



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:30 AM UTC

PDB ID : 8AVD / pdb_00008avd
EMDB ID : EMD-15679
Title : Cryo-EM structure for a 3:3 complex between mouse leptin and the mouse LEP-R ectodomain (local refinement)
Authors : Verstraete, K.; Savvides, S.N.; Verschueren, K.G.; Tsirigotaki, A.
Deposited on : 2022-08-26
Resolution : 4.42 Å(reported)
Based on initial model : 7Z3R

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

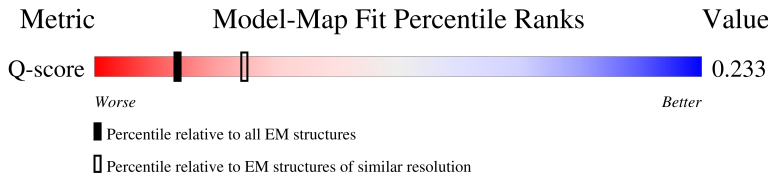
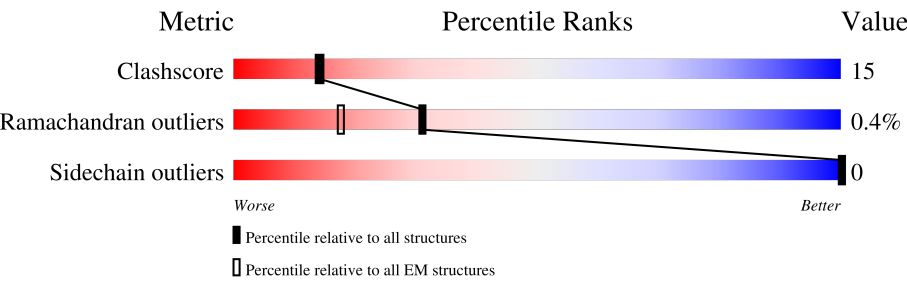
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.42 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	3109 (3.92 - 4.92)

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	174	10% 40% 40% 20%
1	C	174	14% 46% 33% 20%
1	E	174	6% 40% 38% 20%
2	B	868	11% 35% 11% 54%

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Mol	Chain	Length	Quality of chain
2	D	868	14%38%8%54%
2	F	868	6%35%10%54%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12777 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 Leptin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	140	Total	C	N	O	S	0	0
			1077	676	182	216	3		
1	C	140	Total	C	N	O	S	0	0
			1077	676	182	216	3		
1	E	140	Total	C	N	O	S	0	0
			1077	676	182	216	3		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P41160
A	-5	GLY	-	expression tag	UNP P41160
A	-4	SER	-	expression tag	UNP P41160
A	-3	SER	-	expression tag	UNP P41160
A	-2	HIS	-	expression tag	UNP P41160
A	-1	HIS	-	expression tag	UNP P41160
A	0	HIS	-	expression tag	UNP P41160
A	1	HIS	-	expression tag	UNP P41160
A	2	HIS	-	expression tag	UNP P41160
A	3	HIS	-	expression tag	UNP P41160
A	4	PRO	-	expression tag	UNP P41160
A	5	GLY	-	expression tag	UNP P41160
A	6	GLY	-	expression tag	UNP P41160
A	7	PRO	-	expression tag	UNP P41160
A	8	GLY	-	expression tag	UNP P41160
A	9	SER	-	expression tag	UNP P41160
A	10	GLU	-	expression tag	UNP P41160
A	11	ASN	-	expression tag	UNP P41160
A	12	LEU	-	expression tag	UNP P41160
A	13	TYR	-	expression tag	UNP P41160
A	14	PHE	-	expression tag	UNP P41160
A	15	GLN	-	expression tag	UNP P41160
A	16	GLY	-	expression tag	UNP P41160
A	17	GLY	-	expression tag	UNP P41160

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP P41160
A	19	THR	-	expression tag	UNP P41160
A	20	GLY	-	expression tag	UNP P41160
A	21	GLY	ALA	conflict	UNP P41160
C	-6	MET	-	initiating methionine	UNP P41160
C	-5	GLY	-	expression tag	UNP P41160
C	-4	SER	-	expression tag	UNP P41160
C	-3	SER	-	expression tag	UNP P41160
C	-2	HIS	-	expression tag	UNP P41160
C	-1	HIS	-	expression tag	UNP P41160
C	0	HIS	-	expression tag	UNP P41160
C	1	HIS	-	expression tag	UNP P41160
C	2	HIS	-	expression tag	UNP P41160
C	3	HIS	-	expression tag	UNP P41160
C	4	PRO	-	expression tag	UNP P41160
C	5	GLY	-	expression tag	UNP P41160
C	6	GLY	-	expression tag	UNP P41160
C	7	PRO	-	expression tag	UNP P41160
C	8	GLY	-	expression tag	UNP P41160
C	9	SER	-	expression tag	UNP P41160
C	10	GLU	-	expression tag	UNP P41160
C	11	ASN	-	expression tag	UNP P41160
C	12	LEU	-	expression tag	UNP P41160
C	13	TYR	-	expression tag	UNP P41160
C	14	PHE	-	expression tag	UNP P41160
C	15	GLN	-	expression tag	UNP P41160
C	16	GLY	-	expression tag	UNP P41160
C	17	GLY	-	expression tag	UNP P41160
C	18	SER	-	expression tag	UNP P41160
C	19	THR	-	expression tag	UNP P41160
C	20	GLY	-	expression tag	UNP P41160
C	21	GLY	ALA	conflict	UNP P41160
E	-6	MET	-	initiating methionine	UNP P41160
E	-5	GLY	-	expression tag	UNP P41160
E	-4	SER	-	expression tag	UNP P41160
E	-3	SER	-	expression tag	UNP P41160
E	-2	HIS	-	expression tag	UNP P41160
E	-1	HIS	-	expression tag	UNP P41160
E	0	HIS	-	expression tag	UNP P41160
E	1	HIS	-	expression tag	UNP P41160
E	2	HIS	-	expression tag	UNP P41160
E	3	HIS	-	expression tag	UNP P41160

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Chain	Residue	Modelled	Actual	Comment	Reference
E	4	PRO	-	expression tag	UNP P41160
E	5	GLY	-	expression tag	UNP P41160
E	6	GLY	-	expression tag	UNP P41160
E	7	PRO	-	expression tag	UNP P41160
E	8	GLY	-	expression tag	UNP P41160
E	9	SER	-	expression tag	UNP P41160
E	10	GLU	-	expression tag	UNP P41160
E	11	ASN	-	expression tag	UNP P41160
E	12	LEU	-	expression tag	UNP P41160
E	13	TYR	-	expression tag	UNP P41160
E	14	PHE	-	expression tag	UNP P41160
E	15	GLN	-	expression tag	UNP P41160
E	16	GLY	-	expression tag	UNP P41160
E	17	GLY	-	expression tag	UNP P41160
E	18	SER	-	expression tag	UNP P41160
E	19	THR	-	expression tag	UNP P41160
E	20	GLY	-	expression tag	UNP P41160
E	21	GLY	ALA	conflict	UNP P41160

- Molecule 2 is a protein called Leptin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			3181	2033	536	595	17		
2	D	399	Total	C	N	O	S	0	0
			3181	2033	536	595	17		
2	F	399	Total	C	N	O	S	0	0
			3181	2033	536	595	17		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	840	SER	-	expression tag	UNP P48356
B	841	THR	-	expression tag	UNP P48356
B	842	GLY	-	expression tag	UNP P48356
B	843	GLY	-	expression tag	UNP P48356
B	844	SER	-	expression tag	UNP P48356
B	845	GLY	-	expression tag	UNP P48356
B	846	GLY	-	expression tag	UNP P48356
B	847	SER	-	expression tag	UNP P48356
B	848	GLY	-	expression tag	UNP P48356
B	849	GLY	-	expression tag	UNP P48356

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Chain	Residue	Modelled	Actual	Comment	Reference
B	850	SER	-	expression tag	UNP P48356
B	851	GLY	-	expression tag	UNP P48356
B	852	GLY	-	expression tag	UNP P48356
B	853	SER	-	expression tag	UNP P48356
B	854	GLY	-	expression tag	UNP P48356
B	855	GLY	-	expression tag	UNP P48356
B	856	SER	-	expression tag	UNP P48356
B	857	ARG	-	expression tag	UNP P48356
B	858	MET	-	expression tag	UNP P48356
B	859	LYS	-	expression tag	UNP P48356
B	860	GLN	-	expression tag	UNP P48356
B	861	ILE	-	expression tag	UNP P48356
B	862	GLU	-	expression tag	UNP P48356
B	863	ASP	-	expression tag	UNP P48356
B	864	LYS	-	expression tag	UNP P48356
B	865	ILE	-	expression tag	UNP P48356
B	866	GLU	-	expression tag	UNP P48356
B	867	GLU	-	expression tag	UNP P48356
B	868	ILE	-	expression tag	UNP P48356
B	869	LEU	-	expression tag	UNP P48356
B	870	SER	-	expression tag	UNP P48356
B	871	LYS	-	expression tag	UNP P48356
B	872	ILE	-	expression tag	UNP P48356
B	873	TYR	-	expression tag	UNP P48356
B	874	HIS	-	expression tag	UNP P48356
B	875	ILE	-	expression tag	UNP P48356
B	876	GLU	-	expression tag	UNP P48356
B	877	ASN	-	expression tag	UNP P48356
B	878	GLU	-	expression tag	UNP P48356
B	879	ILE	-	expression tag	UNP P48356
B	880	ALA	-	expression tag	UNP P48356
B	881	ARG	-	expression tag	UNP P48356
B	882	ILE	-	expression tag	UNP P48356
B	883	LYS	-	expression tag	UNP P48356
B	884	LYS	-	expression tag	UNP P48356
B	885	LEU	-	expression tag	UNP P48356
B	886	ILE	-	expression tag	UNP P48356
B	887	GLY	-	expression tag	UNP P48356
B	888	GLU	-	expression tag	UNP P48356
B	889	ARG	-	expression tag	UNP P48356
D	840	SER	-	expression tag	UNP P48356
D	841	THR	-	expression tag	UNP P48356

