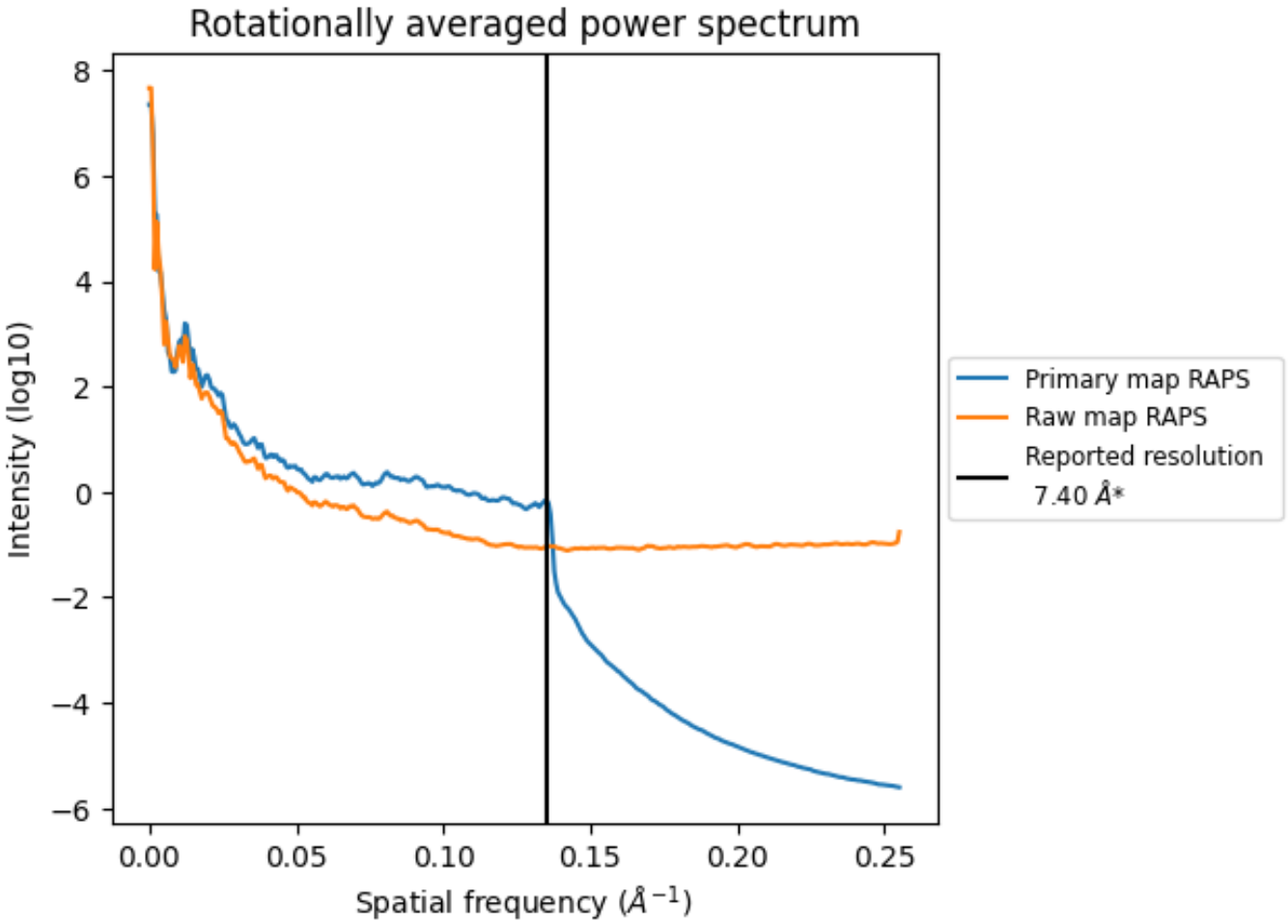
7.2 Volume estimate (i)



The volume at the recommended contour level is 330949 nm^3; this corresponds to an approximate mass of 298955 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 (i)

