



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 09:55 PM UTC

PDB ID : 9L1Q / pdb_00009l1q
EMDB ID : EMD-62752
Title : Cryo-EM structure of the ICT01-BTN2A1/BTN3A1/BTN3A2 complex (2 fabs)
Authors : Xin, W.Z.; Huang, B.D.; Zhou, Q.
Deposited on : 2024-12-15
Resolution : 4.00 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:

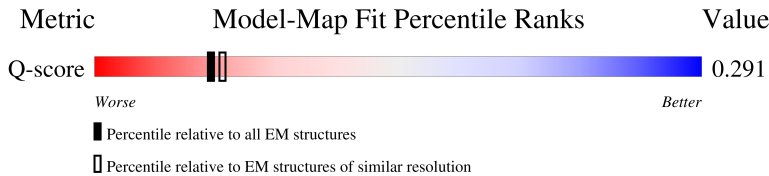
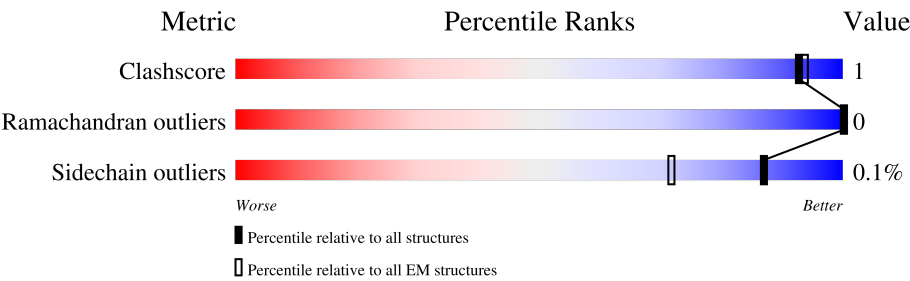
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	534	23% 20% 19% 59%
1	B	534	8% 23% 16% 59%
2	E	340	35% 26% 37%
3	F	539	7% 20% 18% 61%

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Mol	Chain	Length	Quality of chain
4	H	255	30% 54% 33% 12%
4	h	255	66% 50% 36% 12%
5	L	236	31% 50% 40% 9%
5	l	236	55% 57% 30% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13358 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1704	1075	298	320	11		
1	B	217	Total	C	N	O	S	0	0
			1704	1075	298	320	11		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP Q7KYR7
A	8	ASP	-	expression tag	UNP Q7KYR7
A	9	MET	-	expression tag	UNP Q7KYR7
A	10	ARG	-	expression tag	UNP Q7KYR7
A	11	VAL	-	expression tag	UNP Q7KYR7
A	12	PRO	-	expression tag	UNP Q7KYR7
A	13	ALA	-	expression tag	UNP Q7KYR7
A	14	GLN	-	expression tag	UNP Q7KYR7
A	15	LEU	-	expression tag	UNP Q7KYR7
A	16	LEU	-	expression tag	UNP Q7KYR7
A	17	GLY	-	expression tag	UNP Q7KYR7
A	18	LEU	-	expression tag	UNP Q7KYR7
A	19	LEU	-	expression tag	UNP Q7KYR7
A	20	LEU	-	expression tag	UNP Q7KYR7
A	21	LEU	-	expression tag	UNP Q7KYR7
A	22	TRP	-	expression tag	UNP Q7KYR7
A	23	LEU	-	expression tag	UNP Q7KYR7
A	24	SER	-	expression tag	UNP Q7KYR7
A	25	GLY	-	expression tag	UNP Q7KYR7
A	26	ALA	-	expression tag	UNP Q7KYR7
A	27	ARG	-	expression tag	UNP Q7KYR7
A	28	CYS	-	expression tag	UNP Q7KYR7
A	528	GLY	-	expression tag	UNP Q7KYR7
A	529	SER	-	expression tag	UNP Q7KYR7
A	530	SER	-	expression tag	UNP Q7KYR7
A	531	GLY	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	532	MET	-	expression tag	UNP Q7KYR7
A	533	ASP	-	expression tag	UNP Q7KYR7
A	534	TYR	-	expression tag	UNP Q7KYR7
A	535	LYS	-	expression tag	UNP Q7KYR7
A	536	ASP	-	expression tag	UNP Q7KYR7
A	537	ASP	-	expression tag	UNP Q7KYR7
A	538	ASP	-	expression tag	UNP Q7KYR7
A	539	ASP	-	expression tag	UNP Q7KYR7
A	540	LYS	-	expression tag	UNP Q7KYR7
B	7	MET	-	initiating methionine	UNP Q7KYR7
B	8	ASP	-	expression tag	UNP Q7KYR7
B	9	MET	-	expression tag	UNP Q7KYR7
B	10	ARG	-	expression tag	UNP Q7KYR7
B	11	VAL	-	expression tag	UNP Q7KYR7
B	12	PRO	-	expression tag	UNP Q7KYR7
B	13	ALA	-	expression tag	UNP Q7KYR7
B	14	GLN	-	expression tag	UNP Q7KYR7
B	15	LEU	-	expression tag	UNP Q7KYR7
B	16	LEU	-	expression tag	UNP Q7KYR7
B	17	GLY	-	expression tag	UNP Q7KYR7
B	18	LEU	-	expression tag	UNP Q7KYR7
B	19	LEU	-	expression tag	UNP Q7KYR7
B	20	LEU	-	expression tag	UNP Q7KYR7
B	21	LEU	-	expression tag	UNP Q7KYR7
B	22	TRP	-	expression tag	UNP Q7KYR7
B	23	LEU	-	expression tag	UNP Q7KYR7
B	24	SER	-	expression tag	UNP Q7KYR7
B	25	GLY	-	expression tag	UNP Q7KYR7
B	26	ALA	-	expression tag	UNP Q7KYR7
B	27	ARG	-	expression tag	UNP Q7KYR7
B	28	CYS	-	expression tag	UNP Q7KYR7
B	528	GLY	-	expression tag	UNP Q7KYR7
B	529	SER	-	expression tag	UNP Q7KYR7
B	530	SER	-	expression tag	UNP Q7KYR7
B	531	GLY	-	expression tag	UNP Q7KYR7
B	532	MET	-	expression tag	UNP Q7KYR7
B	533	ASP	-	expression tag	UNP Q7KYR7
B	534	TYR	-	expression tag	UNP Q7KYR7
B	535	LYS	-	expression tag	UNP Q7KYR7
B	536	ASP	-	expression tag	UNP Q7KYR7
B	537	ASP	-	expression tag	UNP Q7KYR7
B	538	ASP	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	539	ASP	-	expression tag	UNP Q7KYR7
B	540	LYS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	215	Total	C	N	O	S	0	0
			1624	1024	278	314	8		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	MET	-	initiating methionine	UNP P78410
E	9	ASP	-	expression tag	UNP P78410
E	10	MET	-	expression tag	UNP P78410
E	11	ARG	-	expression tag	UNP P78410
E	12	VAL	-	expression tag	UNP P78410
E	13	PRO	-	expression tag	UNP P78410
E	14	ALA	-	expression tag	UNP P78410
E	15	GLN	-	expression tag	UNP P78410
E	16	LEU	-	expression tag	UNP P78410
E	17	LEU	-	expression tag	UNP P78410
E	18	GLY	-	expression tag	UNP P78410
E	19	LEU	-	expression tag	UNP P78410
E	20	LEU	-	expression tag	UNP P78410
E	21	LEU	-	expression tag	UNP P78410
E	22	LEU	-	expression tag	UNP P78410
E	23	TRP	-	expression tag	UNP P78410
E	24	LEU	-	expression tag	UNP P78410
E	25	SER	-	expression tag	UNP P78410
E	26	GLY	-	expression tag	UNP P78410
E	27	ALA	-	expression tag	UNP P78410
E	28	ARG	-	expression tag	UNP P78410
E	29	CYS	-	expression tag	UNP P78410
E	335	GLY	-	expression tag	UNP P78410
E	336	SER	-	expression tag	UNP P78410
E	337	SER	-	expression tag	UNP P78410
E	338	GLY	-	expression tag	UNP P78410
E	339	MET	-	expression tag	UNP P78410
E	340	ASP	-	expression tag	UNP P78410
E	341	TYR	-	expression tag	UNP P78410
E	342	LYS	-	expression tag	UNP P78410

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	ASP	-	expression tag	UNP P78410
E	344	ASP	-	expression tag	UNP P78410
E	345	ASP	-	expression tag	UNP P78410
E	346	ASP	-	expression tag	UNP P78410
E	347	LYS	-	expression tag	UNP P78410

- Molecule 3 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	212	Total	C	N	O	S	0	0
			1598	1005	274	311	8		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	8	MET	-	initiating methionine	UNP O00481
F	9	ASP	-	expression tag	UNP O00481
F	10	MET	-	expression tag	UNP O00481
F	11	ARG	-	expression tag	UNP O00481
F	12	VAL	-	expression tag	UNP O00481
F	13	PRO	-	expression tag	UNP O00481
F	14	ALA	-	expression tag	UNP O00481
F	15	GLN	-	expression tag	UNP O00481
F	16	LEU	-	expression tag	UNP O00481
F	17	LEU	-	expression tag	UNP O00481
F	18	GLY	-	expression tag	UNP O00481
F	19	LEU	-	expression tag	UNP O00481
F	20	LEU	-	expression tag	UNP O00481
F	21	LEU	-	expression tag	UNP O00481
F	22	LEU	-	expression tag	UNP O00481
F	23	TRP	-	expression tag	UNP O00481
F	24	LEU	-	expression tag	UNP O00481
F	25	SER	-	expression tag	UNP O00481
F	26	GLY	-	expression tag	UNP O00481
F	27	ALA	-	expression tag	UNP O00481
F	28	ARG	-	expression tag	UNP O00481
F	29	CYS	-	expression tag	UNP O00481
F	514	GLY	-	expression tag	UNP O00481
F	515	SER	-	expression tag	UNP O00481
F	516	SER	-	expression tag	UNP O00481
F	517	GLY	-	expression tag	UNP O00481
F	518	ALA	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
F	519	TRP	-	expression tag	UNP O00481
F	520	SER	-	expression tag	UNP O00481
F	521	HIS	-	expression tag	UNP O00481
F	522	PRO	-	expression tag	UNP O00481
F	523	GLN	-	expression tag	UNP O00481
F	524	PHE	-	expression tag	UNP O00481
F	525	GLU	-	expression tag	UNP O00481
F	526	LYS	-	expression tag	UNP O00481
F	527	GLY	-	expression tag	UNP O00481
F	528	GLY	-	expression tag	UNP O00481
F	529	GLY	-	expression tag	UNP O00481
F	530	SER	-	expression tag	UNP O00481
F	531	GLY	-	expression tag	UNP O00481
F	532	GLY	-	expression tag	UNP O00481
F	533	GLY	-	expression tag	UNP O00481
F	534	SER	-	expression tag	UNP O00481
F	535	GLY	-	expression tag	UNP O00481
F	536	GLY	-	expression tag	UNP O00481
F	537	SER	-	expression tag	UNP O00481
F	538	ALA	-	expression tag	UNP O00481
F	539	TRP	-	expression tag	UNP O00481
F	540	SER	-	expression tag	UNP O00481
F	541	HIS	-	expression tag	UNP O00481
F	542	PRO	-	expression tag	UNP O00481
F	543	GLN	-	expression tag	UNP O00481
F	544	PHE	-	expression tag	UNP O00481
F	545	GLU	-	expression tag	UNP O00481
F	546	LYS	-	expression tag	UNP O00481

- Molecule 4 is a protein called ICT01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	225	Total	C	N	O	S	0	0
			1710	1080	285	337	8		
4	h	225	Total	C	N	O	S	0	0
			1710	1080	285	337	8		

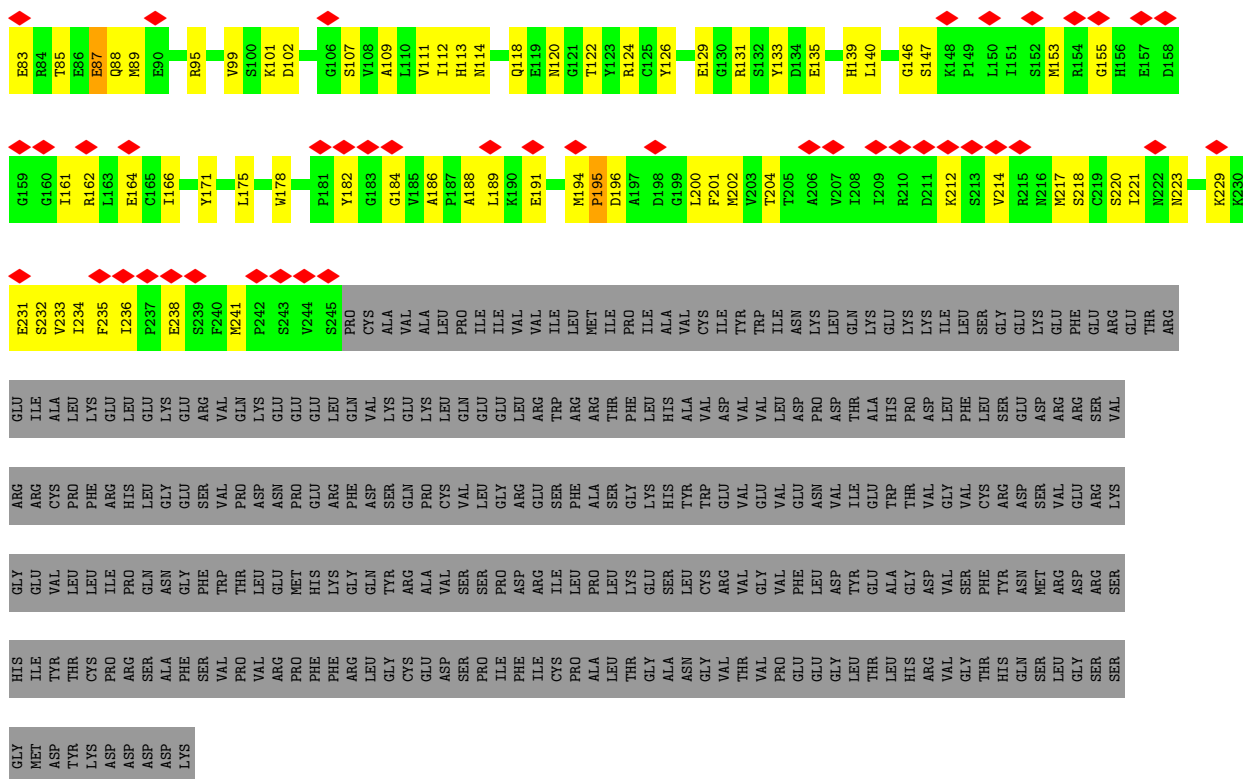
- Molecule 5 is a protein called ICT01 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	214	Total	C	N	O	S	0	0
			1654	1037	278	333	6		

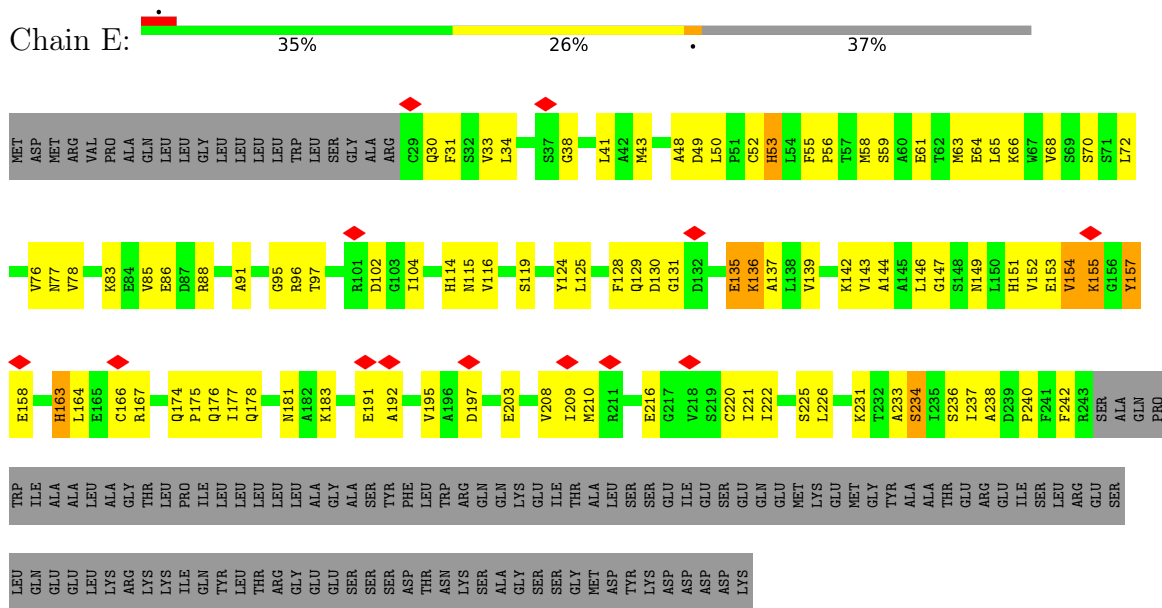
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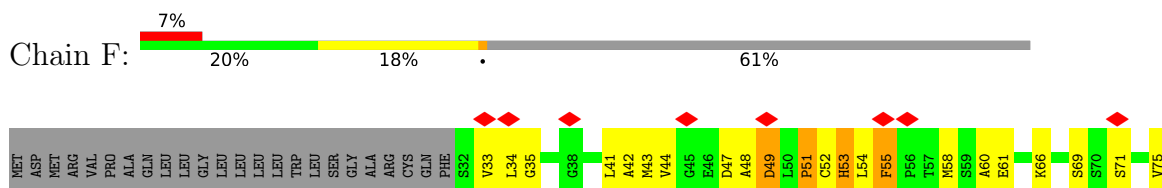
Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	214	Total	C	N	O	S	0	0
			1654	1037	278	333	6		