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Chain	Residue	Modelled	Actual	Comment	Reference
D	842	GLY	-	expression tag	UNP P48356
D	843	GLY	-	expression tag	UNP P48356
D	844	SER	-	expression tag	UNP P48356
D	845	GLY	-	expression tag	UNP P48356
D	846	GLY	-	expression tag	UNP P48356
D	847	SER	-	expression tag	UNP P48356
D	848	GLY	-	expression tag	UNP P48356
D	849	GLY	-	expression tag	UNP P48356
D	850	SER	-	expression tag	UNP P48356
D	851	GLY	-	expression tag	UNP P48356
D	852	GLY	-	expression tag	UNP P48356
D	853	SER	-	expression tag	UNP P48356
D	854	GLY	-	expression tag	UNP P48356
D	855	GLY	-	expression tag	UNP P48356
D	856	SER	-	expression tag	UNP P48356
D	857	ARG	-	expression tag	UNP P48356
D	858	MET	-	expression tag	UNP P48356
D	859	LYS	-	expression tag	UNP P48356
D	860	GLN	-	expression tag	UNP P48356
D	861	ILE	-	expression tag	UNP P48356
D	862	GLU	-	expression tag	UNP P48356
D	863	ASP	-	expression tag	UNP P48356
D	864	LYS	-	expression tag	UNP P48356
D	865	ILE	-	expression tag	UNP P48356
D	866	GLU	-	expression tag	UNP P48356
D	867	GLU	-	expression tag	UNP P48356
D	868	ILE	-	expression tag	UNP P48356
D	869	LEU	-	expression tag	UNP P48356
D	870	SER	-	expression tag	UNP P48356
D	871	LYS	-	expression tag	UNP P48356
D	872	ILE	-	expression tag	UNP P48356
D	873	TYR	-	expression tag	UNP P48356
D	874	HIS	-	expression tag	UNP P48356
D	875	ILE	-	expression tag	UNP P48356
D	876	GLU	-	expression tag	UNP P48356
D	877	ASN	-	expression tag	UNP P48356
D	878	GLU	-	expression tag	UNP P48356
D	879	ILE	-	expression tag	UNP P48356
D	880	ALA	-	expression tag	UNP P48356
D	881	ARG	-	expression tag	UNP P48356
D	882	ILE	-	expression tag	UNP P48356
D	883	LYS	-	expression tag	UNP P48356

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Chain	Residue	Modelled	Actual	Comment	Reference
D	884	LYS	-	expression tag	UNP P48356
D	885	LEU	-	expression tag	UNP P48356
D	886	ILE	-	expression tag	UNP P48356
D	887	GLY	-	expression tag	UNP P48356
D	888	GLU	-	expression tag	UNP P48356
D	889	ARG	-	expression tag	UNP P48356
F	840	SER	-	expression tag	UNP P48356
F	841	THR	-	expression tag	UNP P48356
F	842	GLY	-	expression tag	UNP P48356
F	843	GLY	-	expression tag	UNP P48356
F	844	SER	-	expression tag	UNP P48356
F	845	GLY	-	expression tag	UNP P48356
F	846	GLY	-	expression tag	UNP P48356
F	847	SER	-	expression tag	UNP P48356
F	848	GLY	-	expression tag	UNP P48356
F	849	GLY	-	expression tag	UNP P48356
F	850	SER	-	expression tag	UNP P48356
F	851	GLY	-	expression tag	UNP P48356
F	852	GLY	-	expression tag	UNP P48356
F	853	SER	-	expression tag	UNP P48356
F	854	GLY	-	expression tag	UNP P48356
F	855	GLY	-	expression tag	UNP P48356
F	856	SER	-	expression tag	UNP P48356
F	857	ARG	-	expression tag	UNP P48356
F	858	MET	-	expression tag	UNP P48356
F	859	LYS	-	expression tag	UNP P48356
F	860	GLN	-	expression tag	UNP P48356
F	861	ILE	-	expression tag	UNP P48356
F	862	GLU	-	expression tag	UNP P48356
F	863	ASP	-	expression tag	UNP P48356
F	864	LYS	-	expression tag	UNP P48356
F	865	ILE	-	expression tag	UNP P48356
F	866	GLU	-	expression tag	UNP P48356
F	867	GLU	-	expression tag	UNP P48356
F	868	ILE	-	expression tag	UNP P48356
F	869	LEU	-	expression tag	UNP P48356
F	870	SER	-	expression tag	UNP P48356
F	871	LYS	-	expression tag	UNP P48356
F	872	ILE	-	expression tag	UNP P48356
F	873	TYR	-	expression tag	UNP P48356
F	874	HIS	-	expression tag	UNP P48356
F	875	ILE	-	expression tag	UNP P48356

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Chain	Residue	Modelled	Actual	Comment	Reference
F	876	GLU	-	expression tag	UNP P48356
F	877	ASN	-	expression tag	UNP P48356
F	878	GLU	-	expression tag	UNP P48356
F	879	ILE	-	expression tag	UNP P48356
F	880	ALA	-	expression tag	UNP P48356
F	881	ARG	-	expression tag	UNP P48356
F	882	ILE	-	expression tag	UNP P48356
F	883	LYS	-	expression tag	UNP P48356
F	884	LYS	-	expression tag	UNP P48356
F	885	LEU	-	expression tag	UNP P48356
F	886	ILE	-	expression tag	UNP P48356
F	887	GLY	-	expression tag	UNP P48356
F	888	GLU	-	expression tag	UNP P48356
F	889	ARG	-	expression tag	UNP P48356

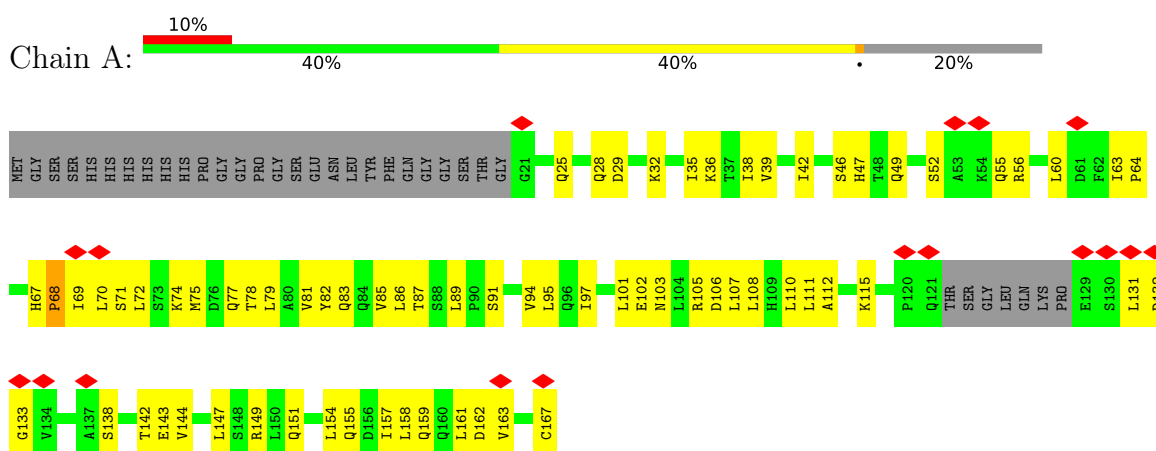
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total Ni 1 1	0
3	D	1	Total Ni 1 1	0
3	F	1	Total Ni 1 1	0

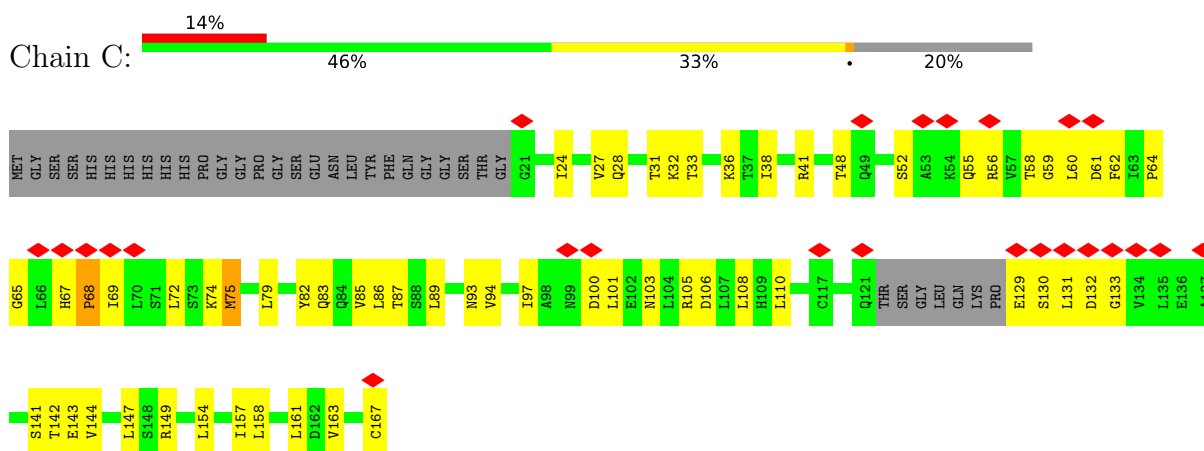
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