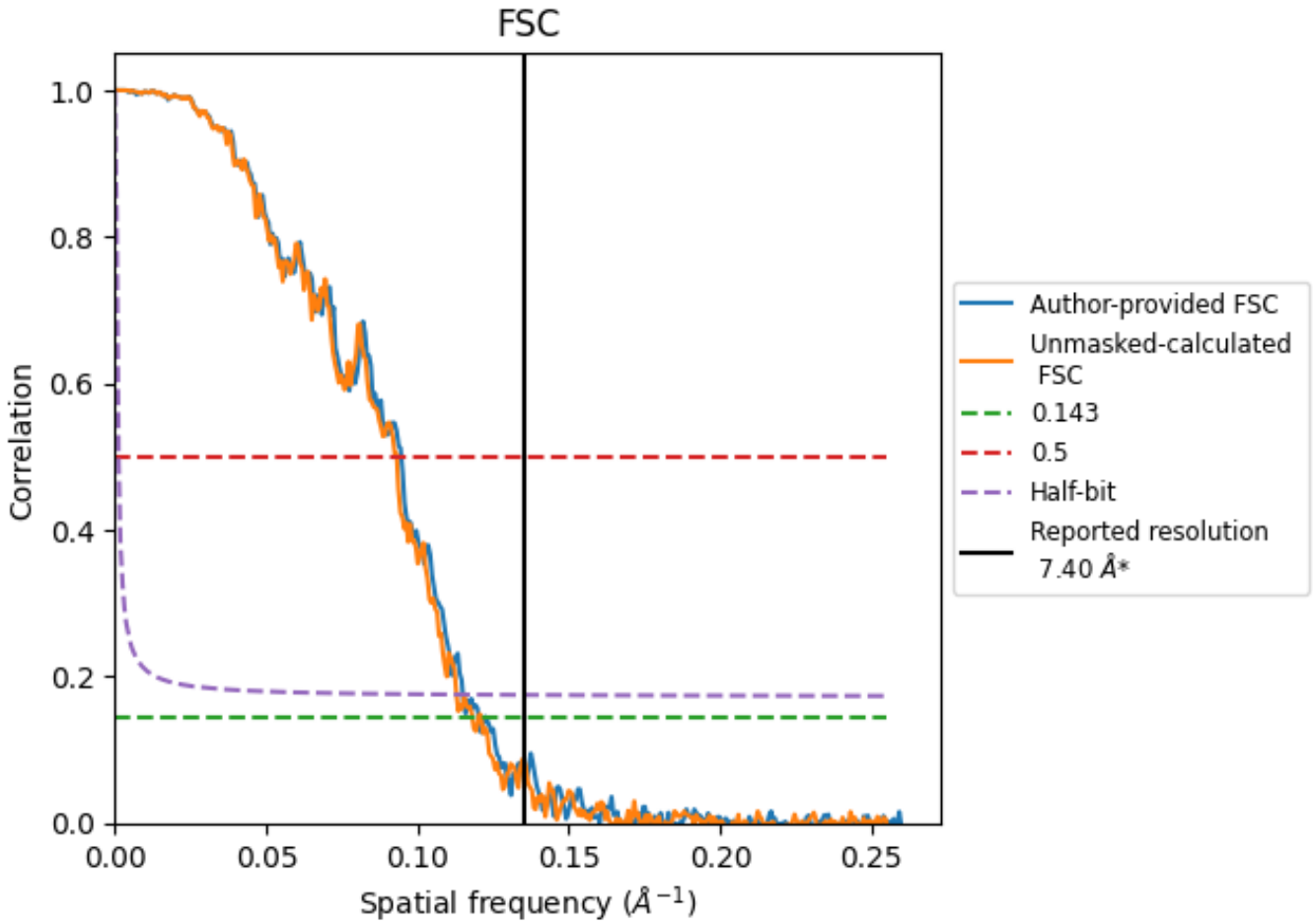


*Reported resolution corresponds to spatial frequency of 0.135 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.135 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.40	-	-
Author-provided FSC curve	8.32	10.57	8.70
Unmasked-calculated*	8.47	10.73	8.86

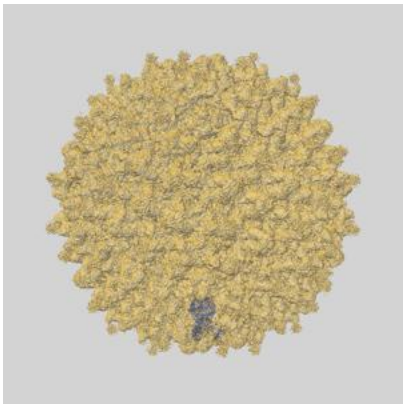
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 7.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.47 differs from the reported value 7.4 by more than 10 %