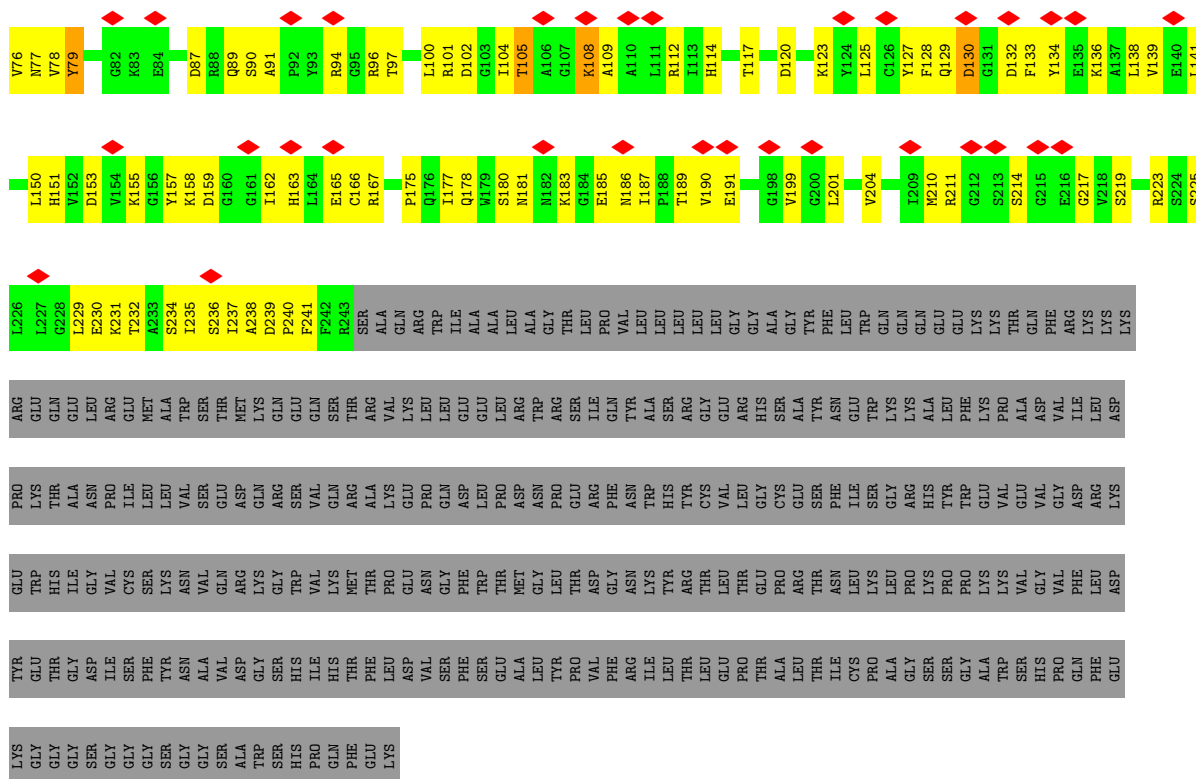


- Molecule 2: Butyrophilin subfamily 3 member A2

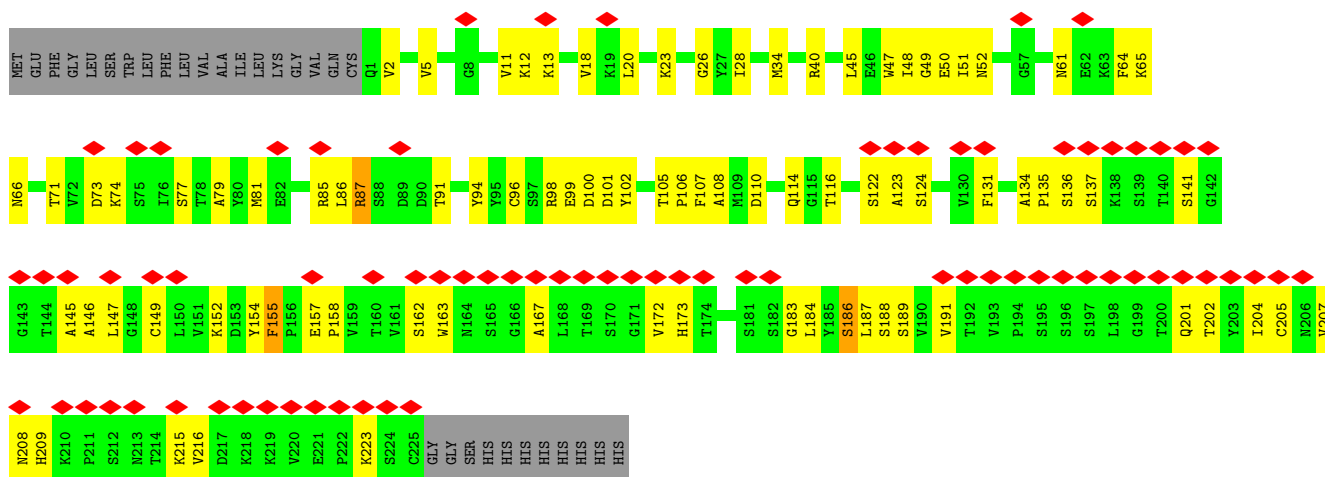


- Molecule 3: Butyrophilin subfamily 3 member A1

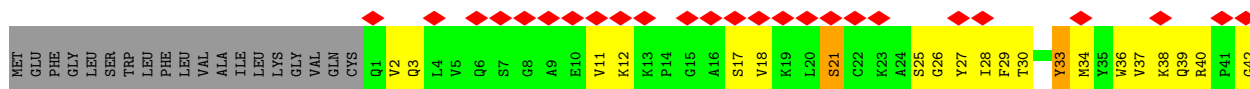




- Molecule 4: ICT01 heavy chain

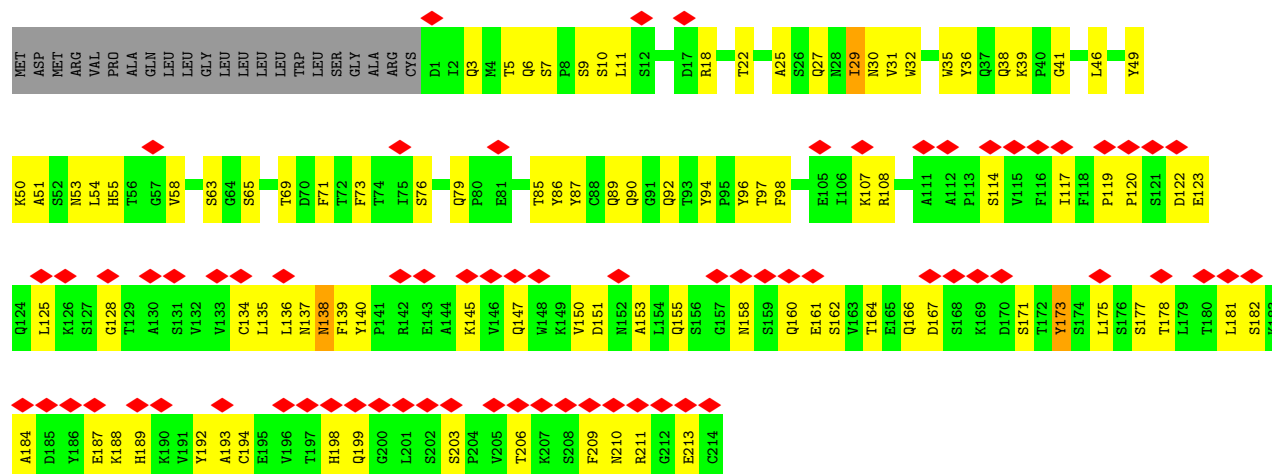


- Molecule 4: ICT01 heavy chain

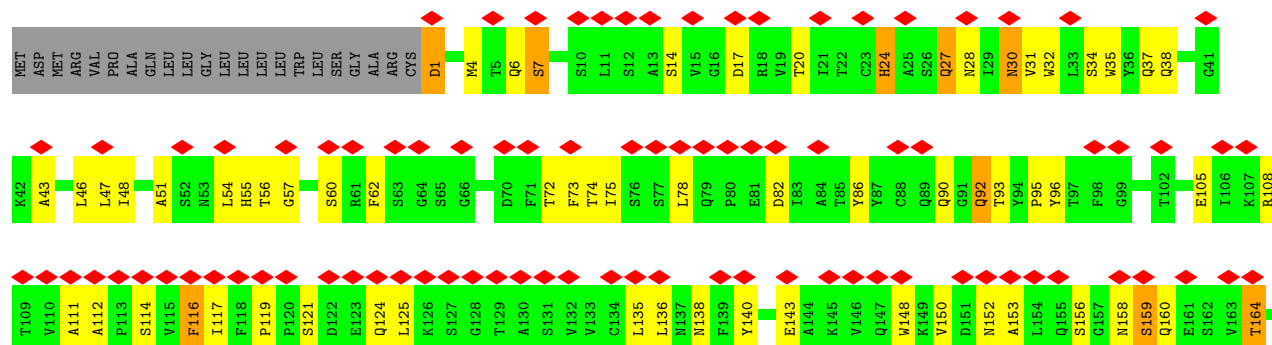




• Molecule 5: ICT01 light chain



• Molecule 5: ICT01 light chain



Y173	S174	L175	S176	S177	T178	L179	T180	L181	S182	K183	A184	D185	Y186	E187	K188	H189	K190	V191	Y192	A193	C194	E195	V196	T197	H198	Q199	G200	L201	S202	S203	P204	V205	T206	K207	S208	F209	N210	R211	G212	E213	C214
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.113	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	2.42	88/1741 (5.1%)	2.02	74/2356 (3.1%)
1	B	2.46	86/1741 (4.9%)	1.84	45/2356 (1.9%)
2	E	2.48	88/1657 (5.3%)	1.90	57/2247 (2.5%)
3	F	2.49	75/1630 (4.6%)	2.07	76/2211 (3.4%)
4	H	2.29	65/1751 (3.7%)	1.71	44/2380 (1.8%)
4	h	2.47	90/1751 (5.1%)	1.85	45/2380 (1.9%)
5	L	2.41	83/1692 (4.9%)	1.85	51/2299 (2.2%)
5	l	2.33	66/1692 (3.9%)	1.81	44/2299 (1.9%)
All	All	2.42	641/13655 (4.7%)	1.88	436/18528 (2.4%)

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	10
1	B	0	7
2	E	0	4
3	F	0	13
4	H	0	4
4	h	0	6
5	L	0	6
5	l	0	6
All	All	0	56