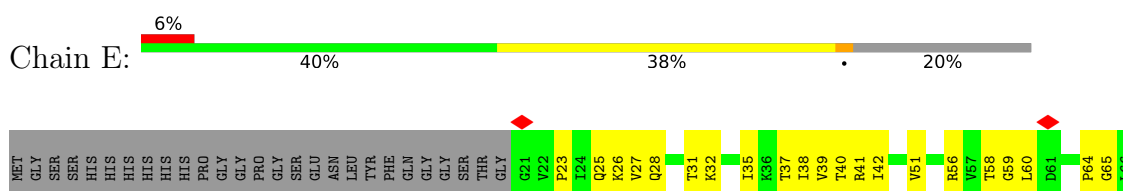
• Molecule 1: Leptin

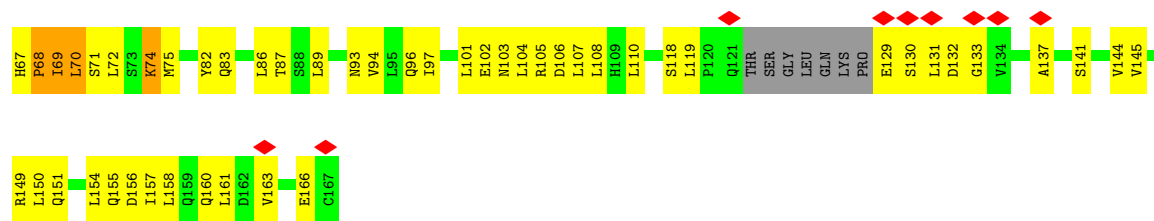


• Molecule 1: Leptin

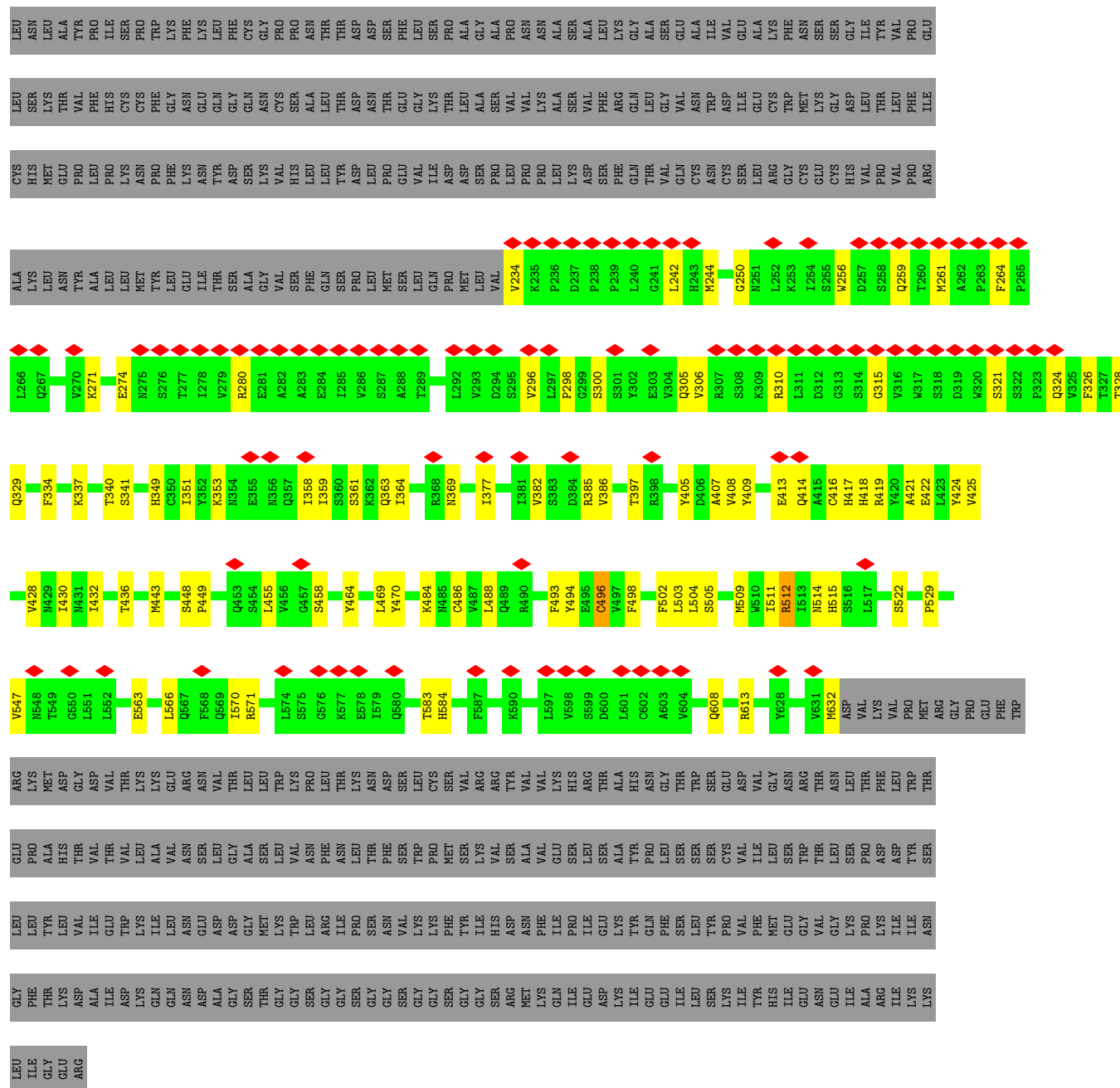
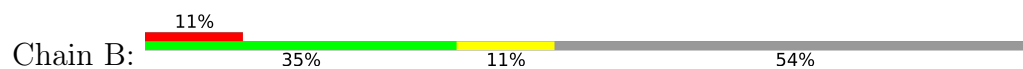


• Molecule 1: Leptin

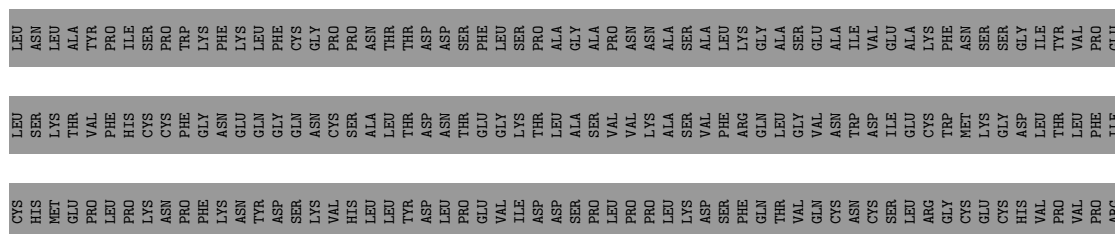
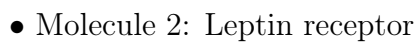