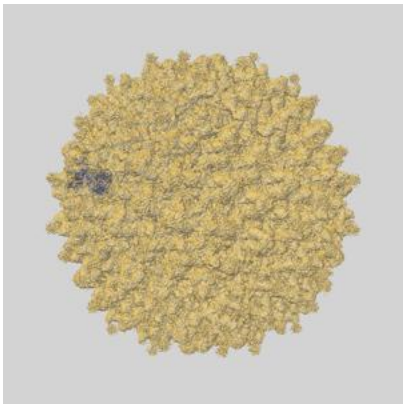
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3821 and PDB model 6EQC. Per-residue inclusion information can be found in section 3 on page 5.

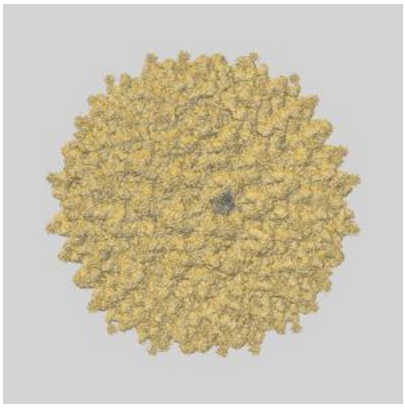
9.1 Map-model overlay



X



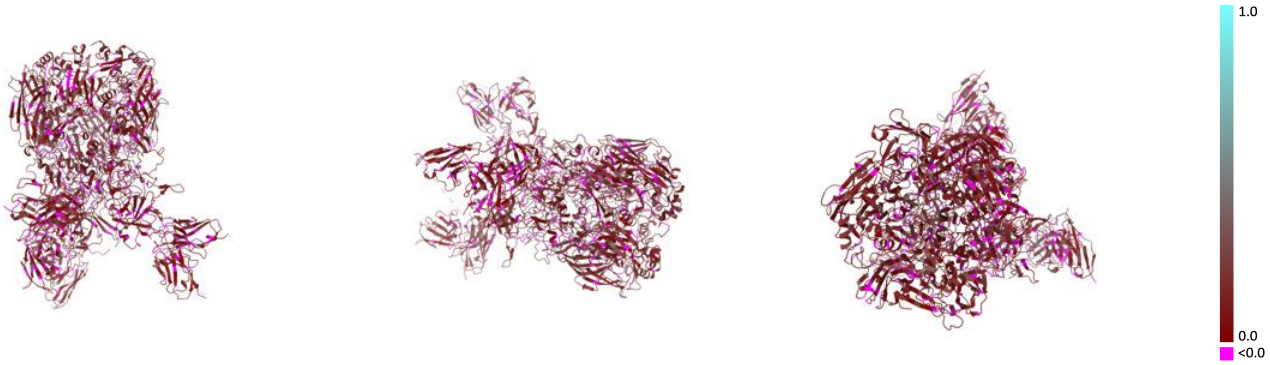
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

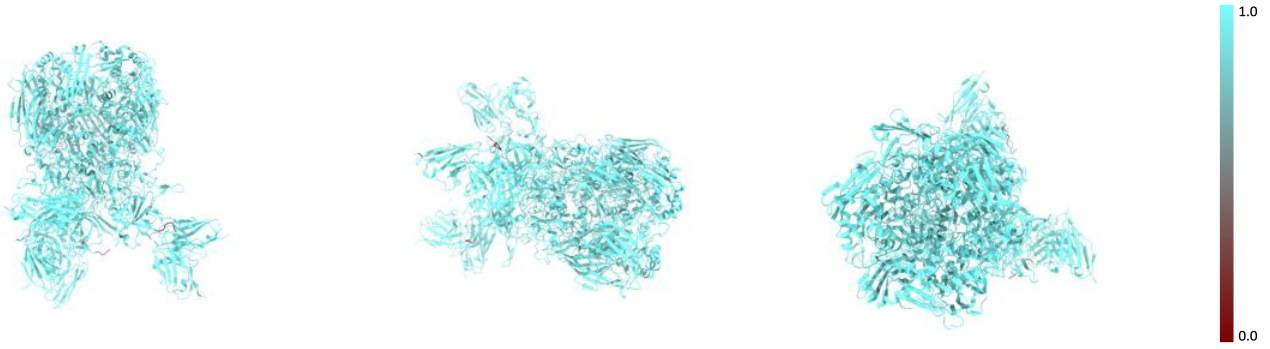
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