All (641) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	105	THR	CA-C	10.82	1.62	1.52
3	F	55	PHE	C-O	-9.94	1.16	1.25
3	F	240	PRO	CA-C	9.61	1.61	1.52
2	E	52	CYS	CA-C	9.60	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	63	MET	SD-CE	-9.53	1.55	1.79
3	F	210	MET	SD-CE	-9.47	1.55	1.79
1	A	64	VAL	CA-C	9.26	1.64	1.52
5	l	24	HIS	CD2-NE2	9.04	1.47	1.37
3	F	185	GLU	CA-C	8.97	1.64	1.52
2	E	240	PRO	CA-C	8.89	1.60	1.52
4	h	55	ASN	CA-C	-8.88	1.41	1.52
1	B	166	ILE	CA-C	8.69	1.63	1.52
2	E	128	PHE	CA-C	-8.65	1.42	1.52
5	L	189	HIS	ND1-CE1	8.61	1.41	1.32
2	E	176	GLN	CA-C	-8.58	1.42	1.52
4	h	93	VAL	CA-C	8.52	1.62	1.52
5	l	4	MET	SD-CE	-8.51	1.58	1.79
4	h	92	ALA	CA-C	-8.50	1.42	1.52
3	F	199	VAL	CA-C	8.47	1.62	1.52
4	H	173	HIS	CA-C	8.31	1.63	1.52
4	h	50	GLU	CA-C	-8.24	1.42	1.52
3	F	108	LYS	CA-C	-8.19	1.44	1.53
1	A	154	ARG	CA-C	-8.16	1.42	1.52
4	H	51	ILE	CA-C	8.15	1.62	1.52
1	B	217	MET	SD-CE	-8.13	1.59	1.79
2	E	144	ALA	CA-C	8.13	1.62	1.52
2	E	203	GLU	CA-C	-8.10	1.43	1.52
4	h	34	MET	SD-CE	8.06	1.99	1.79
5	l	6	GLN	CA-C	-8.05	1.42	1.52
1	A	89	MET	CA-C	-8.05	1.42	1.52
2	E	238	ALA	CA-C	8.03	1.63	1.52
1	A	87	GLU	CA-C	8.02	1.64	1.52
3	F	153	ASP	CA-C	-8.02	1.42	1.52
1	A	215	ARG	CA-C	-7.99	1.42	1.52
1	A	76	PHE	CA-C	7.96	1.62	1.52
1	B	175	LEU	CA-C	7.94	1.62	1.52
1	B	113	HIS	CD2-NE2	7.93	1.46	1.37
4	h	181	SER	CA-C	7.86	1.62	1.52
5	L	203	SER	CA-C	7.83	1.61	1.52
1	A	235	PHE	CA-C	7.80	1.62	1.52
2	E	136	LYS	CA-C	7.79	1.62	1.52
5	l	112	ALA	CA-C	7.76	1.61	1.52
4	H	66	ASN	N-CA	7.69	1.55	1.45
2	E	237	ILE	CA-C	7.63	1.61	1.52
1	B	95	ARG	CA-C	7.60	1.62	1.52
2	E	96	ARG	CA-C	7.59	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ASP	CA-C	7.55	1.62	1.52
4	H	186	SER	CA-C	-7.55	1.43	1.52
3	F	175	PRO	N-CA	7.54	1.53	1.46
4	H	207	VAL	CA-C	7.47	1.61	1.52
1	A	75	VAL	CA-C	-7.46	1.41	1.52
3	F	165	GLU	C-O	-7.44	1.15	1.23
4	h	109	MET	C-O	-7.43	1.15	1.24
1	B	194	MET	SD-CE	-7.42	1.60	1.79
1	B	241	MET	CA-C	7.41	1.61	1.52
2	E	177	ILE	CA-CB	7.41	1.64	1.54
2	E	142	LYS	CA-C	-7.41	1.43	1.52
4	H	102	TYR	N-CA	7.39	1.55	1.46
1	A	82	ARG	CA-C	7.39	1.61	1.52
1	B	89	MET	SD-CE	-7.38	1.61	1.79
3	F	190	VAL	C-O	-7.35	1.16	1.24
4	h	109	MET	CA-C	-7.35	1.43	1.52
4	h	3	GLN	CA-C	-7.35	1.43	1.52
1	B	212	LYS	CA-C	7.30	1.61	1.52
3	F	112	ARG	CA-C	-7.30	1.44	1.52
2	E	225	SER	N-CA	-7.30	1.37	1.46
5	L	51	ALA	CA-C	7.29	1.63	1.52
1	B	52	HIS	ND1-CE1	-7.28	1.25	1.32
4	h	154	TYR	CA-C	-7.28	1.43	1.52
4	h	221	GLU	CA-C	7.28	1.62	1.52
1	B	65	ARG	N-CA	7.27	1.55	1.46
4	H	34	MET	CA-C	7.26	1.61	1.52
2	E	50	LEU	CA-C	7.26	1.61	1.52
3	F	42	ALA	CA-C	7.25	1.62	1.53
3	F	120	ASP	CA-C	7.25	1.62	1.52
2	E	30	GLN	N-CA	7.24	1.55	1.46
3	F	129	GLN	CA-C	7.23	1.61	1.52
3	F	34	LEU	CA-C	7.23	1.61	1.52
4	H	123	ALA	CA-C	7.21	1.61	1.52
1	B	58	ASN	CA-C	7.18	1.62	1.52
1	A	115	ILE	CA-C	-7.17	1.43	1.52
1	B	112	ILE	N-CA	-7.14	1.37	1.46
1	B	118	GLN	N-CA	-7.14	1.39	1.46
1	A	137	ILE	C-O	-7.12	1.16	1.23
1	A	201	PHE	CA-C	-7.12	1.43	1.52
1	B	113	HIS	C-O	-7.11	1.15	1.23
3	F	100	LEU	CA-C	-7.07	1.43	1.53
5	L	92	GLN	N-CA	7.06	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	ILE	C-O	7.06	1.31	1.24
1	B	232	SER	C-O	-7.04	1.16	1.23
1	B	220	SER	CA-C	-7.02	1.44	1.52
5	l	156	SER	C-O	-7.02	1.14	1.23
4	h	53	PRO	C-O	-7.00	1.15	1.24
2	E	216	GLU	C-O	-7.00	1.15	1.23
4	H	191	VAL	CA-C	6.99	1.60	1.52
4	h	178	VAL	N-CA	-6.98	1.38	1.46
3	F	219	SER	CA-C	-6.97	1.43	1.52
2	E	152	VAL	CA-C	6.95	1.60	1.52
5	L	108	ARG	CA-C	-6.93	1.44	1.52
2	E	192	ALA	CA-C	-6.92	1.44	1.52
4	H	202	THR	N-CA	-6.91	1.37	1.45
2	E	53	HIS	ND1-CE1	6.91	1.39	1.32
4	h	112	TRP	N-CA	6.91	1.54	1.45
1	A	226	LEU	CA-C	6.91	1.62	1.52
4	h	12	LYS	N-CA	6.89	1.54	1.46
4	h	153	ASP	CA-C	6.88	1.61	1.53
2	E	191	GLU	CA-C	-6.87	1.44	1.52
2	E	178	GLN	CA-C	-6.87	1.44	1.52
4	h	173	HIS	CE1-NE2	-6.86	1.25	1.32
5	L	153	ALA	CA-C	6.85	1.60	1.52
3	F	163	HIS	CD2-NE2	6.84	1.45	1.37
1	A	233	VAL	C-O	-6.82	1.16	1.23
5	l	175	LEU	CA-C	-6.80	1.44	1.52
1	A	123	TYR	N-CA	-6.80	1.38	1.46
4	H	223	LYS	CA-C	-6.79	1.44	1.52
1	B	217	MET	C-O	-6.79	1.15	1.23
5	l	209	PHE	CA-C	-6.78	1.44	1.52
1	B	202	MET	SD-CE	6.77	1.96	1.79
4	H	87	ARG	CA-C	-6.76	1.43	1.53
3	F	180	SER	C-O	-6.76	1.15	1.23
1	B	201	PHE	N-CA	-6.75	1.37	1.46
3	F	123	LYS	CA-C	-6.74	1.44	1.52
1	A	33	VAL	CA-C	6.74	1.59	1.53
1	A	171	TYR	CA-C	6.74	1.60	1.52
5	L	35	TRP	N-CA	6.73	1.54	1.46
5	L	173	TYR	CA-C	-6.72	1.44	1.53
4	H	61	ASN	CA-C	6.70	1.62	1.53
1	B	58	ASN	N-CA	-6.70	1.37	1.46
1	B	233	VAL	CA-C	-6.70	1.45	1.52
1	B	83	GLU	CA-C	6.69	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	114	GLN	CA-C	-6.69	1.43	1.52
3	F	136	LYS	CA-C	6.69	1.60	1.52
1	B	107	SER	CA-C	-6.68	1.44	1.52
1	A	53	LEU	C-O	-6.68	1.15	1.23
3	F	54	LEU	C-N	6.68	1.42	1.33
4	H	116	THR	CA-C	-6.67	1.44	1.52
5	L	5	THR	CA-C	6.67	1.60	1.52
1	A	157	GLU	CA-C	6.66	1.61	1.52
1	B	88	GLN	CA-C	-6.65	1.44	1.52
3	F	141	LEU	N-CA	-6.65	1.37	1.46
2	E	166	CYS	CA-C	6.64	1.60	1.52
1	B	124	ARG	N-CA	-6.63	1.37	1.46
3	F	47	ASP	CA-C	-6.62	1.44	1.52
4	h	185	TYR	N-CA	-6.62	1.37	1.46
2	E	34	LEU	CA-C	-6.60	1.44	1.52
4	h	63	LYS	CA-C	6.59	1.61	1.52
4	h	113	GLY	C-O	-6.59	1.17	1.23
4	h	209	HIS	N-CA	-6.59	1.37	1.46
3	F	187	ILE	CA-C	6.59	1.59	1.52
4	h	25	SER	C-O	-6.58	1.16	1.23
1	B	62	MET	SD-CE	-6.57	1.63	1.79
2	E	43	MET	N-CA	-6.56	1.38	1.46
4	h	87	ARG	CA-C	-6.56	1.43	1.53
5	L	3	GLN	N-CA	6.55	1.54	1.45
5	L	86	TYR	CA-C	-6.55	1.44	1.52
1	A	150	LEU	CA-C	-6.55	1.44	1.52
3	F	230	GLU	CA-C	6.54	1.60	1.52
5	L	162	SER	CA-C	-6.54	1.44	1.52
1	A	204	THR	N-CA	6.54	1.54	1.46
1	B	153	MET	CA-C	-6.54	1.43	1.53
1	A	30	PHE	N-CA	-6.53	1.37	1.45
3	F	138	LEU	CA-C	-6.53	1.44	1.52
5	l	30	ASN	C-O	6.53	1.31	1.23
4	h	34	MET	C-O	-6.52	1.16	1.24
1	B	140	LEU	N-CA	-6.51	1.38	1.46
3	F	114	HIS	CD2-NE2	6.50	1.45	1.37
2	E	167	ARG	C-O	-6.50	1.15	1.23
4	h	138	LYS	N-CA	6.49	1.54	1.46
1	B	122	THR	CA-C	6.49	1.61	1.52
5	L	18	ARG	C-O	-6.48	1.15	1.23
5	L	92	GLN	C-O	-6.48	1.16	1.24
4	h	95	TYR	CA-C	-6.47	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	186	ASN	CA-C	6.46	1.60	1.52
5	L	25	ALA	N-CA	6.45	1.53	1.45
1	B	241	MET	SD-CE	-6.45	1.63	1.79
2	E	220	CYS	CA-C	6.44	1.60	1.52
5	l	30	ASN	C-N	6.44	1.39	1.33
5	L	150	VAL	C-O	6.43	1.30	1.24
5	L	41	GLY	CA-C	6.42	1.58	1.51
1	A	111	VAL	N-CA	-6.41	1.38	1.46
1	B	122	THR	C-O	6.39	1.31	1.24
2	E	48	ALA	CA-C	6.39	1.60	1.52
3	F	231	LYS	C-O	-6.39	1.15	1.24
1	B	31	ILE	C-O	6.38	1.30	1.24
5	L	53	ASN	CA-C	-6.38	1.45	1.52
5	l	158	ASN	C-O	-6.38	1.15	1.24
5	l	143	GLU	C-O	-6.37	1.16	1.23
1	A	126	TYR	CA-C	6.37	1.60	1.52
3	F	178	GLN	CA-C	-6.37	1.44	1.52
3	F	71	SER	CA-C	6.35	1.60	1.52
5	l	57	GLY	CA-C	-6.35	1.45	1.51
3	F	239	ASP	N-CA	-6.34	1.40	1.46
1	B	59	ALA	CA-C	6.34	1.60	1.53
5	L	194	CYS	N-CA	-6.33	1.38	1.46
5	l	196	VAL	CA-C	6.33	1.60	1.52
1	B	76	PHE	N-CA	-6.32	1.38	1.46
5	L	171	SER	C-O	-6.32	1.15	1.23
1	B	114	ASN	C-N	6.30	1.41	1.33
2	E	220	CYS	C-O	-6.30	1.16	1.24
1	B	204	THR	CA-C	6.30	1.60	1.52
5	L	211	ARG	C-O	-6.30	1.16	1.23
4	H	105	THR	C-O	-6.29	1.18	1.24
1	A	173	LYS	CA-C	6.28	1.60	1.52
2	E	53	HIS	C-O	-6.26	1.16	1.23
4	H	209	HIS	CE1-NE2	-6.26	1.26	1.32
1	B	139	HIS	CA-C	6.26	1.60	1.52
2	E	210	MET	CA-C	6.25	1.61	1.53
2	E	33	VAL	C-O	-6.25	1.17	1.24
1	A	191	GLU	CA-C	6.25	1.60	1.52
4	h	36	TRP	C-O	6.24	1.31	1.24
4	h	209	HIS	CA-C	6.24	1.61	1.53
4	h	89	ASP	N-CA	6.23	1.54	1.46
4	h	140	THR	C-O	-6.23	1.16	1.24
3	F	166	CYS	CA-C	6.23	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	153	ASP	N-CA	-6.22	1.38	1.46
2	E	83	LYS	N-CA	6.22	1.53	1.45
4	h	89	ASP	C-O	-6.21	1.15	1.24
5	l	205	VAL	C-O	6.21	1.31	1.24
2	E	197	ASP	CA-C	-6.20	1.46	1.52
1	A	153	MET	C-O	6.19	1.31	1.23
5	l	114	SER	N-CA	-6.19	1.38	1.46
1	B	52	HIS	CG-ND1	-6.17	1.31	1.38
1	A	67	PHE	CA-C	-6.16	1.45	1.52
5	L	97	THR	C-N	6.15	1.41	1.33
3	F	128	PHE	CA-C	-6.15	1.44	1.52
1	A	78	TYR	CA-C	6.14	1.59	1.53
5	L	135	LEU	C-O	-6.13	1.16	1.23
3	F	133	PHE	CA-C	6.13	1.60	1.53
1	B	120	ASN	C-N	6.13	1.39	1.33
1	A	127	PHE	CA-C	-6.13	1.45	1.52
1	B	155	GLY	CA-C	-6.12	1.45	1.52
5	l	208	SER	CA-C	-6.12	1.45	1.52
1	A	71	PHE	CA-C	6.12	1.60	1.52
2	E	53	HIS	CD2-NE2	6.12	1.44	1.37
1	B	67	PHE	C-O	6.12	1.31	1.23
4	H	187	LEU	N-CA	-6.11	1.39	1.46
5	L	211	ARG	CA-C	6.11	1.60	1.52
1	A	194	MET	C-O	-6.10	1.18	1.24
2	E	174	GLN	N-CA	6.10	1.53	1.45
2	E	61	GLU	N-CA	6.10	1.54	1.46
5	l	17	ASP	CA-C	6.09	1.62	1.53
3	F	87	ASP	N-CA	-6.09	1.38	1.46
1	B	113	HIS	N-CA	-6.09	1.38	1.46
1	B	147	SER	N-CA	-6.08	1.38	1.45
4	H	79	ALA	N-CA	-6.08	1.38	1.46
1	A	32	VAL	C-O	6.08	1.30	1.24
2	E	72	LEU	C-O	-6.08	1.16	1.23
1	B	131	ARG	C-N	6.08	1.41	1.33
1	B	135	GLU	C-N	6.07	1.41	1.33
5	L	49	TYR	CA-C	6.07	1.59	1.52
4	h	40	ARG	CA-C	-6.06	1.44	1.53
4	H	91	THR	C-N	6.04	1.41	1.33
4	H	145	ALA	C-O	-6.03	1.16	1.24
5	L	213	GLU	C-N	6.03	1.41	1.33
5	l	138	ASN	CA-C	-6.02	1.45	1.53
5	L	39	LYS	CA-C	-6.00	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	l	93	THR	C-O	6.00	1.30	1.23
2	E	166	CYS	C-O	-6.00	1.16	1.23
4	h	204	ILE	CA-C	6.00	1.59	1.52
1	B	113	HIS	CG-CD2	-5.98	1.29	1.35
1	A	107	SER	CA-C	5.98	1.59	1.52
5	l	55	HIS	N-CA	-5.98	1.38	1.46
1	B	214	VAL	CA-C	5.98	1.59	1.52
4	H	77	SER	C-O	-5.98	1.17	1.24
5	L	189	HIS	CE1-NE2	-5.97	1.26	1.32
5	l	74	THR	CA-C	-5.97	1.45	1.52
3	F	91	ALA	CA-C	-5.97	1.46	1.52
4	h	106	PRO	C-O	5.97	1.31	1.24
4	h	167	ALA	N-CA	5.96	1.53	1.46
4	h	66	ASN	C-N	5.96	1.41	1.33
1	A	93	ARG	CA-C	-5.95	1.46	1.52
1	A	182	TYR	CA-C	-5.95	1.45	1.53
3	F	49	ASP	N-CA	-5.94	1.39	1.46
3	F	237	ILE	C-O	5.94	1.30	1.23
5	L	55	HIS	CD2-NE2	5.94	1.44	1.37
1	A	239	SER	C-O	-5.93	1.16	1.24
1	B	133	TYR	CA-C	-5.93	1.45	1.52
1	A	180	ASP	CA-C	5.93	1.60	1.53
4	H	134	ALA	N-CA	5.93	1.55	1.45
2	E	226	LEU	CA-C	-5.92	1.45	1.52
2	E	114	HIS	CE1-NE2	-5.92	1.26	1.32
4	H	189	SER	CA-C	5.92	1.59	1.52
3	F	134	TYR	CA-CB	5.91	1.61	1.53
3	F	232	THR	C-N	5.91	1.40	1.33
4	H	183	GLY	CA-C	-5.91	1.45	1.51
5	l	140	TYR	C-O	5.91	1.30	1.24
2	E	76	VAL	C-N	5.91	1.40	1.33
5	L	189	HIS	CD2-NE2	5.90	1.44	1.37
5	l	179	LEU	CA-C	5.89	1.59	1.52
1	A	222	ASN	C-O	-5.89	1.17	1.23
2	E	139	VAL	CA-C	5.89	1.59	1.52
4	H	98	ARG	C-O	5.89	1.30	1.23
4	h	73	ASP	N-CA	5.89	1.53	1.46
2	E	91	ALA	N-CA	-5.88	1.41	1.46
5	l	37	GLN	CA-C	-5.88	1.45	1.52
4	H	215	LYS	N-CA	-5.88	1.39	1.46
2	E	146	LEU	CA-C	5.87	1.59	1.52
3	F	96	ARG	CA-C	-5.87	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	h	48	ILE	CA-C	5.86	1.59	1.52
1	A	213	SER	CA-C	5.86	1.61	1.52
1	B	146	GLY	N-CA	5.86	1.51	1.45
5	L	76	SER	C-N	5.86	1.41	1.33
5	l	46	LEU	C-O	-5.86	1.16	1.23
5	L	192	TYR	N-CA	5.86	1.52	1.45
1	A	190	LYS	N-CA	-5.85	1.39	1.46
4	h	99	GLU	CA-C	5.85	1.60	1.52
4	h	172	VAL	CA-C	5.85	1.59	1.52
5	L	90	GLN	C-N	5.84	1.42	1.33
4	h	202	THR	CA-C	5.84	1.59	1.52
5	L	71	PHE	CA-C	-5.83	1.45	1.52
1	B	161	ILE	C-N	5.83	1.41	1.33
5	l	206	THR	CA-C	-5.83	1.45	1.52
1	B	129	GLU	CA-C	-5.82	1.45	1.52
3	F	225	SER	N-CA	5.82	1.53	1.46
2	E	195	VAL	N-CA	-5.82	1.39	1.46
4	h	27	TYR	C-N	5.82	1.41	1.33
4	h	95	TYR	C-O	5.82	1.31	1.24
2	E	147	GLY	N-CA	5.81	1.51	1.45
4	H	147	LEU	CB-CG	5.81	1.65	1.53
3	F	34	LEU	N-CA	-5.81	1.38	1.45
5	L	150	VAL	CA-C	5.81	1.59	1.52
1	B	124	ARG	C-N	5.81	1.41	1.33
1	A	162	ARG	C-N	5.80	1.41	1.33
5	L	63	SER	CA-C	-5.80	1.45	1.52
5	L	69	THR	N-CA	5.80	1.54	1.46
4	h	178	VAL	CA-C	5.78	1.59	1.52
4	H	116	THR	N-CA	5.78	1.53	1.46
1	A	141	VAL	C-O	-5.78	1.17	1.24
3	F	101	ARG	C-O	5.78	1.30	1.23
1	B	72	SER	N-CA	-5.77	1.41	1.46
4	h	99	GLU	C-O	-5.77	1.16	1.23
2	E	124	TYR	C-N	5.77	1.41	1.33
5	L	158	ASN	C-O	-5.77	1.16	1.24
5	L	107	LYS	CA-C	5.77	1.59	1.52
4	H	204	ILE	N-CA	-5.76	1.39	1.46
4	H	101	ASP	N-CA	-5.75	1.39	1.46
4	h	164	ASN	C-N	5.75	1.41	1.33
1	A	97	THR	CA-C	-5.74	1.45	1.52
1	A	234	ILE	CA-C	5.72	1.58	1.52
2	E	76	VAL	C-O	-5.72	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	TYR	CA-CB	-5.72	1.45	1.52
5	L	178	THR	CA-C	-5.71	1.45	1.52
3	F	97	THR	N-CA	-5.71	1.39	1.46
4	h	2	VAL	C-O	-5.71	1.17	1.24
1	B	217	MET	CA-CB	5.70	1.62	1.53
2	E	125	LEU	C-N	-5.70	1.26	1.33
4	h	195	SER	N-CA	-5.70	1.38	1.46
5	L	65	SER	CA-C	5.70	1.59	1.52
1	B	53	LEU	C-O	-5.70	1.16	1.23
2	E	116	VAL	C-O	-5.69	1.17	1.24
1	A	86	GLU	CA-C	5.69	1.60	1.52
4	H	26	GLY	C-N	5.69	1.40	1.33
1	B	83	GLU	N-CA	-5.68	1.39	1.46
4	h	187	LEU	C-O	5.68	1.30	1.23
5	l	31	VAL	C-O	-5.68	1.16	1.23
5	l	180	THR	N-CA	5.68	1.52	1.46
4	H	149	CYS	CA-C	5.68	1.59	1.52
4	H	108	ALA	N-CA	-5.67	1.39	1.46
1	A	127	PHE	N-CA	5.67	1.53	1.46
4	h	33	TYR	N-CA	5.67	1.53	1.45
5	L	29	ILE	CA-C	5.66	1.59	1.52
2	E	66	LYS	N-CA	-5.65	1.39	1.46
4	h	109	MET	SD-CE	-5.65	1.65	1.79
5	L	160	GLN	C-O	5.65	1.30	1.23
3	F	108	LYS	C-O	5.65	1.29	1.23
5	l	51	ALA	C-O	-5.64	1.16	1.24
1	A	120	ASN	CA-C	-5.64	1.45	1.52
2	E	154	VAL	C-N	5.64	1.41	1.33
3	F	204	VAL	CA-C	-5.64	1.45	1.52
2	E	119	SER	N-CA	5.63	1.53	1.46
5	L	9	SER	N-CA	5.62	1.53	1.46
5	L	58	VAL	CA-C	5.61	1.58	1.52
1	A	233	VAL	N-CA	5.61	1.52	1.46
4	h	203	TYR	C-N	5.61	1.40	1.33
1	A	113	HIS	ND1-CE1	5.60	1.38	1.32
5	L	193	ALA	C-N	5.59	1.40	1.33
2	E	64	GLU	C-O	-5.59	1.17	1.23
2	E	128	PHE	C-O	5.59	1.30	1.24
5	L	155	GLN	CA-C	-5.59	1.45	1.52
2	E	240	PRO	N-CA	-5.58	1.40	1.47
4	H	23	LYS	CA-C	-5.58	1.46	1.52
1	B	51	CYS	C-N	-5.58	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	l	143	GLU	CA-C	5.58	1.59	1.53
5	L	123	GLU	C-O	5.57	1.31	1.24
2	E	64	GLU	C-N	5.57	1.40	1.33
1	A	223	ASN	N-CA	-5.56	1.38	1.46
2	E	153	GLU	CA-C	-5.56	1.45	1.52
4	h	207	VAL	CA-C	5.56	1.59	1.52
1	B	139	HIS	ND1-CE1	5.56	1.38	1.32
3	F	186	ASN	N-CA	-5.56	1.39	1.46
4	h	56	GLY	C-O	-5.55	1.17	1.23
4	H	106	PRO	C-O	5.55	1.28	1.24
1	B	67	PHE	C-N	5.55	1.41	1.33
5	l	7	SER	CA-C	5.55	1.59	1.52
5	l	72	THR	C-O	-5.54	1.17	1.24
5	l	173	TYR	CA-C	-5.54	1.45	1.53
2	E	178	GLN	N-CA	-5.54	1.39	1.46
1	A	127	PHE	C-O	5.54	1.30	1.24
2	E	166	CYS	N-CA	-5.53	1.39	1.46
1	B	238	GLU	CA-C	-5.52	1.45	1.52
4	h	28	ILE	CA-CB	5.52	1.60	1.54
4	H	162	SER	N-CA	-5.52	1.39	1.46
1	A	101	LYS	CA-C	5.50	1.59	1.52
5	L	160	GLN	CA-C	5.50	1.59	1.53
1	A	158	ASP	N-CA	5.50	1.54	1.46
1	B	231	GLU	CA-C	5.50	1.59	1.52
1	B	67	PHE	N-CA	-5.49	1.39	1.45
4	h	200	THR	C-N	5.49	1.41	1.33
3	F	201	LEU	C-N	5.49	1.40	1.33
3	F	229	LEU	C-N	5.49	1.40	1.33
2	E	31	PHE	C-O	-5.49	1.18	1.24
4	h	45	LEU	CA-C	-5.48	1.45	1.53
5	l	168	SER	C-N	5.48	1.40	1.33
5	L	10	SER	C-N	-5.48	1.26	1.33
1	A	139	HIS	ND1-CE1	5.48	1.38	1.32
5	l	48	ILE	C-O	5.48	1.29	1.24
1	A	225	LEU	C-O	-5.47	1.17	1.24
4	H	13	LYS	CA-C	-5.47	1.46	1.52
5	L	73	PHE	C-O	5.47	1.31	1.23
1	A	110	LEU	CA-C	-5.47	1.46	1.52
5	l	24	HIS	CG-CD2	-5.47	1.29	1.35
5	L	128	GLY	CA-C	-5.46	1.45	1.51
3	F	105	THR	CA-C	5.46	1.59	1.52
4	h	21	SER	C-N	5.46	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	94	TYR	CA-C	5.46	1.59	1.52
5	l	82	ASP	C-N	5.46	1.40	1.33
4	H	209	HIS	CD2-NE2	5.45	1.43	1.37
5	l	150	VAL	CA-C	5.45	1.58	1.53
1	A	66	TRP	N-CA	-5.45	1.39	1.46
2	E	59	SER	CA-C	5.44	1.59	1.52
5	L	125	LEU	CA-C	-5.44	1.45	1.52
5	L	187	GLU	N-CA	-5.44	1.39	1.46
5	L	32	TRP	C-O	-5.43	1.17	1.24
5	L	98	PHE	N-CA	-5.43	1.39	1.45
4	H	135	PRO	C-N	5.43	1.41	1.33
3	F	51	PRO	C-O	-5.42	1.17	1.24
4	h	116	THR	C-O	-5.42	1.17	1.24
1	B	235	PHE	C-N	5.42	1.38	1.33
4	h	204	ILE	N-CA	-5.42	1.39	1.46
2	E	43	MET	SD-CE	5.42	1.93	1.79
5	L	161	GLU	CA-C	5.42	1.60	1.53
5	l	28	ASN	C-O	5.41	1.30	1.24
5	l	108	ARG	CA-C	-5.41	1.46	1.52
4	h	219	LYS	N-CA	-5.41	1.39	1.46
5	L	79	GLN	C-O	5.41	1.29	1.23
5	l	82	ASP	CA-C	-5.41	1.46	1.52
1	B	126	TYR	C-O	-5.40	1.17	1.23
1	A	193	SER	CA-C	-5.40	1.46	1.52
2	E	128	PHE	N-CA	5.40	1.52	1.46
4	H	49	GLY	CA-C	-5.40	1.46	1.51
4	h	198	LEU	N-CA	5.40	1.52	1.45
2	E	41	LEU	N-CA	-5.39	1.39	1.46
5	L	137	ASN	C-N	5.39	1.40	1.33
4	H	136	SER	C-O	5.39	1.31	1.23
1	A	144	GLY	C-N	5.39	1.40	1.33
5	L	187	GLU	C-O	-5.39	1.16	1.24
5	l	20	THR	N-CA	-5.39	1.39	1.45
1	A	230	LYS	CA-C	-5.38	1.46	1.52
2	E	78	VAL	C-O	-5.38	1.18	1.24
3	F	100	LEU	C-O	5.38	1.30	1.23
4	h	28	ILE	C-N	5.38	1.39	1.33
1	B	29	GLN	CA-C	5.38	1.64	1.52
3	F	51	PRO	CA-C	-5.38	1.44	1.52
5	L	55	HIS	CA-C	5.38	1.60	1.53
4	h	38	LYS	CA-C	5.38	1.59	1.52
5	L	213	GLU	N-CA	5.37	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	167	ALA	C-O	5.37	1.30	1.24
1	B	191	GLU	CA-C	5.36	1.58	1.52
4	H	110	ASP	C-O	5.36	1.30	1.24
1	A	231	GLU	C-N	5.36	1.40	1.33
3	F	181	ASN	N-CA	-5.36	1.38	1.46
1	A	103	ILE	N-CA	-5.35	1.40	1.46
1	A	167	SER	C-O	5.35	1.30	1.23
1	B	182	TYR	N-CA	5.35	1.53	1.46
4	H	96	CYS	C-N	-5.35	1.26	1.33
1	A	221	ILE	C-O	-5.34	1.17	1.24
5	L	22	THR	C-O	-5.33	1.17	1.23
1	B	234	ILE	CA-C	5.32	1.59	1.52
2	E	78	VAL	CA-C	5.31	1.59	1.52
2	E	221	ILE	N-CA	-5.31	1.40	1.46
4	h	192	THR	CA-C	-5.30	1.46	1.52
5	l	46	LEU	C-N	5.30	1.41	1.33
1	B	188	ALA	N-CA	-5.30	1.39	1.46
1	A	212	LYS	CA-C	-5.29	1.45	1.52
4	h	17	SER	C-N	-5.29	1.27	1.33
1	A	115	ILE	CA-CB	5.29	1.61	1.54
4	h	18	VAL	CA-C	5.29	1.58	1.52
1	B	186	ALA	C-N	5.28	1.40	1.33
2	E	97	THR	N-CA	5.28	1.52	1.46
4	h	190	VAL	CA-C	5.28	1.58	1.52
1	A	114	ASN	C-N	5.28	1.40	1.33
4	h	96	CYS	CA-C	5.27	1.59	1.52
5	l	54	LEU	C-N	5.27	1.40	1.33
3	F	52	CYS	C-O	5.27	1.30	1.23
4	H	172	VAL	C-O	-5.27	1.17	1.24
5	L	164	THR	CA-C	-5.26	1.46	1.52
5	L	87	TYR	C-N	5.26	1.40	1.33
5	L	55	HIS	CE1-NE2	-5.26	1.27	1.32
4	H	28	ILE	C-O	-5.26	1.18	1.24
5	L	209	PHE	C-N	-5.26	1.26	1.33
2	E	68	VAL	N-CA	-5.25	1.40	1.46
5	L	117	ILE	CA-C	-5.25	1.45	1.52
2	E	155	LYS	CA-C	5.25	1.60	1.52
5	L	175	LEU	C-O	5.25	1.30	1.23
5	l	188	LYS	C-N	5.25	1.41	1.33
5	l	159	SER	CA-C	-5.25	1.46	1.52
2	E	222	ILE	C-N	5.25	1.40	1.33
3	F	35	GLY	C-O	-5.24	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	18	VAL	C-O	-5.24	1.18	1.23
4	H	201	GLN	CA-C	-5.24	1.46	1.52
5	l	51	ALA	N-CA	-5.24	1.39	1.46
5	L	182	SER	CA-C	-5.24	1.46	1.53
4	h	207	VAL	N-CA	5.24	1.52	1.46
1	A	65	ARG	CA-C	5.24	1.59	1.52
4	H	163	TRP	C-N	-5.24	1.26	1.33
4	h	86	LEU	CB-CG	-5.23	1.43	1.53
1	B	153	MET	SD-CE	5.23	1.92	1.79
1	B	178	TRP	N-CA	5.23	1.52	1.46
2	E	157	TYR	CA-C	5.23	1.59	1.53
5	L	46	LEU	C-O	-5.23	1.17	1.23
1	B	79	LYS	N-CA	-5.23	1.39	1.46
1	A	77	VAL	C-O	5.22	1.29	1.24
1	B	99	VAL	N-CA	-5.22	1.39	1.46
2	E	195	VAL	C-O	5.22	1.29	1.24
4	h	77	SER	C-N	5.22	1.40	1.33
1	A	161	ILE	N-CA	-5.22	1.39	1.46
1	B	39	ILE	C-N	5.22	1.40	1.33
3	F	177	ILE	CA-C	5.22	1.58	1.52
5	L	31	VAL	C-O	-5.22	1.17	1.24
4	h	181	SER	N-CA	-5.21	1.40	1.46
5	l	111	ALA	C-O	5.21	1.30	1.23
4	h	157	GLU	CA-C	5.21	1.58	1.53
3	F	41	LEU	C-O	5.21	1.30	1.23
4	h	176	PRO	C-N	-5.21	1.26	1.33
1	B	76	PHE	CA-C	-5.21	1.46	1.52
4	h	42	GLY	C-N	5.21	1.40	1.33
4	H	124	SER	N-CA	-5.20	1.39	1.45
2	E	41	LEU	CB-CG	5.20	1.63	1.53
1	A	132	SER	C-O	5.20	1.29	1.23
1	B	46	ASN	CA-CB	5.20	1.61	1.53
4	h	11	VAL	CA-C	5.19	1.59	1.52
1	A	122	THR	CA-C	5.19	1.59	1.53
5	l	1	ASP	C-N	-5.19	1.26	1.33
5	l	148	TRP	C-O	5.18	1.30	1.23
4	H	187	LEU	CB-CG	5.18	1.63	1.53
3	F	120	ASP	C-O	5.18	1.31	1.24
1	B	122	THR	CB-OG1	-5.18	1.35	1.43
1	B	47	THR	C-N	5.17	1.41	1.33
1	A	105	ARG	CA-C	-5.17	1.46	1.52
2	E	58	MET	C-N	5.17	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	154	TYR	CA-C	5.17	1.59	1.52
4	h	185	TYR	C-O	5.17	1.30	1.23
5	l	152	ASN	CG-ND2	-5.17	1.22	1.33
4	H	65	LYS	N-CA	5.16	1.52	1.46
5	l	78	LEU	CA-C	5.16	1.59	1.53
1	B	200	LEU	C-N	5.16	1.40	1.33
3	F	230	GLU	N-CA	-5.16	1.39	1.45
5	l	43	ALA	CA-C	5.16	1.59	1.53
2	E	209	ILE	C-O	5.15	1.30	1.23
3	F	230	GLU	C-O	-5.15	1.17	1.23
3	F	240	PRO	C-O	-5.15	1.18	1.23
4	h	108	ALA	C-N	5.15	1.40	1.33
4	H	141	SER	CA-C	5.14	1.59	1.52
5	l	75	ILE	C-O	-5.14	1.18	1.24
4	h	67	ARG	CA-C	-5.14	1.44	1.52
5	l	35	TRP	C-O	-5.14	1.17	1.24
1	A	55	PRO	C-N	5.13	1.40	1.33
4	H	146	ALA	C-O	-5.13	1.17	1.24
4	h	37	VAL	N-CA	5.13	1.52	1.46
5	L	73	PHE	CA-C	-5.13	1.46	1.52
5	l	125	LEU	C-O	5.13	1.30	1.23
3	F	165	GLU	N-CA	5.13	1.52	1.46
5	L	96	TYR	C-O	5.13	1.30	1.23
5	l	201	LEU	CB-CG	5.12	1.63	1.53
4	h	144	THR	N-CA	-5.12	1.39	1.46
3	F	214	SER	C-N	-5.12	1.27	1.33
5	L	162	SER	C-O	-5.11	1.17	1.23
5	l	56	THR	N-CA	-5.11	1.39	1.45
1	A	128	GLN	CA-C	5.11	1.58	1.52
3	F	78	VAL	C-O	-5.11	1.18	1.24
3	F	210	MET	C-O	-5.11	1.18	1.24
2	E	56	PRO	C-O	5.11	1.27	1.24
5	L	136	LEU	C-N	-5.11	1.26	1.33
2	E	88	ARG	N-CA	5.10	1.52	1.46
2	E	149	ASN	CA-C	5.10	1.59	1.52
5	l	152	ASN	CG-OD1	5.09	1.33	1.23
1	A	86	GLU	C-O	-5.09	1.17	1.24
5	L	97	THR	C-O	-5.09	1.17	1.23
1	A	116	THR	CA-C	5.09	1.59	1.52
2	E	76	VAL	CA-C	5.09	1.59	1.52
4	h	139	SER	N-CA	-5.08	1.39	1.46
1	A	207	VAL	N-CA	5.08	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	77	ASN	CA-C	5.08	1.58	1.52
5	l	37	GLN	C-O	-5.08	1.17	1.23
2	E	88	ARG	CA-C	-5.08	1.46	1.52
1	A	185	VAL	CA-C	5.07	1.59	1.52
4	H	71	THR	CA-C	-5.07	1.46	1.52
4	h	173	HIS	ND1-CE1	5.07	1.37	1.32
5	l	92	GLN	C-O	5.07	1.30	1.24
1	A	31	ILE	C-N	-5.07	1.26	1.33
5	L	114	SER	C-O	5.07	1.30	1.24
4	H	114	GLN	CD-NE2	5.06	1.43	1.33
4	h	81	MET	N-CA	5.06	1.52	1.46
2	E	135	GLU	CA-C	-5.06	1.46	1.52
4	H	173	HIS	CA-CB	-5.06	1.46	1.52
5	L	177	SER	CA-C	-5.06	1.46	1.52
4	h	64	PHE	N-CA	5.06	1.52	1.46
1	A	241	MET	C-O	-5.05	1.17	1.24
3	F	123	LYS	N-CA	5.05	1.52	1.45
4	H	86	LEU	CB-CG	5.05	1.63	1.53
3	F	94	ARG	CA-C	-5.05	1.46	1.52
5	l	93	THR	CB-OG1	-5.05	1.35	1.43
5	l	188	LYS	C-O	-5.05	1.17	1.24
4	H	186	SER	N-CA	5.05	1.52	1.45
1	B	218	SER	C-N	5.05	1.40	1.33
3	F	235	ILE	C-N	5.05	1.40	1.33
5	l	160	GLN	CA-C	-5.04	1.46	1.52
1	A	61	ASP	CA-C	5.04	1.59	1.52
5	l	208	SER	C-N	5.04	1.40	1.33
1	A	60	GLU	N-CA	5.04	1.52	1.46
1	B	229	LYS	C-N	-5.03	1.26	1.33
4	h	200	THR	C-O	-5.03	1.18	1.24
4	h	209	HIS	ND1-CE1	5.03	1.37	1.32
5	l	14	SER	N-CA	-5.03	1.39	1.45
2	E	183	LYS	C-O	-5.02	1.17	1.24
4	h	34	MET	CA-C	-5.02	1.46	1.52
2	E	143	VAL	N-CA	-5.02	1.40	1.46
5	L	119	PRO	CA-C	5.02	1.56	1.52
1	A	34	GLY	N-CA	5.02	1.51	1.44
4	h	215	LYS	CA-C	5.01	1.58	1.52
5	L	198	HIS	ND1-CE1	5.01	1.37	1.32
5	L	38	GLN	CA-C	-5.01	1.46	1.52
1	A	179	ARG	N-CA	5.01	1.52	1.46
5	L	145	LYS	CG-CD	-5.01	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ASP	CA-C	-5.01	1.46	1.52
1	B	221	ILE	C-O	-5.01	1.18	1.24
3	F	43	MET	SD-CE	5.01	1.92	1.79
4	H	45	LEU	CA-C	-5.01	1.46	1.52
2	E	129	GLN	C-O	-5.00	1.18	1.23
3	F	210	MET	CA-C	5.00	1.59	1.52
4	H	50	GLU	CA-C	5.00	1.58	1.52