• Molecule 2: Leptin receptor



• Molecule 2: Leptin receptor



ALA	LYS	LEU	ASN	ASN	TYR	ALA	LEU	LEU	MET	TYR	LEU	GLU	ILE	THR	SER	ALA	GLY	VAL	SER	PHE	GLN	SER	PRO	LEU	MET	SER	LEU	GLN	PRO	MET	LEU	VAL	V294	K235	P236	D237	P238	P239	L240	L241	L242	H243	M244	E245	D248	L252	K253	I254	D257	S258	Q259	T260	M261	A262	P263	F264	P265
L266	Q267				Y272	S276	T277	I278	V279	R280	E281	A282	A283	E284	I285	V286	S287	A288		L292		L297	Y302	F303	V304	Q305	V306		R310	L311	D312	G313	S314	G315	V316	W317	S318	D319		S322	P323	Q324	V325	Q329	D330	T340	S341		H349	C350	I351	Y352	K353		N356	Q357	I358
I359	K362	W366	W367	S276	N369	L370	A371	E372	K373	I374		I377	V382	S383	D384	R385	V386		T397	R400	Y406	D406	A407	V408	Y409	C410	N411	N412	A415	C416	H417	H418	R419	Y420	A421	Y424	V425	T436	Y439	L440	T441	R446	W447	S448	P449		Q453	S454	L455								
V456	G457	S458	Y464	S468	L469		C486	V487	L488	D491	G492	F493	Y494	E495	C496	F502		Y507	T508	N509	H515	V532	V533		I545	T546	V547	N548	T549	G550	L551	L552		F561	L566	I570	K577	H584		F587	D588	A589	K590		L596	L597	V598	S599	D600								
L601	V609	R613	V631	M632	ASP	VAL	LYS	ARG	THR	VAL	THR	PRO	ASN	MET	ARG	GLY	THR	VAL	THR	VAL	LYS	ALA	GLY	VAL	THR	LEU	ASN	ARG	ASN	VAL	THR	LEU	ASN	THR	LYS	ASP	SER	THR	PRO	CYS	SER	VAL	ARG	THR	TYR	VAL	ALA	VAL	GLU	LYS	HIS	ARG	THR	ALA			
HIS	ASN	GLY	THR	TRP	SER	GLU	ASP	VAL	VAL	GLY	ASN	VAL	ASP	THR	TRP	THR	GLU	PRO	ALA	HIS	THR	VAL	THR	VAL	THR	LEU	ALA	GLY	VAL	THR	LEU	ASN	ARG	ASN	VAL	THR	LEU	ASN	PRO	MET	SER	VAL	ARG	THR	ASN	VAL	ALA	VAL	GLU	LYS	THR	ALA					
TYR	PRO	LEU	SER	SER	CYS	VAL	VAL	ASP	GLY	SER	ASN	VAL	ASP	THR	TRP	THR	GLU	LEU	PRO	TYR	LEU	HIS	VAL	ILE	VAL	THR	TRP	VAL	ASN	LEU	ARG	PHE	LEU	ILE	PRO	THR	ASN	PHE	LYS	PRO	PHE	LYS	HIS	ASP	ASN	VAL	PHE	ILE	PRO	ILE	GLU	LYS					
TYR	GLN	PHE	SER	LEU	TYR	PRO	VAL	PHE	GLU	GLY	VAL	ASN	GLY	GLY	ASN	PHE	THR	ASP	ALA	ASP	LYS	THR	GLY	THR	ALA	ILE	GLU	TRP	VAL	ILE	GLN	ASN	ASP	GLU	GLY	ASP	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
ILE	GLU	GLU	ILE	LEU	SER	LYS	ILE	TYR	HIS	ILE	GLU	ASN	GLU	GLU	ASN	GLU	GLY	PHE	THR	LYS	ASP	ALA	ILE	ILE	ASP	GLY	THR	THR	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54708	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.733	Depositor
Minimum map value	-0.392	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.256	Depositor
Map size (Å)	371.392, 371.392, 371.392	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.658, 1.658, 1.658	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.30	0/1088	0.72	0/1477
1	C	0.23	0/1088	0.62	1/1477 (0.1%)
1	E	0.34	0/1088	0.82	5/1477 (0.3%)
2	B	0.21	0/3267	0.60	2/4457 (0.0%)
2	D	0.16	0/3267	0.53	0/4457
2	F	0.16	0/3267	0.61	6/4457 (0.1%)
All	All	0.21	0/13065	0.62	14/17802 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	486	CYS	CA-CB-SG	12.99	144.29	114.40
2	F	496	CYS	CA-CB-SG	8.94	134.97	114.40
2	F	496	CYS	CB-CA-C	7.22	122.15	110.16
1	E	74	LYS	CG-CD-CE	-6.86	95.52	111.30
2	F	486	CYS	CB-CA-C	6.84	121.89	109.37
1	E	74	LYS	CB-CG-CD	6.64	126.58	111.30
2	F	440	LEU	CA-CB-CG	6.27	138.24	116.30
2	B	496	CYS	CA-CB-SG	5.93	128.04	114.40
1	E	69	ILE	CA-CB-CG1	5.47	119.70	110.40
1	C	75	MET	CB-CG-SD	5.21	128.33	112.70
1	E	74	LYS	CD-CE-NZ	5.15	128.39	111.90
2	F	330	ASP	N-CA-C	5.12	116.67	111.14
1	E	70	LEU	N-CA-C	5.07	119.42	112.88
2	B	512	ARG	CB-CG-CD	5.07	122.95	111.30

There are no chirality outliers.

There are no planarity outliers.

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	1077	0	1109	66	0
1	C	1077	0	1109	64	0
1	E	1077	0	1109	87	0
2	B	3181	0	3135	87	0
2	D	3181	0	3135	64	0
2	F	3181	0	3135	75	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
All	All	12777	0	12732	395	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 15.