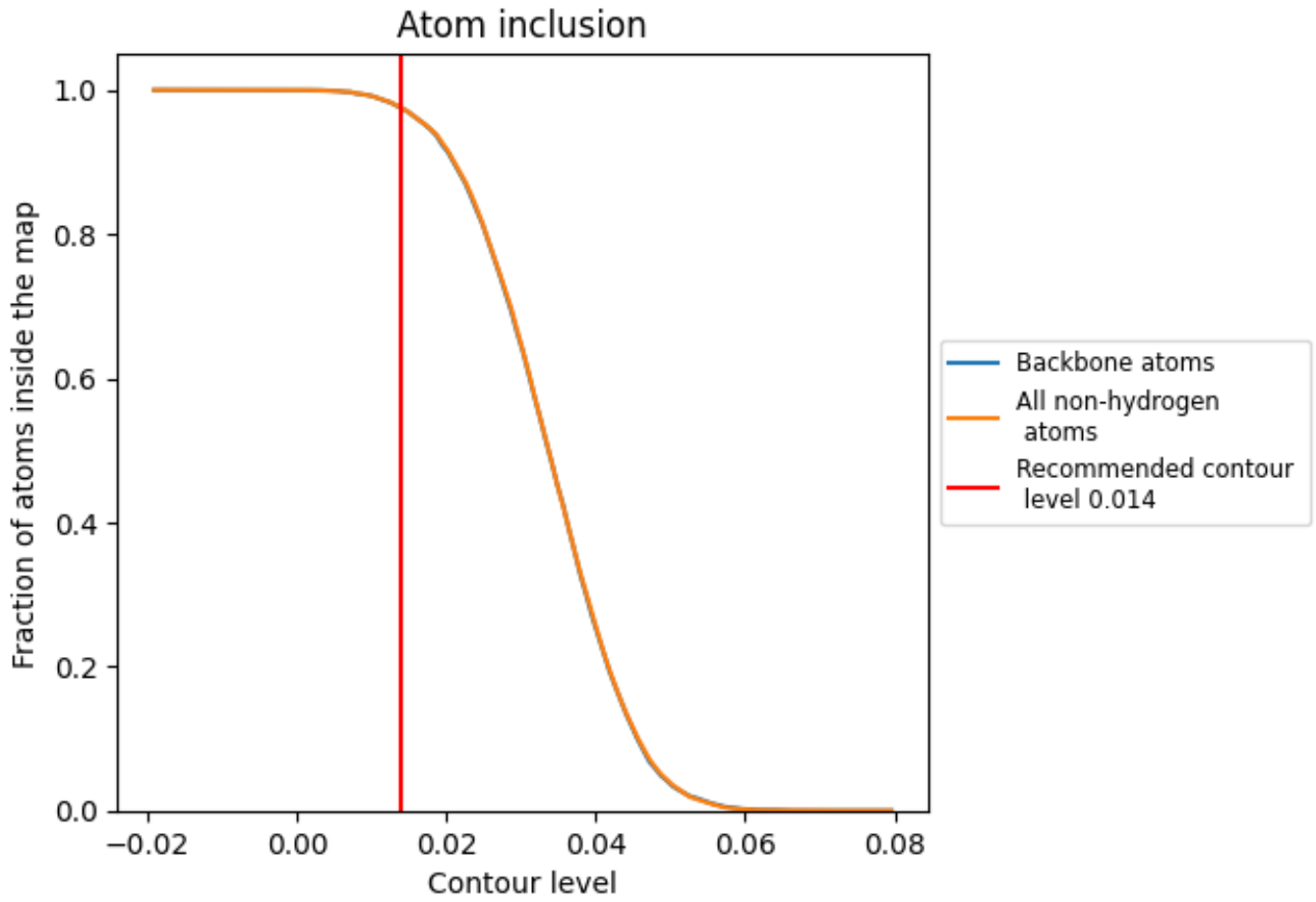
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9751	0.1270
A	0.9817	0.1340
B	0.9776	0.1310
C	0.9781	0.1240
D	0.9671	0.1200
E	0.9500	0.1120
F	0.9676	0.1250