All (436) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ILE	N-CA-C	16.31	122.41	107.56
5	L	50	LYS	N-CA-C	-11.60	99.07	113.23
2	E	181	ASN	OD1-CG-ND2	-10.54	112.06	122.60
4	H	137	SER	N-CA-C	-10.19	100.92	113.97
2	E	176	GLN	OE1-CD-NE2	-9.95	112.66	122.60
5	L	89	GLN	OE1-CD-NE2	-9.60	113.00	122.60
1	A	222	ASN	OD1-CG-ND2	-9.56	113.04	122.60
2	E	129	GLN	OE1-CD-NE2	-9.45	113.16	122.60
1	A	105	ARG	N-CA-C	9.29	121.41	111.28
2	E	181	ASN	CA-CB-CG	9.17	121.77	112.60
3	F	130	ASP	CA-CB-CG	9.16	121.76	112.60
1	B	223	ASN	CA-CB-CG	9.10	121.69	112.60
5	L	167	ASP	CA-CB-CG	9.05	121.65	112.60
2	E	130	ASP	CA-CB-CG	8.99	121.59	112.60
1	B	46	ASN	N-CA-C	8.99	122.20	110.43
4	h	107	PHE	CA-CB-CG	8.99	122.79	113.80
2	E	221	ILE	N-CA-C	8.78	120.40	108.11
5	l	30	ASN	CA-C-N	-8.73	113.44	121.65
5	l	30	ASN	C-N-CA	-8.73	113.44	121.65
4	H	73	ASP	CA-CB-CG	8.72	121.32	112.60
5	l	28	ASN	CA-CB-CG	8.66	121.26	112.60
3	F	89	GLN	OE1-CD-NE2	-8.64	113.96	122.60
3	F	94	ARG	N-CA-C	8.60	122.89	110.24
1	B	131	ARG	N-CA-C	8.60	121.79	111.82
4	h	164	ASN	OD1-CG-ND2	8.58	131.18	122.60
3	F	105	THR	CA-C-O	-8.55	111.89	120.70
5	L	210	ASN	OD1-CG-ND2	-8.55	114.05	122.60
5	l	92	GLN	CA-C-O	-8.39	110.93	120.24
4	h	52	ASN	CA-C-O	8.34	125.88	119.46
3	F	159	ASP	CA-CB-CG	8.32	120.92	112.60
4	h	55	ASN	CA-C-N	8.28	130.73	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	55	ASN	C-N-CA	8.28	130.73	120.22
1	A	124	ARG	N-CA-C	8.18	122.57	109.24
1	B	114	ASN	CA-CB-CG	8.16	120.76	112.60
1	A	71	PHE	CA-CB-CG	-8.16	105.64	113.80
1	B	162	ARG	N-CA-C	8.11	122.12	109.96
5	L	137	ASN	OD1-CG-ND2	-8.10	114.50	122.60
3	F	47	ASP	CA-CB-CG	8.09	120.69	112.60
2	E	158	GLU	CB-CG-CD	8.09	126.34	112.60
1	B	61	ASP	CA-CB-CG	7.95	120.55	112.60
1	A	180	ASP	CA-C-O	-7.94	112.46	120.64
2	E	85	VAL	N-CA-C	7.93	120.08	109.37
4	H	48	ILE	CA-C-O	-7.91	112.39	120.69
1	A	235	PHE	CA-C-O	-7.88	111.79	120.38
1	B	63	GLU	N-CA-C	7.86	122.06	109.24
1	A	62	MET	N-CA-C	7.84	120.43	110.24
5	L	90	GLN	OE1-CD-NE2	-7.83	114.77	122.60
5	L	54	LEU	N-CA-C	7.82	122.56	110.20
3	F	129	GLN	CA-C-O	-7.79	112.46	120.71
1	A	124	ARG	CA-C-O	-7.73	112.00	120.43
5	l	62	PHE	CA-CB-CG	7.72	121.52	113.80
1	A	68	ARG	CA-C-O	-7.72	112.26	121.60
5	l	31	VAL	N-CA-CB	-7.71	104.58	112.28
5	l	189	HIS	CE1-NE2-CD2	-7.69	101.31	109.00
5	l	6	GLN	OE1-CD-NE2	-7.68	114.92	122.60
3	F	163	HIS	CE1-NE2-CD2	-7.64	101.36	109.00
1	A	153	MET	CA-C-O	-7.61	112.30	121.28
1	A	171	TYR	N-CA-C	-7.59	101.32	108.07
1	A	76	PHE	CA-C-O	-7.55	113.23	121.31
5	l	189	HIS	ND1-CE1-NE2	7.53	115.93	108.40
2	E	153	GLU	CB-CG-CD	7.51	125.37	112.60
3	F	114	HIS	CE1-NE2-CD2	-7.51	101.49	109.00
5	l	158	ASN	CA-C-O	7.35	127.16	119.51
5	L	30	ASN	CA-C-O	-7.25	113.18	120.80
4	H	5	VAL	N-CA-C	7.25	119.52	108.71
5	l	116	PHE	CA-CB-CG	7.23	121.03	113.80
1	B	85	THR	N-CA-C	-7.21	104.48	113.28
5	l	38	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	B	196	ASP	N-CA-C	7.16	120.23	110.35
5	l	24	HIS	CE1-NE2-CD2	-7.16	101.84	109.00
2	E	203	GLU	N-CA-C	7.09	120.45	108.90
2	E	158	GLU	N-CA-C	7.07	118.98	111.28
2	E	178	GLN	CG-CD-NE2	7.05	126.98	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	77	ASN	OD1-CG-ND2	-7.05	115.55	122.60
5	L	173	TYR	N-CA-C	7.05	119.84	110.53
1	A	228	GLN	N-CA-C	7.05	119.88	109.24
5	l	116	PHE	CA-C-O	-7.05	113.72	121.33
2	E	236	SER	N-CA-C	7.01	119.83	109.24
1	B	236	ILE	N-CA-CB	-7.01	103.42	111.20
5	L	203	SER	O-C-N	7.01	127.80	121.35
1	A	120	ASN	N-CA-C	7.00	120.53	110.24
3	F	90	SER	CA-C-O	-6.99	113.47	121.72
5	L	117	ILE	N-CA-C	6.98	118.45	109.30
2	E	34	LEU	N-CA-C	6.92	121.59	109.96
2	E	77	ASN	CA-CB-CG	6.90	119.50	112.60
3	F	49	ASP	N-CA-C	-6.86	103.21	112.26
1	A	234	ILE	CA-C-N	-6.84	113.56	123.00
1	A	234	ILE	C-N-CA	-6.84	113.56	123.00
3	F	185	GLU	N-CA-C	-6.83	99.23	108.86
4	H	114	GLN	N-CA-C	6.83	119.59	111.33
3	F	130	ASP	CA-C-O	-6.80	112.33	120.56
3	F	94	ARG	CA-C-O	-6.78	113.56	120.96
1	B	83	GLU	N-CA-C	-6.78	100.25	110.28
2	E	125	LEU	CA-C-O	-6.76	113.48	121.11
1	B	102	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	95	ARG	N-CA-C	-6.72	102.56	113.19
3	F	114	HIS	ND1-CE1-NE2	6.70	115.10	108.40
5	L	192	TYR	N-CA-C	6.70	120.95	110.17
4	H	52	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	88	GLN	OE1-CD-NE2	-6.66	115.94	122.60
3	F	66	LYS	N-CA-C	-6.66	99.36	109.95
4	H	131	PHE	CA-CB-CG	-6.66	107.14	113.80
5	L	161	GLU	N-CA-C	-6.65	101.57	110.55
3	F	77	ASN	CB-CG-ND2	6.64	126.36	116.40
4	H	81	MET	N-CA-C	6.61	119.71	109.07
4	H	107	PHE	CA-C-O	-6.60	111.09	118.69
1	B	72	SER	N-CA-C	6.60	121.73	112.75
3	F	102	ASP	CA-CB-CG	6.59	119.19	112.60
3	F	163	HIS	ND1-CE1-NE2	6.59	114.99	108.40
5	l	34	SER	CA-C-O	-6.58	111.09	120.11
4	h	98	ARG	CA-C-O	-6.57	113.76	121.44
2	E	55	PHE	N-CA-C	6.53	121.64	112.75
4	h	209	HIS	CA-CB-CG	6.53	120.33	113.80
5	L	181	LEU	N-CA-C	6.53	118.07	108.86
3	F	79	TYR	N-CA-C	6.52	118.69	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	CA-CB-CG	6.48	119.08	112.60
3	F	109	ALA	N-CA-C	-6.48	99.18	109.23
1	A	67	PHE	N-CA-C	6.48	119.96	109.40
4	H	172	VAL	N-CA-C	6.48	118.02	109.21
5	L	49	TYR	N-CA-C	-6.44	99.32	109.50
1	B	37	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	114	ASN	OD1-CG-ND2	-6.43	116.17	122.60
4	H	50	GLU	N-CA-C	-6.42	98.93	109.40
4	h	39	GLN	OE1-CD-NE2	-6.39	116.21	122.60
3	F	238	ALA	CA-C-O	-6.37	114.44	121.89
5	L	184	ALA	N-CA-C	-6.35	104.41	111.71
4	h	45	LEU	CA-C-O	6.32	129.20	121.99
1	A	37	ASP	CA-CB-CG	6.32	118.92	112.60
3	F	181	ASN	OD1-CG-ND2	6.31	128.91	122.60
3	F	132	ASP	CA-C-O	-6.31	111.66	118.79
4	h	62	GLU	CA-C-O	-6.27	113.90	120.92
3	F	61	GLU	CB-CG-CD	6.26	123.25	112.60
5	l	1	ASP	CA-CB-CG	6.26	118.86	112.60
4	H	47	TRP	CA-C-N	-6.26	115.18	122.63
4	H	47	TRP	C-N-CA	-6.26	115.18	122.63
2	E	181	ASN	CB-CG-ND2	6.25	125.77	116.40
3	F	129	GLN	N-CA-C	-6.25	99.53	109.59
1	A	222	ASN	N-CA-C	6.23	119.70	108.48
4	h	73	ASP	N-CA-C	6.22	118.86	108.96
1	B	140	LEU	N-CA-C	6.21	119.02	108.90
2	E	178	GLN	CA-C-O	-6.20	114.59	121.23
3	F	150	LEU	N-CA-C	6.19	119.21	110.23
1	A	110	LEU	O-C-N	-6.19	115.83	123.44
5	l	92	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	182	TYR	N-CA-C	6.19	121.34	111.81
4	h	217	ASP	N-CA-C	6.19	118.78	108.20
5	l	196	VAL	N-CA-C	-6.18	99.25	108.46
5	L	135	LEU	N-CA-C	6.17	119.95	110.20
5	l	105	GLU	CA-C-O	-6.15	114.16	121.60
2	E	102	ASP	CA-CB-CG	6.14	118.74	112.60
3	F	138	LEU	N-CA-C	6.14	119.56	110.48
3	F	211	ARG	CA-C-O	-6.13	113.94	121.67
1	B	194	MET	O-C-N	6.13	128.38	121.94
1	B	66	TRP	N-CA-C	6.12	119.63	109.46
3	F	167	ARG	O-C-N	-6.12	116.27	123.25
5	l	24	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	A	160	GLY	CA-C-O	-6.09	115.05	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	GLU	CA-C-O	-6.07	113.69	120.66
2	E	208	VAL	N-CA-C	6.04	116.21	107.88
5	L	160	GLN	CB-CG-CD	-6.04	102.34	112.60
2	E	242	PHE	N-CA-C	-6.03	105.23	112.59
2	E	236	SER	CA-C-N	-6.01	114.85	123.03
2	E	236	SER	C-N-CA	-6.01	114.85	123.03
4	H	152	LYS	CG-CD-CE	6.01	125.13	111.30
1	A	46	ASN	OD1-CG-ND2	-6.01	116.59	122.60
4	H	186	SER	O-C-N	-6.01	116.40	123.25
3	F	47	ASP	N-CA-C	6.00	118.93	110.23
5	L	122	ASP	CA-C-O	-5.97	114.55	120.70
1	A	113	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
1	B	87	GLU	N-CA-C	5.96	117.59	110.44
1	A	180	ASP	O-C-N	5.95	129.20	121.64
1	B	107	SER	N-CA-C	5.95	118.44	108.73
1	A	170	TRP	N-CA-C	5.95	118.20	110.53
4	H	134	ALA	CA-C-O	-5.95	114.33	120.87
4	H	188	SER	N-CA-C	-5.93	100.23	109.72
5	L	89	GLN	CG-CD-NE2	5.91	125.27	116.40
4	H	11	VAL	N-CA-C	5.91	116.44	108.17
4	H	49	GLY	N-CA-C	5.91	119.71	110.91
5	l	24	HIS	CA-CB-CG	5.91	119.71	113.80
4	h	66	ASN	N-CA-C	-5.90	101.72	110.46
3	F	241	PHE	CA-C-O	5.90	125.28	118.97
5	l	160	GLN	N-CA-C	5.90	119.14	109.76
2	E	64	GLU	N-CA-C	5.89	119.00	110.28
4	H	40	ARG	N-CA-C	-5.87	103.38	110.13
5	L	11	LEU	CD1-CG-CD2	5.87	123.72	110.80
1	A	65	ARG	O-C-N	5.86	129.84	123.10
5	l	112	ALA	CA-C-N	-5.86	113.90	119.76
5	l	112	ALA	C-N-CA	-5.86	113.90	119.76
3	F	163	HIS	N-CA-C	5.85	118.25	108.96
5	L	203	SER	CA-C-N	-5.85	113.74	119.76
5	L	203	SER	C-N-CA	-5.85	113.74	119.76
1	A	170	TRP	CA-C-O	-5.84	115.22	121.94
1	A	201	PHE	CA-CB-CG	5.84	119.64	113.80
3	F	96	ARG	O-C-N	-5.84	115.91	122.10
1	A	204	THR	N-CA-C	-5.83	98.90	108.76
5	L	134	CYS	O-C-N	-5.83	116.39	123.27
5	l	119	PRO	CA-C-N	-5.82	114.75	120.98
5	l	119	PRO	C-N-CA	-5.82	114.75	120.98
1	A	32	VAL	CA-C-O	-5.81	113.87	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	HIS	CE1-NE2-CD2	-5.79	103.21	109.00
1	A	228	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	E	129	GLN	CG-CD-NE2	5.79	125.08	116.40
2	E	191	GLU	N-CA-C	5.78	118.92	108.69
1	A	239	SER	N-CA-C	5.78	120.05	112.89
3	F	191	GLU	CA-C-O	-5.76	114.84	121.82
4	h	67	ARG	N-CA-CB	-5.76	105.18	113.65
4	h	96	CYS	N-CA-C	-5.76	100.50	109.72
4	h	27	TYR	CA-C-N	-5.76	115.17	122.37
4	h	27	TYR	C-N-CA	-5.76	115.17	122.37
4	h	157	GLU	N-CA-C	5.75	116.95	109.64
4	H	61	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	E	234	SER	CA-C-N	5.74	130.72	122.45
2	E	234	SER	C-N-CA	5.74	130.72	122.45
4	H	99	GLU	CB-CG-CD	5.74	122.36	112.60
4	H	99	GLU	N-CA-C	-5.73	102.44	110.35
5	L	5	THR	CA-CB-OG1	-5.73	101.01	109.60
2	E	64	GLU	CB-CG-CD	5.72	122.33	112.60
3	F	158	LYS	N-CA-C	-5.72	100.81	109.85
1	B	52	HIS	N-CA-C	5.71	117.08	108.46
2	E	38	GLY	CA-C-N	-5.71	114.38	120.03
2	E	38	GLY	C-N-CA	-5.71	114.38	120.03
2	E	151	HIS	ND1-CG-CD2	-5.71	100.39	106.10
2	E	136	LYS	CA-C-O	-5.71	114.10	120.66
3	F	76	VAL	CA-C-O	-5.71	114.70	120.69
2	E	136	LYS	N-CA-C	-5.70	99.73	109.24
4	h	17	SER	CA-C-N	-5.70	114.03	122.23
4	h	17	SER	C-N-CA	-5.70	114.03	122.23
4	h	64	PHE	N-CA-C	5.68	120.56	111.81
4	H	74	LYS	N-CA-C	-5.68	106.23	114.12
2	E	65	LEU	CA-C-O	-5.67	114.23	120.24
4	H	13	LYS	O-C-N	-5.66	116.08	121.57
4	h	174	THR	CA-C-O	5.66	126.95	120.84
1	A	234	ILE	CA-C-O	-5.65	115.78	121.49
2	E	237	ILE	N-CA-C	-5.63	100.48	108.65
1	A	201	PHE	N-CA-C	5.63	118.44	110.50
5	L	203	SER	CA-C-O	-5.63	115.15	119.32
5	l	73	PHE	CA-CB-CG	5.63	119.43	113.80
5	L	128	GLY	N-CA-C	5.63	120.91	113.37
4	h	160	THR	CA-CB-OG1	-5.63	101.16	109.60
5	l	164	THR	N-CA-C	5.63	118.90	109.95
1	A	156	HIS	N-CA-C	-5.62	101.12	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	122	ASP	O-C-N	5.62	128.16	122.09
5	l	135	LEU	CA-C-O	-5.62	114.20	120.66
3	F	234	SER	N-CA-C	5.62	118.06	108.90
3	F	162	ILE	CA-C-N	5.61	129.87	122.30
3	F	162	ILE	C-N-CA	5.61	129.87	122.30
1	A	167	SER	CA-CB-OG	5.61	122.31	111.10
1	A	133	TYR	N-CA-C	-5.59	100.85	109.52
1	A	129	GLU	CB-CG-CD	5.57	122.07	112.60
1	B	195	PRO	CA-C-O	-5.57	114.40	120.92
2	E	175	PRO	CA-C-N	5.57	130.18	122.77
2	E	175	PRO	C-N-CA	5.57	130.18	122.77
2	E	115	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	161	ILE	N-CA-CB	-5.56	103.41	111.52
1	B	220	SER	N-CA-C	5.56	118.46	109.40
4	h	29	PHE	N-CA-C	5.55	119.81	111.81
3	F	231	LYS	CA-C-O	5.55	126.70	120.70
4	h	202	THR	N-CA-C	-5.55	102.41	110.24
5	L	108	ARG	O-C-N	-5.55	117.44	123.26
3	F	187	ILE	CA-C-O	-5.54	112.52	119.95
5	L	139	PHE	N-CA-C	-5.54	101.33	109.81
2	E	233	ALA	CA-C-O	-5.54	115.14	121.40
5	l	17	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	208	ILE	CA-C-O	-5.53	114.47	120.67
1	A	182	TYR	N-CA-CB	-5.53	103.17	111.25
4	h	84	SER	CA-C-N	-5.53	114.55	122.68
4	h	84	SER	C-N-CA	-5.53	114.55	122.68
1	A	233	VAL	CA-C-N	-5.53	115.60	123.17
1	A	233	VAL	C-N-CA	-5.53	115.60	123.17
3	F	217	GLY	N-CA-C	5.53	121.75	112.85
1	A	66	TRP	CB-CA-C	-5.52	104.19	111.42
2	E	102	ASP	N-CA-C	5.52	120.89	114.04
4	h	60	PHE	N-CA-C	-5.52	101.27	109.94
4	H	155	PHE	CA-C-O	-5.52	112.60	120.16
2	E	59	SER	CA-C-O	-5.51	114.58	120.92
3	F	125	LEU	CA-C-O	-5.50	113.27	119.98
5	l	86	TYR	N-CA-C	5.50	118.45	109.59
1	A	222	ASN	CB-CG-ND2	5.50	124.65	116.40
5	l	27	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	B	109	ALA	N-CA-C	5.50	117.62	108.99
1	A	126	TYR	N-CA-C	5.49	118.77	110.64
3	F	109	ALA	CA-C-N	-5.49	114.28	122.74
3	F	109	ALA	C-N-CA	-5.49	114.28	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	3	GLN	OE1-CD-NE2	5.49	128.09	122.60
5	L	36	TYR	N-CA-C	-5.49	100.93	109.72
2	E	95	GLY	O-C-N	5.49	127.79	122.41
2	E	177	ILE	N-CA-C	-5.48	100.58	108.48
4	h	167	ALA	N-CA-C	5.48	120.08	112.90
2	E	178	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	B	46	ASN	O-C-N	5.47	129.15	122.75
1	A	141	VAL	CA-C-N	-5.46	113.55	120.98
1	A	141	VAL	C-N-CA	-5.46	113.55	120.98
4	H	184	LEU	CA-C-O	-5.46	115.34	121.40
4	H	216	VAL	CA-C-O	5.45	126.14	120.36
2	E	70	SER	CA-CB-OG	-5.44	100.22	111.10
3	F	236	SER	CA-CB-OG	5.44	121.98	111.10
3	F	219	SER	CA-C-O	-5.43	113.86	120.54
1	A	170	TRP	CA-C-N	-5.43	114.18	122.06
1	A	170	TRP	C-N-CA	-5.43	114.18	122.06
1	A	46	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	61	ASP	N-CA-CB	-5.42	104.48	112.78
4	h	39	GLN	O-C-N	-5.42	116.74	123.36
5	L	138	ASN	N-CA-C	5.42	118.72	111.24
5	l	46	LEU	CD1-CG-CD2	-5.42	98.89	110.80
4	h	114	GLN	N-CA-C	5.41	119.60	112.89
3	F	117	THR	CA-C-N	5.41	128.28	120.38
3	F	117	THR	C-N-CA	5.41	128.28	120.38
1	A	38	PRO	CA-C-O	-5.41	115.18	121.34
1	A	79	LYS	N-CA-C	5.41	117.71	108.90
4	h	21	SER	O-C-N	-5.41	116.67	123.27
4	H	154	TYR	N-CA-C	-5.40	101.15	109.52
4	h	148	GLY	O-C-N	-5.40	118.74	123.92
5	L	6	GLN	N-CA-C	-5.39	100.39	109.07
5	l	121	SER	N-CA-C	5.39	118.04	110.23
3	F	44	VAL	O-C-N	-5.38	116.81	122.68
5	L	53	ASN	OD1-CG-ND2	-5.38	117.22	122.60
3	F	69	SER	O-C-N	-5.37	116.96	123.03
3	F	241	PHE	N-CA-C	-5.37	107.10	113.97
2	E	183	LYS	N-CA-C	5.36	119.90	112.45
3	F	90	SER	CA-CB-OG	-5.36	100.38	111.10
5	L	199	GLN	O-C-N	-5.36	117.11	123.22
5	l	47	LEU	CA-C-O	-5.36	113.18	119.24
1	A	226	LEU	O-C-N	5.36	129.85	122.46
5	L	151	ASP	CA-CB-CG	5.36	117.95	112.60
5	l	152	ASN	CB-CG-ND2	5.36	124.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	27	GLN	OE1-CD-NE2	-5.35	117.25	122.60
5	L	65	SER	O-C-N	5.35	129.14	123.42
5	l	148	TRP	CA-C-O	-5.34	113.26	120.47
4	H	122	SER	N-CA-C	-5.32	107.34	113.88
5	l	121	SER	CA-CB-OG	-5.32	100.46	111.10
2	E	76	VAL	N-CA-C	-5.31	105.54	110.53
2	E	178	GLN	CB-CG-CD	5.30	121.61	112.60
3	F	223	ARG	N-CA-C	5.30	117.97	110.50
1	B	79	LYS	CA-C-N	5.29	130.66	120.66
1	B	79	LYS	C-N-CA	5.29	130.66	120.66
1	B	99	VAL	N-CA-C	5.29	115.47	107.75
3	F	128	PHE	N-CA-C	5.29	116.76	109.15
1	B	241	MET	O-C-N	5.28	127.83	121.60
1	B	64	VAL	N-CA-C	5.28	116.33	108.46
4	H	208	ASN	CA-CB-CG	5.28	117.88	112.60
5	L	175	LEU	N-CA-C	5.28	117.41	109.23
1	A	75	VAL	CA-C-N	-5.28	113.34	122.10
1	A	75	VAL	C-N-CA	-5.28	113.34	122.10
3	F	234	SER	CA-C-O	-5.28	114.66	120.36
4	h	215	LYS	N-CA-C	-5.27	100.10	109.06
3	F	189	THR	OG1-CB-CG2	5.26	119.83	109.30
5	l	117	ILE	CB-CG1-CD1	5.26	124.84	113.80
3	F	91	ALA	CA-C-N	-5.25	114.91	121.00
3	F	91	ALA	C-N-CA	-5.25	114.91	121.00
1	B	45	GLU	N-CA-C	-5.25	101.44	109.41
1	B	101	LYS	N-CA-C	-5.24	106.39	112.89
5	L	160	GLN	CG-CD-NE2	-5.24	108.54	116.40
5	L	49	TYR	CA-C-O	5.24	127.24	121.11
1	A	132	SER	CA-C-O	-5.23	114.73	120.70
2	E	91	ALA	CA-C-O	-5.23	113.61	118.73
4	H	209	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	A	210	ARG	N-CA-C	5.23	121.94	110.80
3	F	183	LYS	N-CA-C	5.22	119.65	113.12
4	H	64	PHE	CA-CB-CG	-5.22	108.58	113.80
3	F	163	HIS	CB-CG-CD2	-5.22	124.42	131.20
3	F	230	GLU	CA-C-O	-5.21	115.52	121.40
2	E	231	LYS	O-C-N	5.20	129.72	123.16
3	F	90	SER	CA-C-N	5.20	127.19	120.44
3	F	90	SER	C-N-CA	5.20	127.19	120.44
5	L	30	ASN	OD1-CG-ND2	-5.19	117.41	122.60
4	H	20	LEU	CA-C-O	-5.19	115.16	121.28
4	H	100	ASP	O-C-N	-5.19	117.13	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	33	TYR	CA-C-N	5.18	130.30	122.99
4	h	33	TYR	C-N-CA	5.18	130.30	122.99
4	H	101	ASP	CA-CB-CG	5.18	117.78	112.60
5	L	188	LYS	N-CA-C	-5.18	106.96	113.28
1	A	68	ARG	N-CA-C	-5.18	102.24	109.69
2	E	102	ASP	N-CA-CB	-5.18	103.15	110.81
4	h	73	ASP	CA-CB-CG	5.17	117.77	112.60
5	l	124	GLN	N-CA-C	-5.17	106.80	113.01
1	A	96	THR	CA-C-O	-5.17	115.31	121.16
1	A	66	TRP	O-C-N	-5.17	117.56	123.40
5	L	69	THR	N-CA-C	-5.17	106.92	113.43
1	A	213	SER	CA-C-O	-5.17	113.48	120.15
4	H	98	ARG	CA-C-O	-5.17	115.04	121.50
5	l	31	VAL	CA-C-O	5.15	127.11	122.63
1	A	161	ILE	CA-CB-CG1	5.14	119.14	110.40
3	F	153	ASP	CA-CB-CG	5.14	117.74	112.60
5	l	54	LEU	N-CA-C	5.14	117.62	109.96
4	H	28	ILE	CB-CG1-CD1	5.14	124.59	113.80
4	h	83	LEU	O-C-N	-5.14	117.00	123.27
2	E	49	ASP	N-CA-C	5.13	118.09	110.14
2	E	104	ILE	CB-CG1-CD1	5.13	124.57	113.80
5	l	60	SER	CA-CB-OG	5.13	121.35	111.10
5	L	36	TYR	CA-C-O	-5.12	115.32	121.11
5	L	85	THR	CA-C-N	5.12	130.22	123.05
5	L	85	THR	C-N-CA	5.12	130.22	123.05
4	h	30	THR	CA-CB-OG1	-5.11	101.93	109.60
3	F	129	GLN	CG-CD-NE2	5.11	124.06	116.40
4	h	26	GLY	N-CA-C	5.10	122.47	115.27
1	A	226	LEU	CA-C-O	-5.10	112.99	119.31
3	F	96	ARG	N-CA-CB	-5.10	104.22	111.00
2	E	137	ALA	O-C-N	5.09	129.77	123.15
3	F	139	VAL	N-CA-C	5.09	114.58	108.06
5	L	54	LEU	N-CA-CB	-5.09	102.37	110.06
4	h	64	PHE	N-CA-CB	-5.09	103.81	111.25
1	A	119	GLU	CA-C-N	-5.09	113.77	121.05
1	A	119	GLU	C-N-CA	-5.09	113.77	121.05
4	H	2	VAL	N-CA-C	5.09	116.96	109.63
4	H	205	CYS	N-CA-C	5.09	117.26	107.44
1	B	189	LEU	CA-C-O	-5.09	115.16	120.55
4	h	162	SER	CA-C-O	-5.09	115.16	121.06
3	F	75	VAL	CA-C-N	-5.08	116.59	122.63
3	F	75	VAL	C-N-CA	-5.08	116.59	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLN	O-C-N	-5.08	116.27	122.11
1	A	100	SER	CA-C-O	-5.08	113.28	119.32
1	B	161	ILE	CB-CG1-CD1	5.08	124.46	113.80
1	A	124	ARG	CA-C-N	-5.07	115.01	123.33
1	A	124	ARG	C-N-CA	-5.07	115.01	123.33
4	H	152	LYS	CB-CG-CD	5.07	122.95	111.30
5	L	206	THR	N-CA-C	5.07	117.87	107.69
4	H	86	LEU	CA-C-N	5.06	130.10	121.29
4	H	86	LEU	C-N-CA	5.06	130.10	121.29
1	B	184	GLY	CA-C-O	-5.06	117.92	122.57
5	L	140	TYR	CA-C-O	-5.06	113.23	120.16
1	A	78	TYR	CB-CA-C	-5.06	104.05	111.23
4	H	12	LYS	CG-CD-CE	5.05	122.92	111.30
3	F	104	ILE	CA-CB-CG1	5.05	118.99	110.40
4	h	28	ILE	CB-CG1-CD1	5.05	124.41	113.80
1	B	111	VAL	CA-C-N	5.04	130.00	122.99
1	B	111	VAL	C-N-CA	5.04	130.00	122.99
3	F	141	LEU	N-CA-C	5.04	117.61	109.40
3	F	166	CYS	CA-C-N	-5.02	113.07	121.75
3	F	166	CYS	C-N-CA	-5.02	113.07	121.75
5	l	153	ALA	O-C-N	-5.01	117.53	123.25
5	L	206	THR	CA-CB-OG1	5.01	117.12	109.60
1	B	241	MET	CA-C-N	-5.01	114.62	119.78
1	B	241	MET	C-N-CA	-5.01	114.62	119.78
1	B	164	GLU	CA-C-O	5.01	126.34	120.43
2	E	86	GLU	CA-C-O	5.01	125.59	119.78
4	h	83	LEU	CA-C-O	5.00	126.42	120.66