All (395) 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)
1:A:103:ASN:ND2	2:B:504:LEU:H	1.08	1.46
2:B:409:TYR:OH	1:C:141:SER:HB3	1.05	1.22
1:A:103:ASN:ND2	2:B:504:LEU:N	1.89	1.19
1:E:41:ARG:NH2	2:F:439:TYR:O	1.78	1.16
2:B:409:TYR:OH	1:C:141:SER:CB	1.97	1.11
2:D:417:HIS:ND1	1:E:58:THR:HG23	1.69	1.06
2:B:417:HIS:ND1	1:C:58:THR:HG23	1.69	1.06
1:C:24:ILE:HG22	1:C:28:GLN:HE22	1.35	0.91
2:B:486:CYS:HA	2:B:496:CYS:HB3	1.51	0.90
1:A:115:LYS:NZ	1:A:167:CYS:SG	2.44	0.89
1:A:56:ARG:HH22	2:F:415:ALA:HA	1.39	0.88
2:B:512:ARG:NH1	2:B:514:ASN:OD1	2.07	0.86
1:A:70:LEU:H	1:A:74:LYS:HE3	1.39	0.85
1:C:79:LEU:HD12	1:C:101:LEU:HD11	1.57	0.84
2:B:274:GLU:OE1	2:B:280:ARG:NH1	2.13	0.82
1:A:103:ASN:HD22	2:B:504:LEU:H	0.84	0.81
2:B:409:TYR:HH	1:C:141:SER:HB3	1.45	0.81
1:A:103:ASN:HD22	2:B:504:LEU:N	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LEU:HG	1:E:145:VAL:HG11	1.63	0.80
1:E:38:ILE:HD11	1:E:97:ILE:HG23	1.63	0.80
1:C:68:PRO:O	1:C:74:LYS:NZ	2.14	0.79
1:E:151:GLN:O	1:E:155:GLN:NE2	2.17	0.78
2:F:278:ILE:HB	2:F:280:ARG:HH11	1.47	0.78
1:E:69:ILE:C	1:E:74:LYS:HE3	2.08	0.77
2:B:234:VAL:O	2:B:310:ARG:NH1	2.18	0.75
1:E:71:SER:O	1:E:74:LYS:NZ	2.18	0.74
1:C:103:ASN:HD21	2:D:502:PHE:HB3	1.53	0.73
2:F:276:SER:OG	2:F:280:ARG:NH1	2.21	0.73
1:A:25:GLN:NE2	1:A:29:ASP:OD2	2.22	0.73
1:A:103:ASN:HB3	2:B:504:LEU:HB2	1.72	0.72
1:A:69:ILE:HD11	1:A:75:MET:HA	1.71	0.72
1:E:83:GLN:O	1:E:87:THR:HG23	1.91	0.71
2:D:299:GLY:HA3	2:D:353:LYS:HE2	1.73	0.71
1:E:23:PRO:HG2	1:E:26:LYS:HG2	1.72	0.71
1:E:101:LEU:HD13	1:E:104:LEU:HD21	1.71	0.71
1:E:25:GLN:HA	1:E:28:GLN:HG2	1.73	0.70
2:B:408:VAL:HG23	2:B:421:ALA:HB3	1.74	0.70
1:E:103:ASN:HD21	2:F:502:PHE:HB3	1.57	0.70
2:F:368:ARG:NH1	2:F:372:GLU:OE2	2.25	0.70
1:C:24:ILE:O	1:C:28:GLN:NE2	2.24	0.69
1:A:155:GLN:O	1:A:159:GLN:NE2	2.25	0.69
2:D:359:ILE:HB	2:D:363:GLN:HE21	1.58	0.69
2:F:547:VAL:HG22	2:F:632:MET:HE2	1.75	0.68
2:B:329:GLN:OE1	2:B:419:ARG:NH2	2.27	0.67
2:D:351:ILE:HD11	2:D:386:VAL:HG22	1.77	0.67
1:A:42:ILE:HD13	1:A:151:GLN:HB2	1.77	0.66
2:B:271:LYS:NZ	2:B:305:GLN:OE1	2.20	0.66
2:D:358:ILE:HG21	2:D:385:ARG:HE	1.60	0.65
1:C:60:LEU:HD21	1:C:142:THR:HG22	1.77	0.65
1:A:70:LEU:H	1:A:74:LYS:CE	2.09	0.65
2:B:417:HIS:ND1	1:C:58:THR:CG2	2.54	0.64
1:E:151:GLN:HG3	1:E:155:GLN:HE22	1.62	0.64
2:F:351:ILE:HD11	2:F:386:VAL:HG22	1.80	0.64
2:D:334:PHE:HB2	2:D:349:HIS:HB2	1.78	0.64
1:E:41:ARG:HH21	2:F:440:LEU:HG	1.63	0.64
2:D:455:LEU:HD21	2:D:515:HIS:HD2	1.64	0.63
1:A:94:VAL:HA	1:A:97:ILE:HG12	1.80	0.63
1:A:103:ASN:HD21	2:B:502:PHE:C	2.07	0.63
1:E:101:LEU:HA	1:E:104:LEU:HG	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:ILE:HB	2:D:363:GLN:NE2	2.14	0.62
2:D:415:ALA:HB2	1:E:56:ARG:HH22	1.62	0.62
2:D:415:ALA:CB	1:E:56:ARG:HH12	2.11	0.62
2:B:310:ARG:NH2	2:B:315:GLY:HA2	2.14	0.62
2:B:397:THR:HG23	2:B:425:VAL:HB	1.81	0.62
2:F:366:TRP:CZ3	2:F:410:CYS:HB3	2.34	0.62
1:E:157:ILE:O	1:E:161:LEU:HG	1.99	0.62
1:E:27:VAL:HG11	1:E:110:LEU:HD11	1.80	0.62
1:E:71:SER:O	1:E:74:LYS:HG2	1.99	0.62
2:B:503:LEU:HD22	2:B:504:LEU:HD22	1.81	0.62
1:A:70:LEU:N	1:A:74:LYS:HE3	2.14	0.61
2:B:455:LEU:HD21	2:B:515:HIS:HD2	1.65	0.61
2:B:351:ILE:HD11	2:B:386:VAL:HG22	1.83	0.61
2:F:488:LEU:HB2	2:F:494:TYR:CE1	2.35	0.61
2:B:334:PHE:HB2	2:B:349:HIS:HB2	1.81	0.61
1:A:69:ILE:HG12	1:A:75:MET:HG2	1.81	0.61
2:F:408:VAL:HG23	2:F:421:ALA:HB3	1.82	0.61
2:D:418:HIS:HD2	1:E:59:GLY:HA3	1.64	0.61
2:D:419:ARG:NH2	2:D:420:TYR:O	2.34	0.61
1:C:72:LEU:HA	1:C:75:MET:HE2	1.83	0.61
2:B:405:TYR:CD2	2:B:422:GLU:HG3	2.35	0.60
2:D:397:THR:HG23	2:D:425:VAL:HB	1.83	0.60
2:B:469:LEU:HG	2:B:470:TYR:CD2	2.36	0.60
2:F:397:THR:HG23	2:F:425:VAL:HB	1.83	0.60
2:F:455:LEU:HD21	2:F:515:HIS:HD2	1.67	0.60
1:A:60:LEU:HB3	1:A:63:ILE:HD12	1.83	0.60
1:C:56:ARG:NH2	1:C:61:ASP:OD2	2.34	0.60
1:A:79:LEU:HD12	1:A:101:LEU:HD22	1.84	0.59
1:E:71:SER:H	1:E:74:LYS:CE	2.16	0.59
2:D:417:HIS:ND1	1:E:58:THR:CG2	2.58	0.59
1:E:42:ILE:HD12	1:E:151:GLN:HB2	1.85	0.59
1:A:83:GLN:O	1:A:87:THR:HG23	2.03	0.58
1:A:155:GLN:HG3	1:A:159:GLN:HE22	1.68	0.58
2:D:360:SER:H	2:D:363:GLN:HE22	1.51	0.58
1:C:83:GLN:O	1:C:87:THR:HG23	2.02	0.58
2:F:357:GLN:NE2	2:F:358:ILE:O	2.36	0.58
1:E:141:SER:O	1:E:145:VAL:HG12	2.03	0.58
2:B:340:THR:HG22	2:B:341:SER:H	1.69	0.58
1:E:154:LEU:HA	1:E:157:ILE:HG22	1.86	0.58
1:A:72:LEU:HA	1:A:75:MET:HE3	1.85	0.57
2:D:367:TRP:CE2	2:D:373:LYS:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ARG:NH2	2:F:440:LEU:HG	2.20	0.57
2:B:430:ILE:HD13	2:B:511:ILE:HG13	1.86	0.57
2:F:340:THR:HG22	2:F:341:SER:H	1.70	0.57
2:B:305:GLN:NE2	2:B:321:SER:O	2.34	0.57
2:B:417:HIS:CG	1:C:58:THR:HG23	2.37	0.57
1:C:33:THR:HG23	1:C:36:LYS:HE3	1.87	0.57
2:B:443:MET:HG3	2:B:498:PHE:HB2	1.86	0.57
1:E:71:SER:N	1:E:74:LYS:HZ2	2.03	0.57
2:D:417:HIS:CG	1:E:58:THR:HG23	2.39	0.56
1:C:158:LEU:HD12	1:C:161:LEU:HD21	1.88	0.56
2:B:369:ASN:OD1	2:B:407:ALA:N	2.35	0.56
1:E:71:SER:H	1:E:74:LYS:HD3	1.69	0.56
2:F:436:THR:HG23	2:F:532:VAL:HG23	1.87	0.56
1:C:52:SER:HB3	1:C:55:GLN:HB2	1.87	0.55
2:F:570:ILE:HG22	2:F:609:VAL:HG22	1.89	0.55
2:B:436:THR:HG22	2:B:443:MET:HB3	1.89	0.55
1:C:48:THR:HG22	1:C:144:VAL:HA	1.88	0.55
1:E:23:PRO:O	1:E:26:LYS:HG3	2.06	0.55
1:E:51:VAL:HG21	1:E:144:VAL:HG21	1.89	0.55
1:A:29:ASP:HA	1:A:32:LYS:HE2	1.88	0.55
1:C:72:LEU:HB2	1:C:167:CYS:HA	1.89	0.55
2:D:332:VAL:CG2	2:D:351:ILE:HB	2.37	0.55
1:A:56:ARG:NH2	2:F:415:ALA:HA	2.16	0.55
1:A:102:GLU:HG3	2:B:502:PHE:HE2	1.71	0.55
2:B:418:HIS:HD2	1:C:59:GLY:HA3	1.71	0.54
1:C:69:ILE:HG22	1:C:75:MET:SD	2.47	0.54
2:B:432:ILE:HD11	2:B:511:ILE:HG12	1.88	0.54
1:E:71:SER:H	1:E:74:LYS:NZ	2.04	0.54
1:E:89:LEU:HD22	1:E:94:VAL:HG21	1.89	0.54
1:C:129:GLU:HG2	1:C:130:SER:H	1.73	0.54
1:C:86:LEU:HD22	1:C:94:VAL:HG13	1.88	0.54
1:E:71:SER:H	1:E:74:LYS:CD	2.21	0.54
2:F:244:MET:HG3	2:F:254:ILE:HG12	1.89	0.54
2:F:310:ARG:NH1	2:F:315:GLY:HA2	2.23	0.54
1:E:74:LYS:HG3	1:E:75:MET:N	2.23	0.54
2:B:488:LEU:HB2	2:B:494:TYR:CE1	2.43	0.54
1:E:28:GLN:O	1:E:32:LYS:HD3	2.08	0.54
1:E:72:LEU:HA	1:E:75:MET:HG2	1.89	0.54
2:B:259:GLN:HB3	2:B:261:MET:SD	2.48	0.54
1:C:69:ILE:HD13	1:C:74:LYS:HE2	1.91	0.53
1:E:67:HIS:O	1:E:68:PRO:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:GLY:HA3	1:E:149:ARG:HE	1.74	0.53
2:D:366:TRP:CD2	2:D:389:VAL:HB	2.43	0.53
1:E:27:VAL:O	1:E:31:THR:HG23	2.08	0.53
1:A:46:SER:O	1:A:49:GLN:HG3	2.08	0.53
1:E:97:ILE:O	1:E:101:LEU:HD23	2.09	0.53
2:F:552:LEU:HD23	2:F:596:LEU:HD12	1.89	0.53
1:E:37:THR:HG23	2:F:561:PHE:CZ	2.44	0.53
2:B:244:MET:HE1	2:B:324:GLN:CG	2.38	0.53
2:B:486:CYS:CA	2:B:496:CYS:HB3	2.23	0.53
1:E:26:LYS:HE3	1:E:27:VAL:HG23	1.91	0.53
2:F:436:THR:OG1	2:F:533:VAL:HA	2.09	0.53
1:E:69:ILE:CA	1:E:74:LYS:HE3	2.40	0.52
2:B:298:PRO:HG2	2:B:353:LYS:HD3	1.91	0.52
1:C:32:LYS:HE2	1:C:158:LEU:HD11	1.92	0.52
2:B:417:HIS:HA	1:C:58:THR:HG23	1.92	0.52
2:F:329:GLN:HG3	2:F:419:ARG:HH22	1.74	0.52
1:C:69:ILE:HD13	1:C:74:LYS:HZ3	1.74	0.52
1:E:129:GLU:HG2	1:E:130:SER:H	1.74	0.52
2:F:409:TYR:CE2	2:F:420:TYR:HB3	2.45	0.52
2:D:250:GLY:HA3	2:D:334:PHE:CE1	2.46	0.51
1:A:35:ILE:O	1:A:39:VAL:HG23	2.11	0.51
2:B:488:LEU:HA	2:B:494:TYR:HA	1.93	0.51
2:D:448:SER:HB2	2:D:493:PHE:CE2	2.45	0.51
1:C:36:LYS:HD3	2:D:563:GLU:HG3	1.92	0.51
1:C:132:ASP:OD1	1:C:133:GLY:N	2.43	0.51
1:C:32:LYS:HE3	1:C:161:LEU:HD11	1.92	0.51
1:C:36:LYS:HZ3	2:D:563:GLU:H	1.58	0.51
2:F:570:ILE:HD12	2:F:596:LEU:HD11	1.91	0.51
1:A:158:LEU:HD12	1:A:161:LEU:HD21	1.93	0.51
1:C:27:VAL:O	1:C:31:THR:HG23	2.11	0.51
2:D:349:HIS:CE1	2:D:382:VAL:HG21	2.45	0.51
1:E:74:LYS:CG	1:E:75:MET:N	2.74	0.51
2:B:264:PHE:CE1	2:B:310:ARG:HG2	2.46	0.51
1:C:33:THR:O	1:C:36:LYS:HG3	2.11	0.51
2:F:417:HIS:HD2	2:F:419:ARG:HB2	1.75	0.51
1:C:89:LEU:HB2	1:C:94:VAL:HG11	1.93	0.51
2:D:419:ARG:NH1	1:E:137:ALA:O	2.44	0.50
1:A:28:GLN:O	1:A:32:LYS:HD3	2.12	0.50
2:D:409:TYR:CE2	2:D:420:TYR:HB3	2.47	0.50
1:E:35:ILE:O	1:E:38:ILE:HG22	2.12	0.50
1:A:154:LEU:HA	1:A:157:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:PRO:HD2	1:E:82:TYR:CZ	2.45	0.50
1:A:154:LEU:O	1:A:157:ILE:HG22	2.12	0.50
1:A:108:LEU:HA	1:A:111:LEU:HG	1.94	0.50
1:C:36:LYS:NZ	2:D:563:GLU:H	2.09	0.49
2:D:529:PRO:HA	2:D:532:VAL:HG12	1.94	0.49
2:B:242:LEU:HD11	2:B:306:VAL:HG23	1.93	0.49
2:B:566:LEU:HD23	2:B:613:ARG:HA	1.92	0.49
2:D:509:MET:HE1	2:D:527:VAL:HG22	1.93	0.49
1:E:107:LEU:HD23	1:E:110:LEU:HD21	1.94	0.49
2:D:426:ILE:HG23	2:D:428:VAL:HG23	1.94	0.49
2:F:243:HIS:ND1	2:F:245:GLU:OE2	2.45	0.49
1:A:72:LEU:HD21	1:A:111:LEU:HD11	1.94	0.49
2:B:250:GLY:O	2:B:296:VAL:HG22	2.12	0.49
2:B:361:SER:HA	2:B:364:ILE:HD12	1.93	0.49
2:B:502:PHE:CB	2:B:505:SER:HB2	2.42	0.49
1:C:41:ARG:HD2	1:C:97:ILE:HD11	1.95	0.49
2:F:566:LEU:HD23	2:F:613:ARG:HA	1.94	0.49
2:B:300:SER:H	2:B:328:THR:HG1	1.60	0.49
2:B:570:ILE:HD12	2:B:608:GLN:O	2.13	0.49
1:E:102:GLU:O	1:E:105:ARG:HG2	2.12	0.49
1:A:52:SER:HB3	1:A:55:GLN:HB2	1.95	0.49
2:B:349:HIS:CE1	2:B:382:VAL:HG21	2.48	0.49
1:C:143:GLU:O	1:C:147:LEU:HD13	2.12	0.49
2:F:349:HIS:CE1	2:F:382:VAL:HG21	2.48	0.49
1:A:32:LYS:C	1:A:36:LYS:HZ2	2.21	0.49
1:E:132:ASP:OD1	1:E:133:GLY:N	2.46	0.49
1:C:67:HIS:O	1:C:68:PRO:C	2.55	0.49
2:D:319:ASP:OD2	2:D:319:ASP:N	2.44	0.49
2:D:332:VAL:HG23	2:D:351:ILE:HB	1.95	0.49
2:D:361:SER:HB2	2:D:381:ILE:HG12	1.95	0.49
2:D:566:LEU:HD23	2:D:613:ARG:HA	1.94	0.49
1:C:82:TYR:O	1:C:86:LEU:HG	2.13	0.48
1:C:154:LEU:HA	1:C:157:ILE:HG22	1.94	0.48
2:D:416:CYS:O	1:E:58:THR:HG22	2.12	0.48
1:A:71:SER:OG	1:A:74:LYS:HG2	2.14	0.48
2:F:369:ASN:CG	2:F:400:ARG:HH22	2.21	0.48
2:B:359:ILE:HD12	2:B:363:GLN:HB2	1.95	0.48
2:F:264:PHE:CE1	2:F:310:ARG:HG2	2.49	0.48
1:A:28:GLN:HB3	1:A:32:LYS:HZ2	1.78	0.48
1:A:69:ILE:HA	1:A:74:LYS:HE3	1.94	0.48
1:A:64:PRO:HG3	1:A:81:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:HD11	1:A:147:LEU:O	2.13	0.48
2:F:446:ARG:NH1	2:F:491:ASP:OD2	2.42	0.48
1:A:36:LYS:HG3	2:B:563:GLU:HG3	1.96	0.48
1:A:63:ILE:HG22	1:A:149:ARG:HD2	1.96	0.48
2:D:443:MET:SD	2:D:445:CYS:SG	3.12	0.48
2:F:242:LEU:HD21	2:F:306:VAL:HG23	1.96	0.48
2:F:304:VAL:O	2:F:323:PRO:HA	2.14	0.48
2:B:443:MET:CG	2:B:498:PHE:HB2	2.43	0.48
1:E:69:ILE:CD1	1:E:74:LYS:HE2	2.44	0.48
1:A:91:SER:O	1:A:95:LEU:HD23	2.14	0.48
2:B:448:SER:HB2	2:B:493:PHE:CE2	2.49	0.47
2:D:570:ILE:O	2:D:583:THR:HA	2.14	0.47
2:F:370:LEU:HG	2:F:409:TYR:CE1	2.49	0.47
1:E:71:SER:N	1:E:74:LYS:NZ	2.60	0.47
1:A:67:HIS:O	1:A:68:PRO:C	2.56	0.47
2:B:340:THR:HG22	2:B:341:SER:N	2.28	0.47
1:A:106:ASP:O	1:A:110:LEU:HD23	2.14	0.47
1:A:155:GLN:HG3	1:A:159:GLN:NE2	2.29	0.47
1:E:69:ILE:HD12	1:E:74:LYS:HE2	1.97	0.47
1:E:156:ASP:O	1:E:160:GLN:HG2	2.15	0.47
2:F:340:THR:HG22	2:F:341:SER:N	2.29	0.47
2:F:359:ILE:HG21	2:F:412:ASN:ND2	2.29	0.47
1:E:71:SER:C	1:E:74:LYS:HZ3	2.16	0.47
1:A:35:ILE:O	1:A:38:ILE:HG22	2.15	0.47
2:F:417:HIS:CD2	2:F:419:ARG:H	2.32	0.47
1:E:37:THR:HG23	2:F:561:PHE:CE1	2.50	0.46
2:F:302:TYR:O	2:F:325:VAL:HA	2.15	0.46
2:F:448:SER:HB2	2:F:493:PHE:CE2	2.50	0.46
1:A:72:LEU:HD23	1:A:75:MET:HE3	1.96	0.46
1:E:75:MET:SD	1:E:108:LEU:HD23	2.55	0.46
2:B:377:ILE:H	2:B:377:ILE:HD12	1.81	0.46
1:C:62:PHE:HE2	1:C:131:LEU:HD13	1.81	0.46
2:F:464:TYR:HB3	2:F:509:MET:HG3	1.98	0.46
1:A:47:HIS:HD2	1:A:144:VAL:HG12	1.80	0.46
1:E:107:LEU:O	1:E:110:LEU:HG	2.14	0.46
2:D:428:VAL:HG12	2:D:522:SER:HA	1.97	0.46
1:E:72:LEU:HD23	1:E:166:GLU:O	2.16	0.46
2:F:377:ILE:HD12	2:F:377:ILE:H	1.81	0.46
2:F:455:LEU:HD21	2:F:515:HIS:CD2	2.48	0.46
2:D:377:ILE:HD12	2:D:377:ILE:H	1.81	0.46
2:F:234:VAL:HB	2:F:310:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLY:HA3	1:C:149:ARG:HD3	1.98	0.45
2:F:486:CYS:HB2	2:F:496:CYS:HB3	1.17	0.45
2:D:337:LYS:HG2	2:D:422:GLU:HB2	1.98	0.45
2:F:369:ASN:OD1	2:F:407:ALA:N	2.42	0.45
1:A:60:LEU:HD11	1:A:142:THR:HA	1.99	0.45
2:F:468:SER:O	2:F:469:LEU:HD22	2.17	0.45
1:E:41:ARG:HH12	2:F:441:THR:HG22	1.81	0.45
2:B:417:HIS:HA	1:C:58:THR:CG2	2.46	0.45
1:C:157:ILE:HD12	1:C:157:ILE:HA	1.86	0.45
1:E:72:LEU:HD13	1:E:75:MET:SD	2.56	0.45
2:D:364:ILE:HA	2:D:411:CYS:O	2.18	0.45
2:F:570:ILE:CG1	2:F:584:HIS:HB3	2.47	0.45
1:C:69:ILE:HD13	1:C:74:LYS:NZ	2.31	0.44
1:C:93:ASN:OD1	1:C:94:VAL:N	2.50	0.44
1:E:70:LEU:N	1:E:74:LYS:HE3	2.32	0.44
1:A:89:LEU:HB2	1:A:94:VAL:HG11	1.99	0.44
1:E:41:ARG:NH1	1:E:96:GLN:HG2	2.32	0.44
2:B:547:VAL:HG22	2:B:632:MET:HE3	1.98	0.44
2:F:278:ILE:O	2:F:280:ARG:NH1	2.51	0.44
1:C:69:ILE:HD13	1:C:74:LYS:CE	2.47	0.44
2:F:244:MET:HE1	2:F:324:GLN:HB3	1.99	0.44
2:B:428:VAL:HG12	2:B:522:SER:HA	2.00	0.44
1:E:35:ILE:HG21	1:E:158:LEU:HD13	1.99	0.44
1:E:150:LEU:O	1:E:154:LEU:HD23	2.18	0.44
2:F:310:ARG:CZ	2:F:315:GLY:HA2	2.48	0.44
2:D:415:ALA:CA	1:E:56:ARG:HH12	2.31	0.44
2:F:507:TYR:HB3	2:F:509:MET:SD	2.58	0.44
2:B:443:MET:CE	2:B:529:PRO:HG3	2.47	0.44
2:F:366:TRP:CE3	2:F:410:CYS:HB3	2.53	0.44
2:D:282:ALA:HB1	2:D:284:GLU:OE2	2.18	0.43
1:E:35:ILE:O	1:E:39:VAL:HG23	2.19	0.43
1:E:72:LEU:O	1:E:75:MET:HG2	2.18	0.43
1:A:82:TYR:O	1:A:86:LEU:HD13	2.18	0.43
1:C:103:ASN:OD1	2:D:504:LEU:C	2.61	0.43
2:B:503:LEU:CD2	2:B:504:LEU:HD22	2.48	0.43
2:D:415:ALA:HB2	1:E:56:ARG:HH12	1.83	0.43
2:F:330:ASP:OD1	2:F:353:LYS:HE2	2.19	0.43
1:A:138:SER:O	1:A:142:THR:HG23	2.17	0.43
1:E:28:GLN:O	1:E:31:THR:OG1	2.31	0.43
2:F:486:CYS:HB3	2:F:496:CYS:HB2	1.72	0.43
1:C:105:ARG:O	1:C:108:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:TYR:HB3	2:B:509:MET:HG3	2.01	0.43
1:C:101:LEU:HD12	1:C:101:LEU:HA	1.58	0.43
1:E:93:ASN:O	1:E:97:ILE:HG12	2.19	0.43
1:E:118:SER:C	1:E:119:LEU:HD22	2.43	0.43
2:B:502:PHE:HB2	2:B:505:SER:HB2	2.00	0.43
2:F:244:MET:HB3	2:F:252:LEU:HD11	2.01	0.43
2:B:422:GLU:HG2	2:B:424:TYR:CE1	2.54	0.42
1:C:85:VAL:HG22	1:C:131:LEU:HD22	2.01	0.42
1:A:132:ASP:OD1	1:A:133:GLY:N	2.53	0.42
2:D:366:TRP:CZ3	2:D:410:CYS:HB3	2.54	0.42
2:D:415:ALA:HA	1:E:56:ARG:HH12	1.84	0.42
2:B:244:MET:HE1	2:B:324:GLN:HG2	2.00	0.42
2:B:244:MET:HE1	2:B:324:GLN:HG3	2.00	0.42
2:B:418:HIS:CE1	2:B:419:ARG:HG3	2.54	0.42
2:D:405:TYR:HB3	2:D:424:TYR:CD2	2.54	0.42
2:F:362:LYS:HE3	2:F:362:LYS:HB2	1.78	0.42
2:B:484:LYS:HG2	2:B:498:PHE:CZ	2.54	0.42
2:F:280:ARG:NH2	2:F:297:LEU:HD12	2.34	0.42
1:A:103:ASN:CB	2:B:504:LEU:HB2	2.45	0.42
1:C:106:ASP:O	1:C:110:LEU:HD23	2.20	0.42
2:F:278:ILE:HB	2:F:280:ARG:NH1	2.23	0.42
1:C:62:PHE:CE2	1:C:131:LEU:HD13	2.55	0.42
1:C:93:ASN:OD1	1:C:94:VAL:HG23	2.19	0.42
2:D:417:HIS:HA	1:E:58:THR:HG23	2.00	0.42
1:C:158:LEU:HA	1:C:161:LEU:CD2	2.49	0.42
2:F:366:TRP:HB3	2:F:374:ILE:HD12	2.00	0.42
2:B:244:MET:HG3	2:B:326:PHE:HB2	2.01	0.42
2:B:358:ILE:CG2	2:B:385:ARG:HB2	2.49	0.42
2:B:250:GLY:HA3	2:B:334:PHE:CE2	2.55	0.42
2:D:252:LEU:HD22	2:D:254:ILE:HG13	2.01	0.42
1:E:69:ILE:O	1:E:69:ILE:HG23	2.20	0.42
2:F:449:PRO:HG3	2:F:494:TYR:CE2	2.55	0.42
2:B:413:GLU:HG3	2:B:414:GLN:H	1.85	0.42
2:B:570:ILE:O	2:B:583:THR:HA	2.19	0.42
2:D:304:VAL:O	2:D:323:PRO:HA	2.20	0.42
2:D:418:HIS:CE1	2:D:419:ARG:HG2	2.55	0.42
1:A:103:ASN:OD1	2:B:505:SER:OG	2.22	0.41
2:B:469:LEU:HD12	2:B:504:LEU:O	2.19	0.41
1:C:141:SER:HA	1:C:144:VAL:HG22	2.01	0.41
1:E:107:LEU:HA	1:E:110:LEU:HG	2.01	0.41
1:C:154:LEU:O	1:C:157:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:MET:O	1:A:78:THR:OG1	2.35	0.41
1:A:83:GLN:NE2	1:A:105:ARG:HD3	2.35	0.41
2:B:458:SER:HB2	2:B:515:HIS:HA	2.02	0.41
1:C:64:PRO:O	1:C:82:TYR:OH	2.32	0.41
2:D:359:ILE:HD12	2:D:363:GLN:HG2	2.02	0.41
2:D:370:LEU:HG	2:D:409:TYR:CE1	2.56	0.41
2:D:509:MET:SD	2:D:509:MET:N	2.93	0.41
2:F:439:TYR:O	2:F:441:THR:HG23	2.20	0.41
1:E:82:TYR:O	1:E:86:LEU:HG	2.21	0.41
1:A:103:ASN:O	1:A:107:LEU:HD13	2.21	0.41
2:B:337:LYS:HG2	2:B:422:GLU:HB3	2.02	0.41
2:B:417:HIS:CB	1:C:58:THR:HG23	2.50	0.41
1:E:72:LEU:HA	1:E:75:MET:HE3	2.02	0.41
1:E:131:LEU:HD12	1:E:132:ASP:N	2.35	0.41
1:A:72:LEU:HD13	1:A:112:ALA:HB2	2.03	0.41
2:B:449:PRO:HG3	2:B:494:TYR:CE2	2.56	0.41
2:F:280:ARG:HH22	2:F:297:LEU:HD12	1.86	0.41
2:F:468:SER:C	2:F:469:LEU:HD22	2.46	0.41
1:A:69:ILE:O	1:A:69:ILE:HG23	2.21	0.41
2:B:512:ARG:HD3	2:B:514:ASN:OD1	2.21	0.41
2:B:570:ILE:CG2	2:B:584:HIS:HB3	2.51	0.41
2:B:571:ARG:NH2	2:B:608:GLN:OE1	2.37	0.41
2:D:426:ILE:HG23	2:D:428:VAL:CG2	2.50	0.41
2:D:612:ARG:HB2	2:D:620:TRP:CD2	2.56	0.41
1:E:37:THR:O	1:E:40:THR:HG22	2.21	0.41
1:A:72:LEU:HD12	1:A:167:CYS:SG	2.61	0.41
1:C:69:ILE:HA	1:C:74:LYS:HD3	2.03	0.41
2:D:349:HIS:ND1	2:D:382:VAL:HG21	2.36	0.41
2:D:360:SER:N	2:D:363:GLN:HE22	2.17	0.41
1:E:106:ASP:OD2	2:F:468:SER:HB3	2.21	0.41
1:A:74:LYS:HA	1:A:77:GLN:HG2	2.02	0.40
1:A:143:GLU:OE2	1:A:147:LEU:HD12	2.21	0.40
2:D:434:CYS:HB3	2:D:443:MET:SD	2.61	0.40
2:F:408:VAL:CG2	2:F:421:ALA:HB3	2.49	0.40
1:A:162:ASP:N	1:A:162:ASP:OD1	2.54	0.40
1:C:38:ILE:HD11	1:C:100:ASP:CB	2.51	0.40
1:C:64:PRO:HD2	1:C:82:TYR:HE1	1.86	0.40
2:D:405:TYR:HB3	2:D:424:TYR:CE2	2.57	0.40
2:B:242:LEU:HD23	2:B:256:TRP:HB3	2.03	0.40
2:D:312:ASP:OD2	2:D:312:ASP:N	2.42	0.40
2:D:374:ILE:O	2:D:379:TYR:OH	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:PRO:HG2	1:E:26:LYS:CG	2.46	0.40
2:F:272:TYR:CZ	2:F:282:ALA:HB3	2.56	0.40
2:F:405:TYR:HB3	2:F:424:TYR:CE2	2.57	0.40
2:B:416:CYS:O	1:C:58:THR:HG22	2.20	0.40
2:F:373:LYS:HE3	2:F:373:LYS:HB3	1.90	0.40
2:F:458:SER:HB2	2:F:515:HIS:CD2	2.56	0.40
1:A:85:VAL:HA	1:A:131:LEU:HD21	2.04	0.40
1:E:83:GLN:NE2	1:E:105:ARG:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	136/174 (78%)	122 (90%)	12 (9%)	2 (2%)	8	38
1	C	136/174 (78%)	122 (90%)	12 (9%)	2 (2%)	8	38
1	E	136/174 (78%)	122 (90%)	12 (9%)	2 (2%)	8	38
2	B	397/868 (46%)	381 (96%)	16 (4%)	0	100	100
2	D	397/868 (46%)	382 (96%)	15 (4%)	0	100	100
2	F	397/868 (46%)	380 (96%)	17 (4%)	0	100	100
All	All	1599/3126 (51%)	1509 (94%)	84 (5%)	6 (0%)	31	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	C	68	PRO
1	E	68	PRO
1	A	163	VAL