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	SER	Peptide
1	A	113	HIS	Sidechain
1	A	123	TYR	Sidechain
1	A	125	CYS	Peptide
1	A	126	TYR	Sidechain
1	A	171	TYR	Peptide
1	A	182	TYR	Peptide
1	A	69	SER	Peptide
1	A	72	SER	Peptide
1	A	94	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	171	TYR	Peptide
1	B	195	PRO	Peptide
1	B	53	LEU	Peptide
1	B	60	GLU	Peptide
1	B	62	MET	Peptide
1	B	65	ARG	Peptide
1	B	70	GLN	Peptide
2	E	131	GLY	Peptide
2	E	135	GLU	Peptide
2	E	157	TYR	Peptide
2	E	53	HIS	Sidechain
3	F	105	THR	Peptide
3	F	127	TYR	Peptide
3	F	130	ASP	Peptide
3	F	155	LYS	Peptide
3	F	157	TYR	Sidechain
3	F	33	VAL	Peptide
3	F	48	ALA	Peptide
3	F	49	ASP	Peptide
3	F	51	PRO	Peptide
3	F	55	PHE	Peptide
3	F	58	MET	Peptide
3	F	60	ALA	Peptide
3	F	79	TYR	Sidechain
4	H	155	PHE	Peptide
4	H	157	GLU	Peptide
4	H	158	PRO	Peptide
4	H	186	SER	Peptide
5	L	120	PRO	Peptide
5	L	147	GLN	Peptide
5	L	166	GLN	Peptide
5	L	29	ILE	Peptide
5	L	7	SER	Peptide
5	L	94	TYR	Peptide
4	h	106	PRO	Peptide
4	h	155	PHE	Peptide
4	h	158	PRO	Peptide
4	h	202	THR	Peptide
4	h	21	SER	Peptide
4	h	33	TYR	Sidechain
5	l	116	PHE	Peptide
5	l	136	LEU	Peptide