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Mol	Chain	Res	Type
1	C	163	VAL
1	E	163	VAL

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	129/155 (83%)	129 (100%)	0	100	100
1	C	129/155 (83%)	129 (100%)	0	100	100
1	E	129/155 (83%)	129 (100%)	0	100	100
2	B	367/781 (47%)	367 (100%)	0	100	100
2	D	367/781 (47%)	367 (100%)	0	100	100
2	F	367/781 (47%)	367 (100%)	0	100	100
All	All	1488/2808 (53%)	1488 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	159	GLN
2	B	461	GLN
1	C	28	GLN
1	C	83	GLN
1	C	109	HIS
1	C	151	GLN
1	C	160	GLN
1	E	43	ASN
1	E	155	GLN
2	F	412	ASN
2	F	417	HIS
2	F	465	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

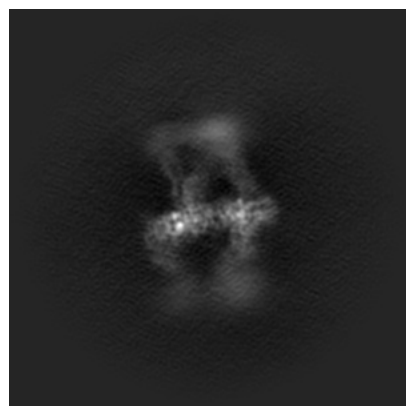
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15679. These allow visual inspection of the internal detail of the map and identification of artifacts.