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Mol	Chain	Res	Type	Group
5	l	159	SER	Peptide
5	l	164	THR	Peptide
5	l	24	HIS	Sidechain
5	l	7	SER	Peptide

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	1704	0	1686	0	0
1	B	1704	0	1686	2	0
2	E	1624	0	1591	17	0
3	F	1598	0	1574	4	0
4	H	1710	0	1680	1	0
4	h	1710	0	1683	11	0
5	L	1654	0	1602	1	0
5	l	1654	0	1603	15	0
All	All	13358	0	13105	38	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 1.

All (38) 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)
4:h:225:CYS:SG	5:l:214:CYS:SG	2.46	1.09
2:E:155:LYS:HB3	2:E:163:HIS:CE1	1.91	1.05
2:E:234:SER:HB3	3:F:151:HIS:CD2	1.97	0.99
2:E:234:SER:HB3	3:F:151:HIS:HD2	1.34	0.90
4:h:149:CYS:SG	4:h:220:VAL:HG22	2.12	0.89
2:E:154:VAL:HB	2:E:164:LEU:HD23	1.57	0.85
2:E:155:LYS:CB	2:E:163:HIS:CE1	2.61	0.82
2:E:154:VAL:HB	2:E:164:LEU:CD2	2.09	0.82
2:E:154:VAL:HG23	2:E:163:HIS:O	1.82	0.79
2:E:155:LYS:CB	2:E:163:HIS:HE1	1.96	0.78
2:E:154:VAL:CB	2:E:164:LEU:HD23	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:137:SER:HB2	5:l:214:CYS:SG	2.29	0.72
4:h:47:TRP:CE2	5:l:96:TYR:CE2	2.79	0.70
5:l:30:ASN:HB2	5:l:32:TRP:CD1	2.27	0.69
4:h:47:TRP:CD2	5:l:96:TYR:CE2	2.81	0.69
2:E:234:SER:CB	3:F:151:HIS:CD2	2.78	0.66
2:E:155:LYS:HG2	2:E:155:LYS:O	1.95	0.65
4:h:47:TRP:HZ3	5:l:95:PRO:HB3	1.65	0.61
4:h:47:TRP:CZ3	5:l:95:PRO:HB3	2.36	0.60
2:E:154:VAL:CG2	2:E:164:LEU:HD23	2.34	0.57
4:h:149:CYS:SG	4:h:220:VAL:CG2	2.93	0.55
5:l:1:ASP:CB	5:l:95:PRO:O	2.56	0.53
2:E:155:LYS:HB2	2:E:163:HIS:HE1	1.69	0.53
4:H:85:ARG:HH12	4:H:87:ARG:HH11	1.59	0.51
4:h:107:PHE:CD2	5:l:32:TRP:HE3	2.31	0.49
4:h:47:TRP:CE2	5:l:96:TYR:HE2	2.30	0.48
5:l:30:ASN:HB2	5:l:32:TRP:NE1	2.29	0.47
5:l:27:GLN:NE2	5:l:92:GLN:HE22	2.14	0.46
5:l:90:GLN:NE2	5:l:96:TYR:HA	2.30	0.46
2:E:163:HIS:ND1	2:E:163:HIS:C	2.74	0.45
3:F:53:HIS:HD2	3:F:108:LYS:HG2	1.82	0.45
2:E:154:VAL:HG23	2:E:164:LEU:HD23	1.98	0.44
2:E:163:HIS:O	2:E:163:HIS:ND1	2.51	0.44
4:h:107:PHE:CD2	5:l:32:TRP:CE3	3.07	0.43
5:L:138:ASN:HA	5:L:173:TYR:O	2.20	0.41
1:B:68:ARG:HG3	1:B:75:VAL:CG2	2.51	0.41
5:l:1:ASP:HB3	5:l:95:PRO:O	2.20	0.41
1:B:87:GLU:OE2	2:E:136:LYS:HE2	2.22	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	215/534 (40%)	211 (98%)	4 (2%)	0	100	100
1	B	215/534 (40%)	214 (100%)	1 (0%)	0	100	100
2	E	213/340 (63%)	212 (100%)	1 (0%)	0	100	100
3	F	210/539 (39%)	210 (100%)	0	0	100	100
4	H	223/255 (88%)	221 (99%)	2 (1%)	0	100	100
4	h	223/255 (88%)	223 (100%)	0	0	100	100
5	L	212/236 (90%)	212 (100%)	0	0	100	100
5	l	212/236 (90%)	211 (100%)	1 (0%)	0	100	100
All	All	1723/2929 (59%)	1714 (100%)	9 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	188/472 (40%)	188 (100%)	0	100	100
1	B	188/472 (40%)	188 (100%)	0	100	100
2	E	172/278 (62%)	171 (99%)	1 (1%)	78	81
3	F	172/451 (38%)	171 (99%)	1 (1%)	78	81
4	H	193/218 (88%)	193 (100%)	0	100	100
4	h	193/218 (88%)	193 (100%)	0	100	100
5	L	189/207 (91%)	189 (100%)	0	100	100
5	l	189/207 (91%)	189 (100%)	0	100	100
All	All	1484/2523 (59%)	1482 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	163	HIS
3	F	53	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	113	HIS
2	E	30	GLN
3	F	53	HIS
3	F	129	GLN
3	F	151	HIS
4	H	180	GLN
5	L	160	GLN
5	L	210	ASN
4	h	206	ASN
5	l	27	GLN
5	l	124	GLN

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](#)

There are no chain breaks in this entry.

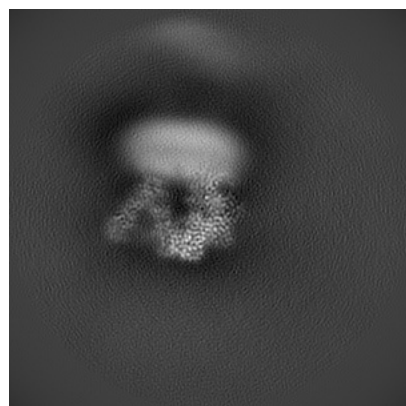
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62752. These allow visual inspection of the internal detail of the map and identification of artifacts.

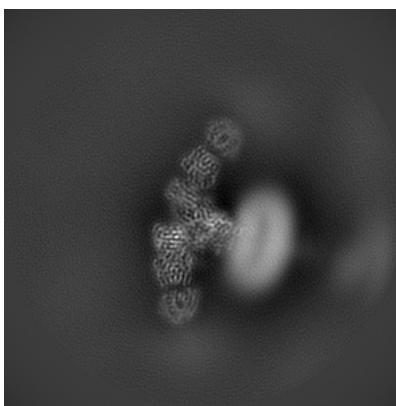
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

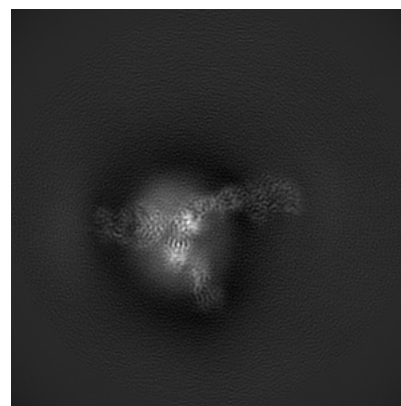
6.1.1 Primary map



X

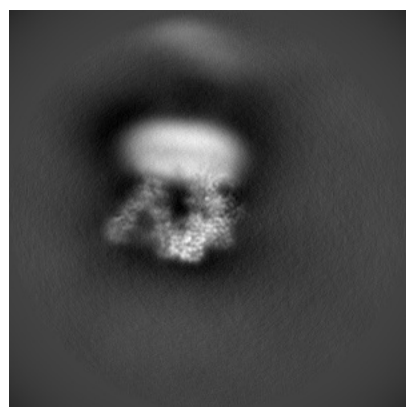


Y

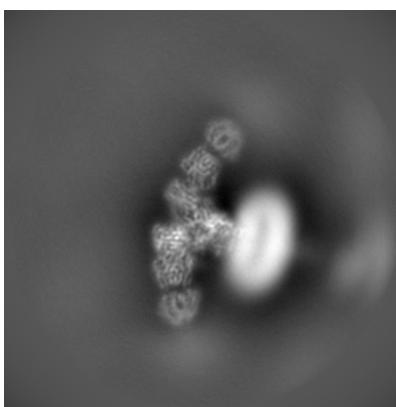


Z

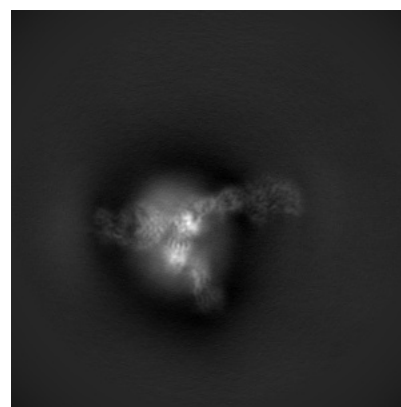
6.1.2 Raw map



X



Y

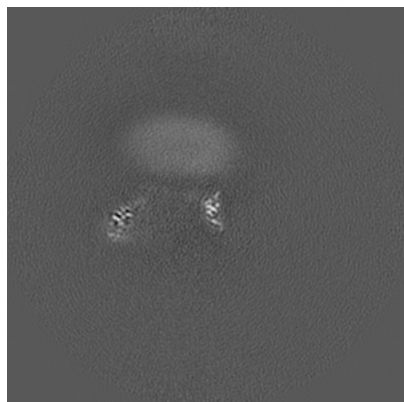


Z

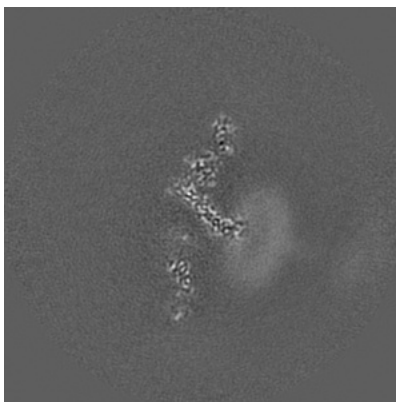
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

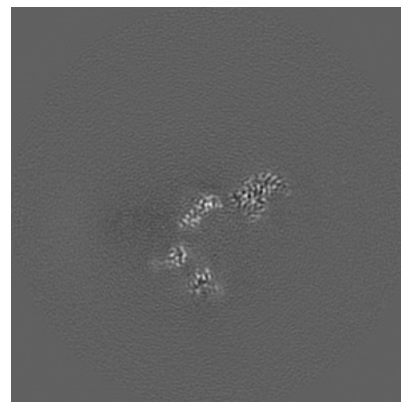
6.2.1 Primary map



X Index: 180

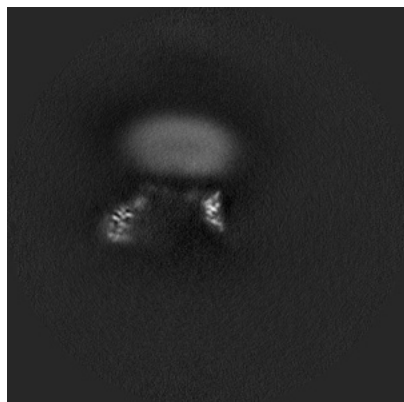


Y Index: 180

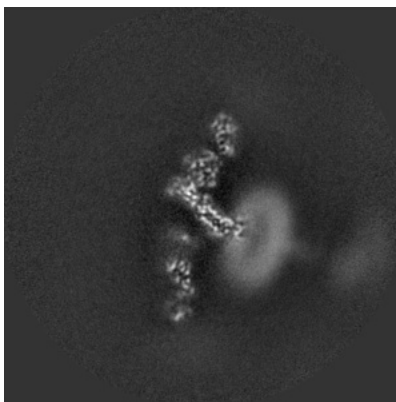


Z Index: 180

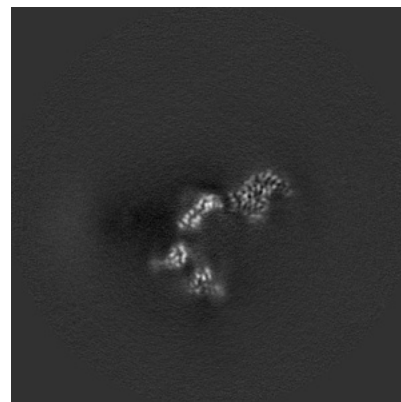
6.2.2 Raw map



X Index: 180



Y Index: 180

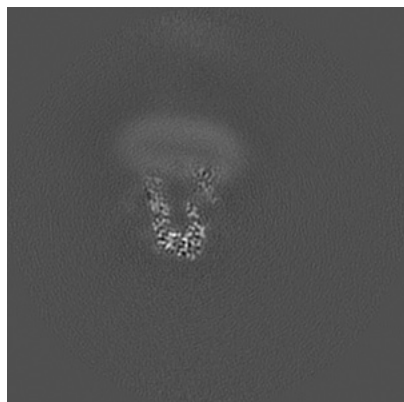


Z Index: 180

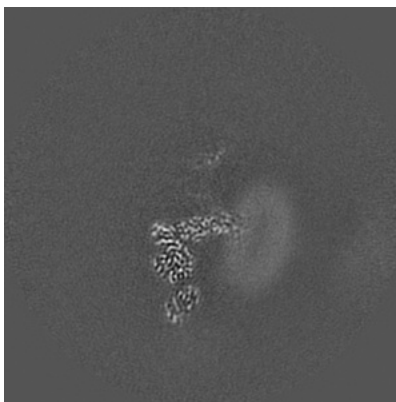
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

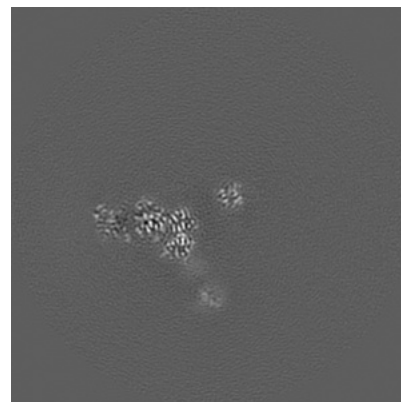
6.3.1 Primary map



X Index: 154

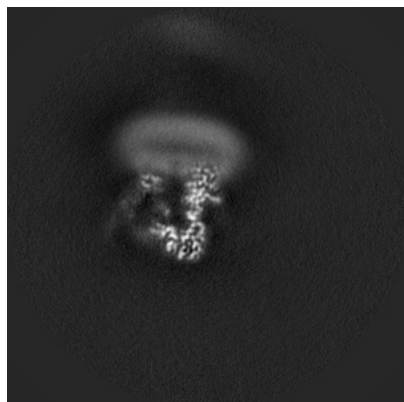


Y Index: 168

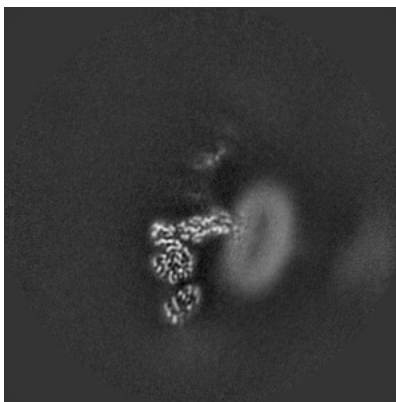


Z Index: 155

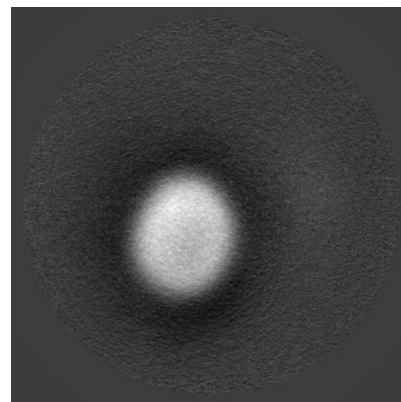
6.3.2 Raw map



X Index: 159



Y Index: 168

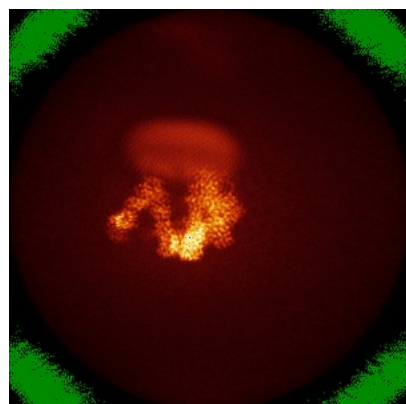


Z Index: 243

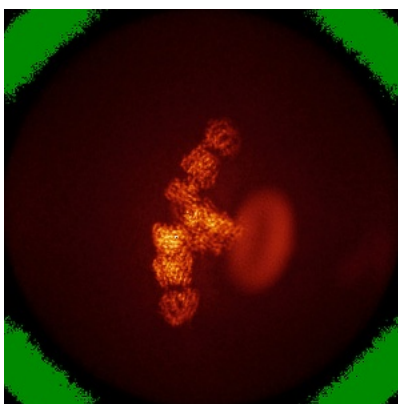
The images above show the largest variance slices of the map in three orthogonal directions.

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

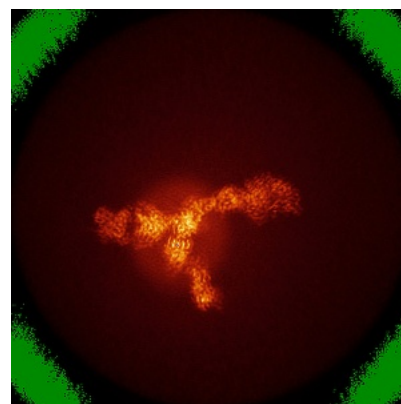
6.4.1 Primary map



X



Y

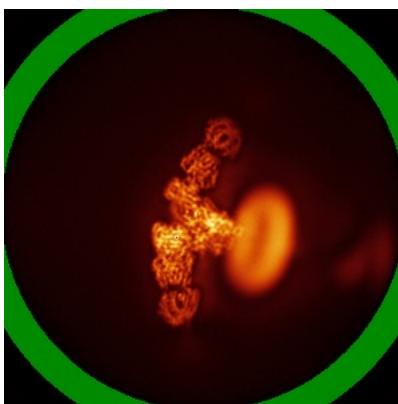


Z

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 0.02. 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.

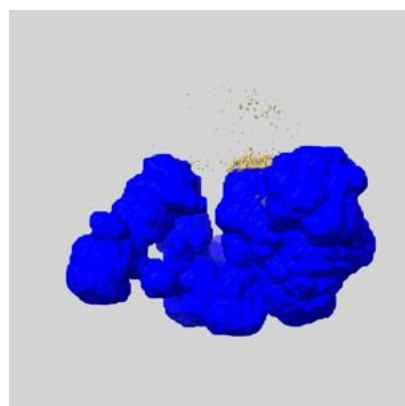
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

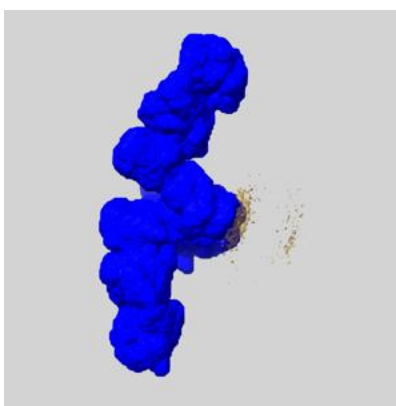
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

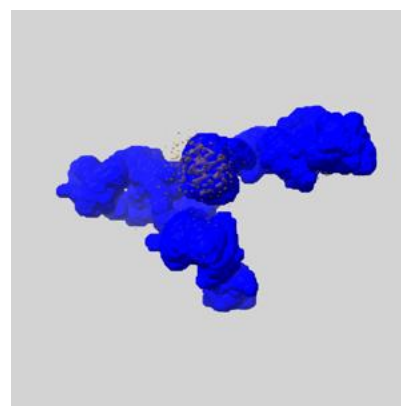
6.6.1 emd_62752_msk_1.map [i](#)



X



Y

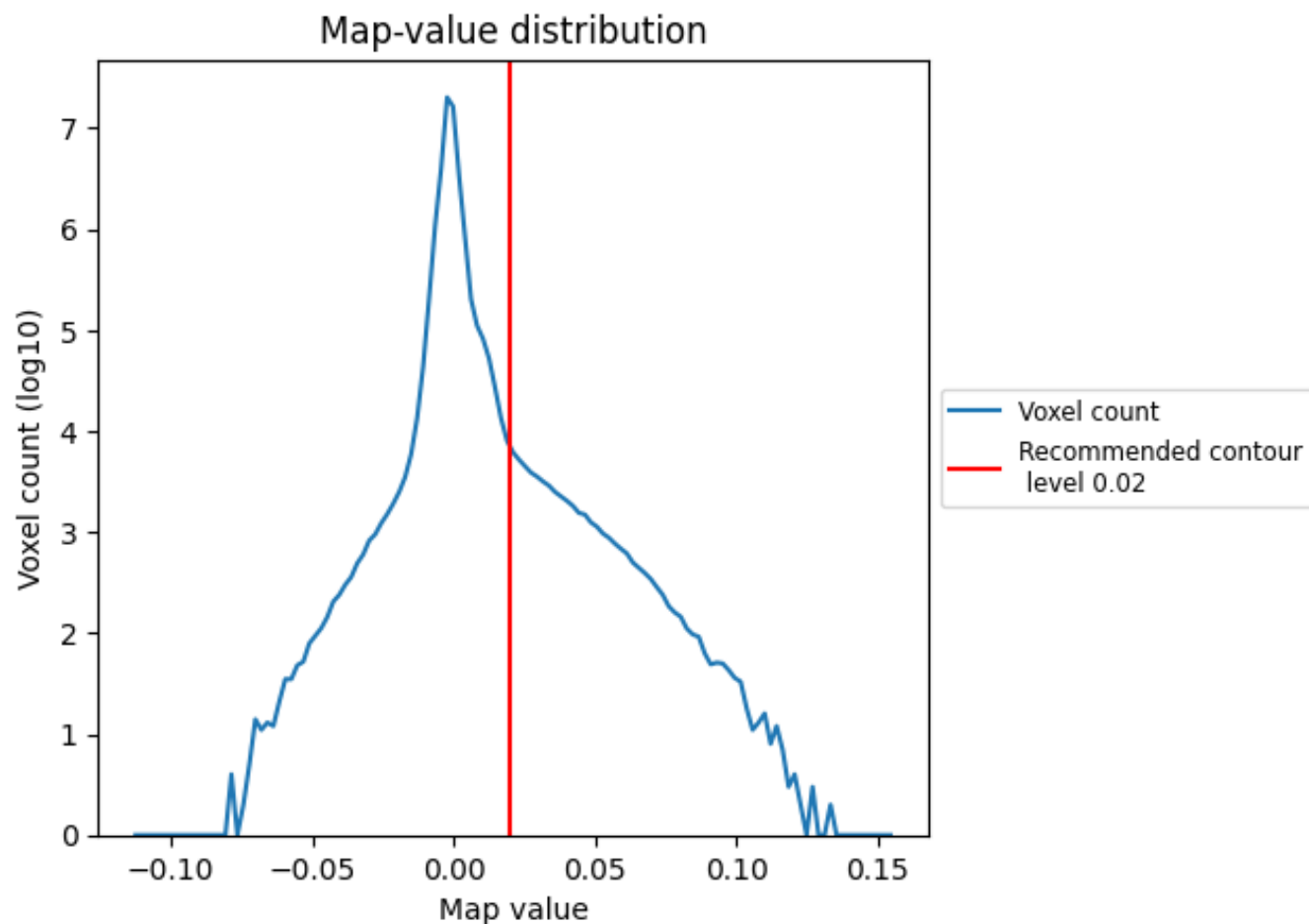


Z

7 Map analysis [i](#)

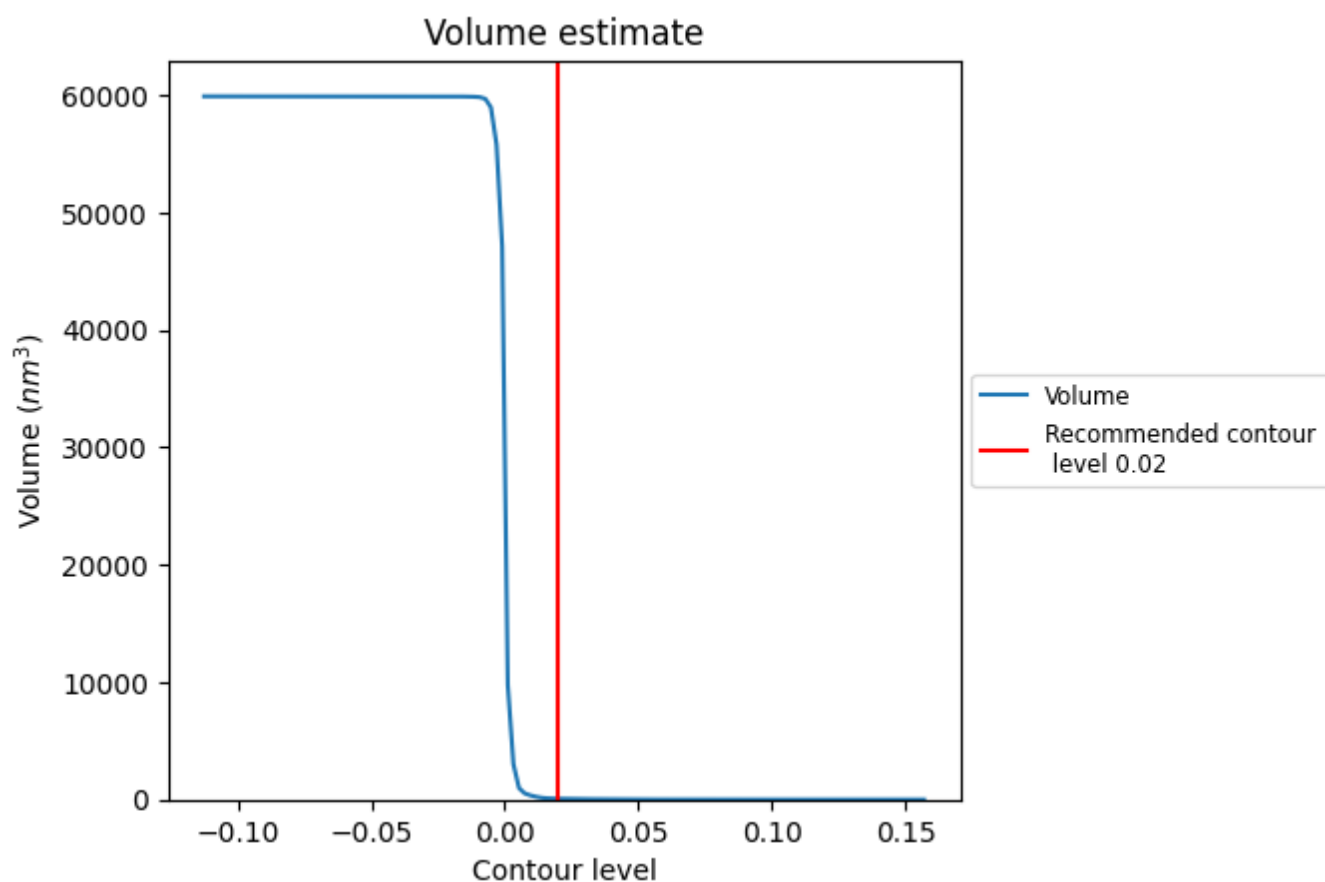
This section contains the results of statistical analysis of the map.

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.

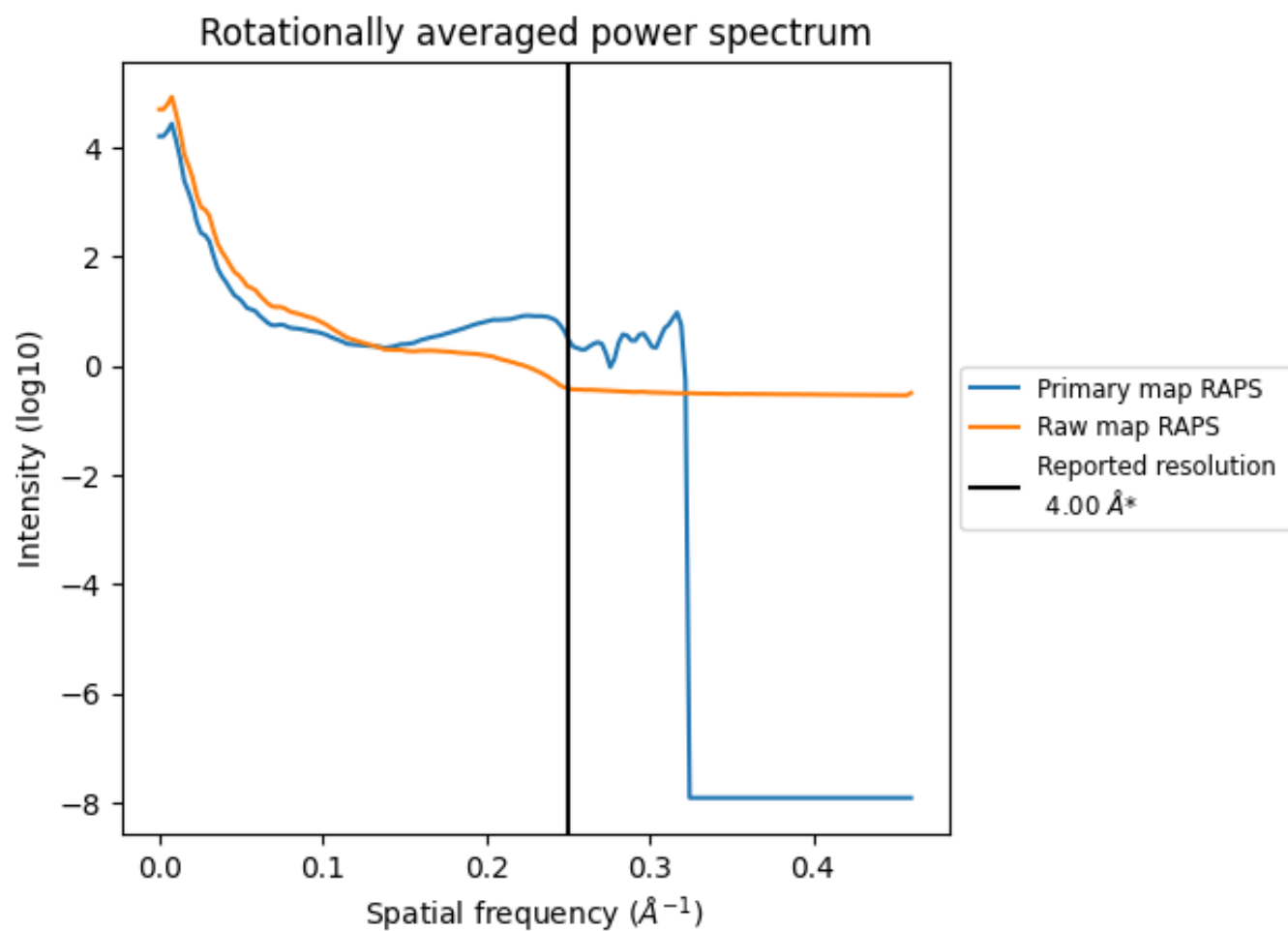
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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 ⓘ

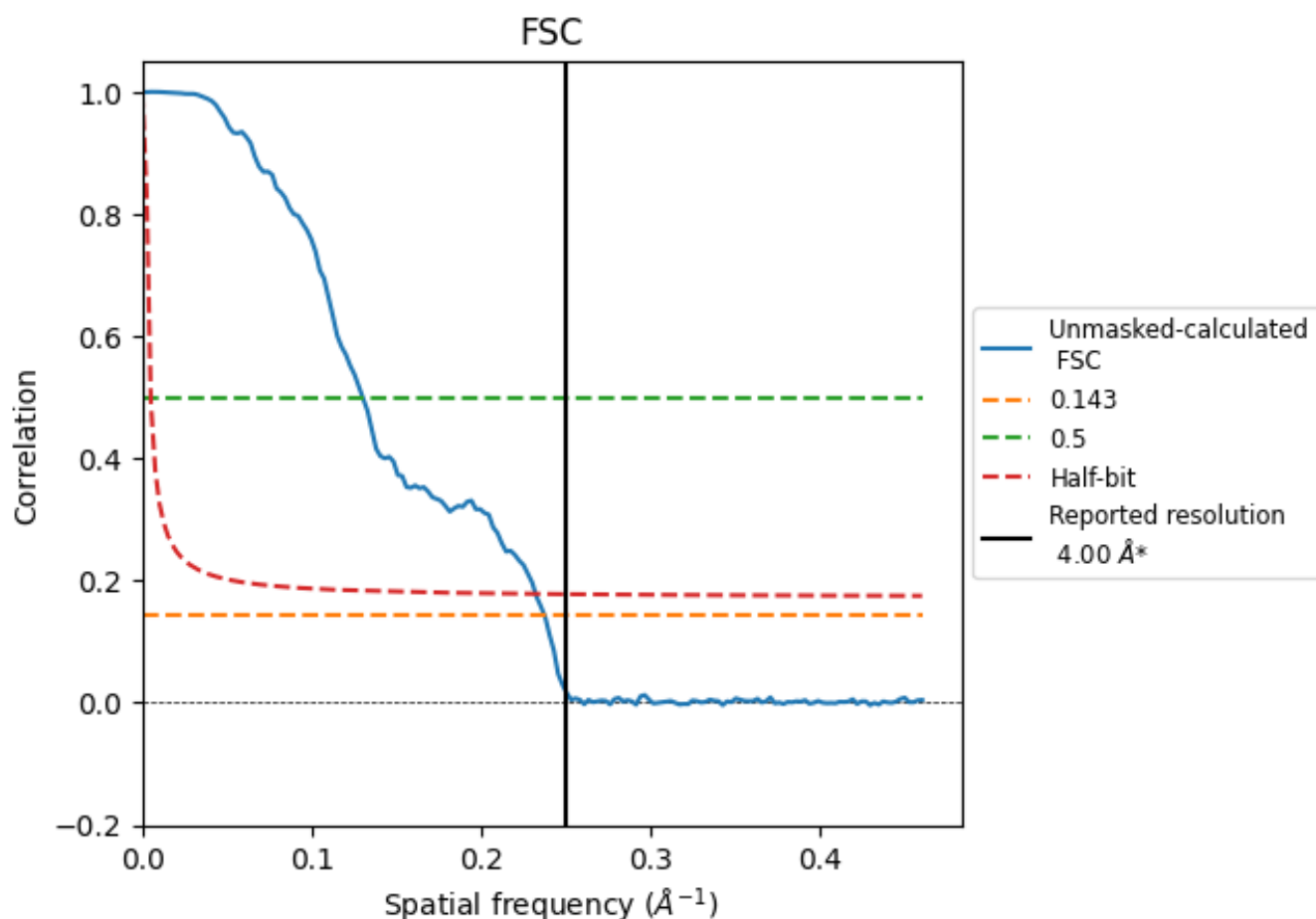


*Reported resolution corresponds to spatial frequency of $0.250 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.250 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

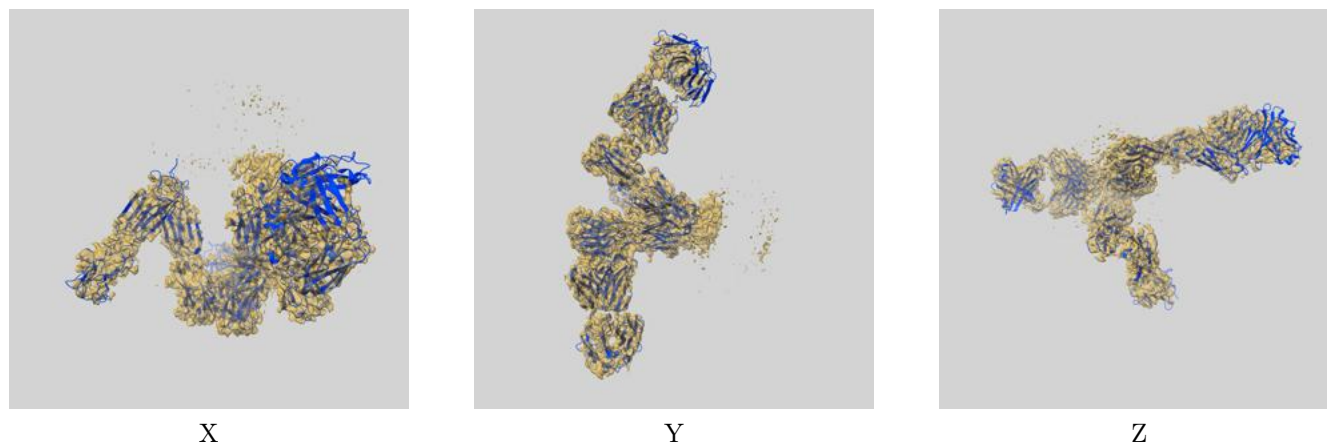
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	7.70	4.31

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

9 Map-model fit [i](#)

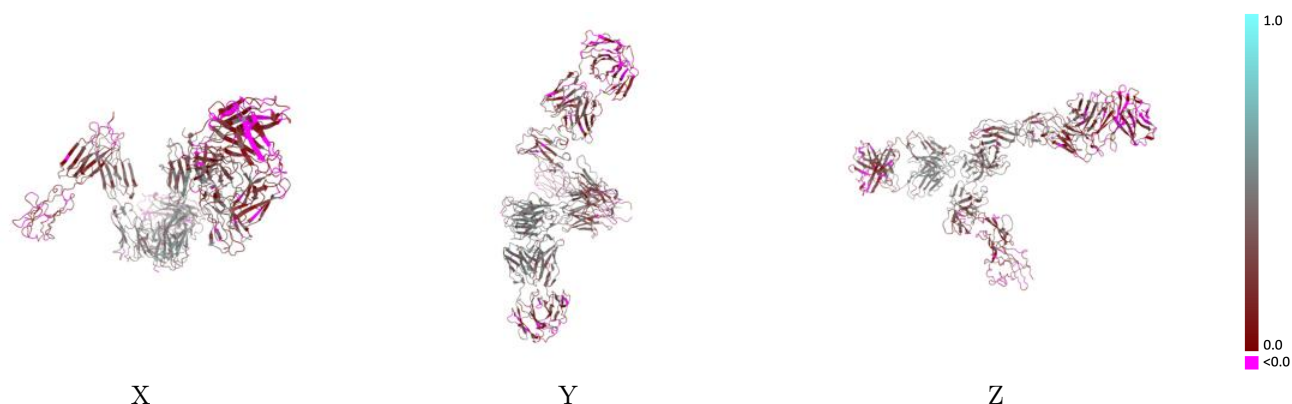
This section contains information regarding the fit between EMDB map EMD-62752 and PDB model 9L1Q. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



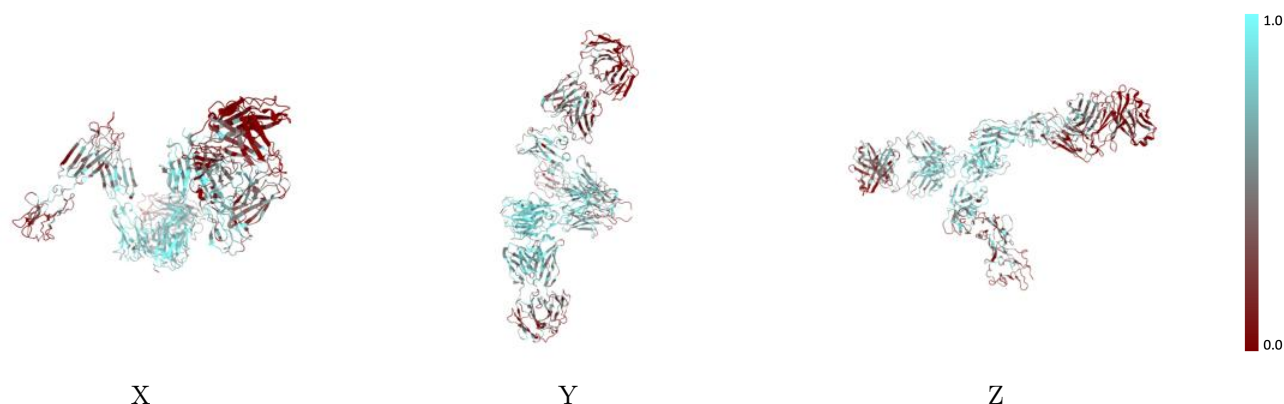
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



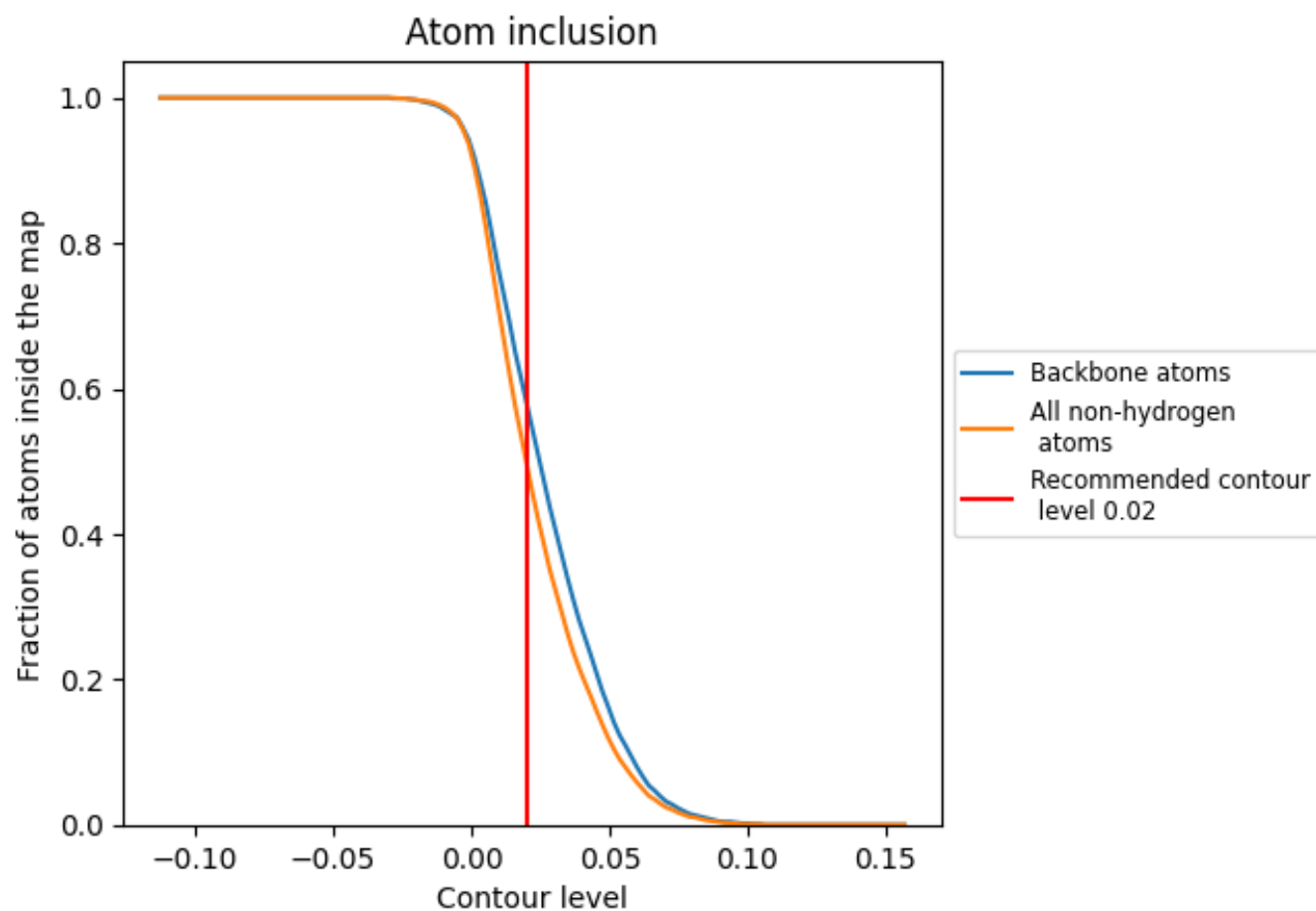
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 50% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4970	0.2910
A	0.3630	0.1920
B	0.6450	0.3640
E	0.7530	0.4230
F	0.6320	0.3390
H	0.5120	0.3340
L	0.5300	0.3220
h	0.2380	0.2000
l	0.3180	0.1640

1.0

0.0

<0.0