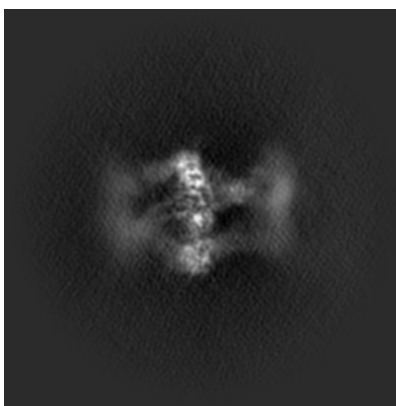
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

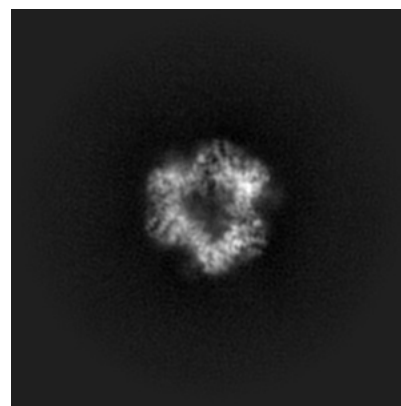
6.1.1 Primary map



X

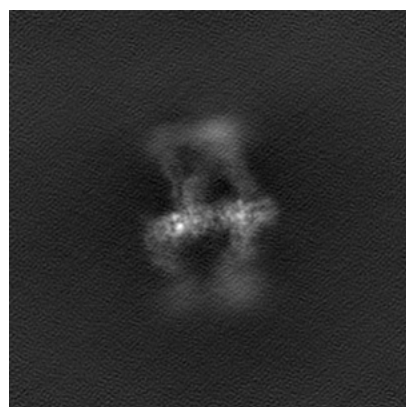


Y

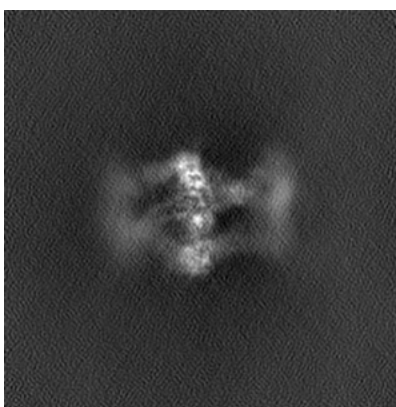


Z

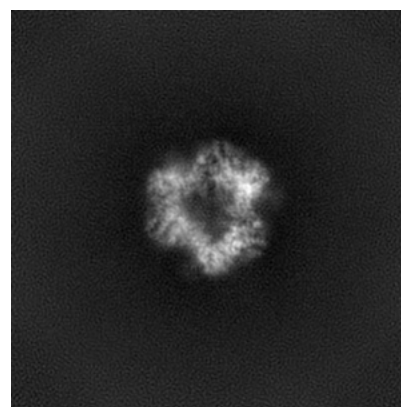
6.1.2 Raw map



X



Y

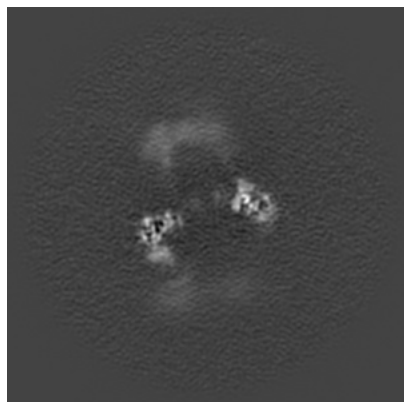


Z

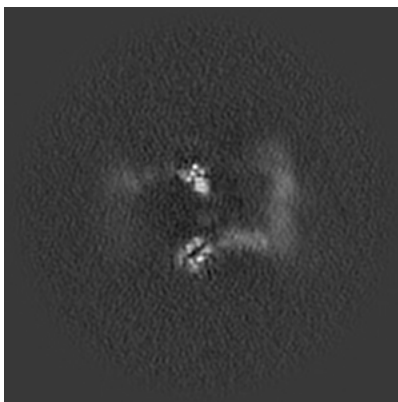
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

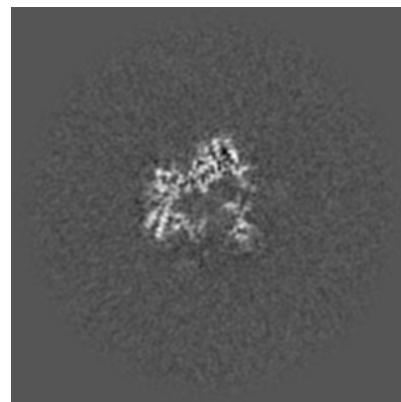
6.2.1 Primary map



X Index: 112

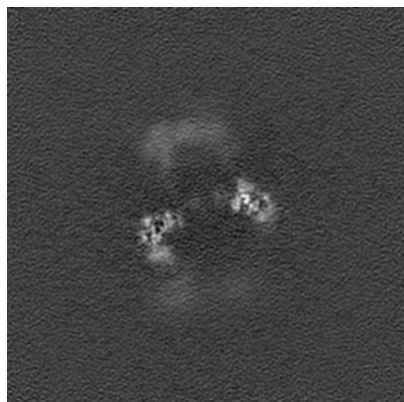


Y Index: 112

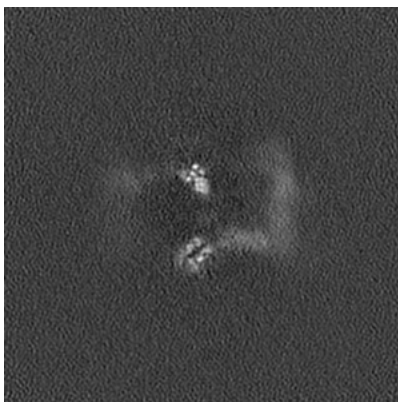


Z Index: 112

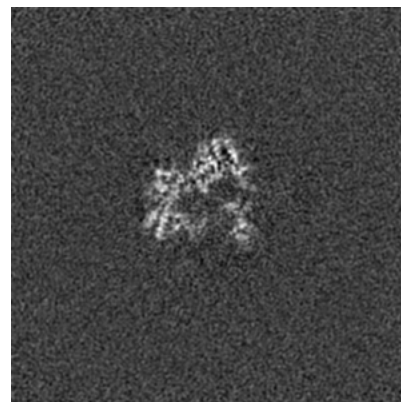
6.2.2 Raw map



X Index: 112



Y Index: 112

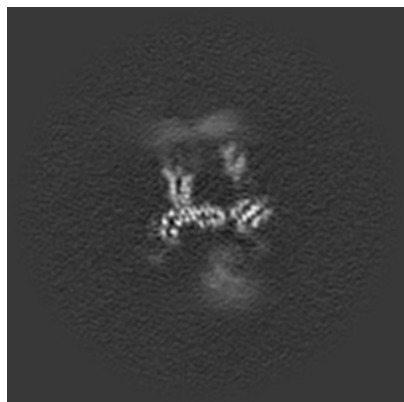


Z Index: 112

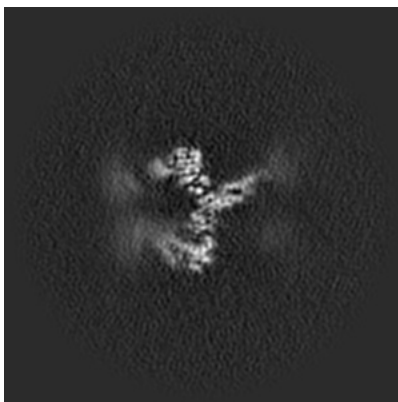
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

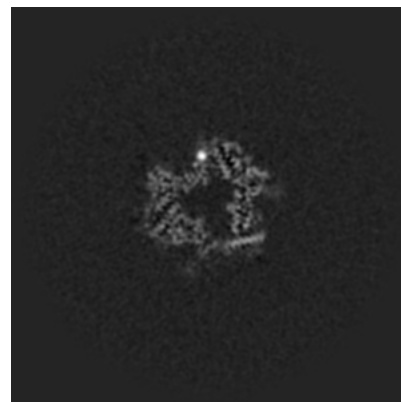
6.3.1 Primary map



X Index: 126

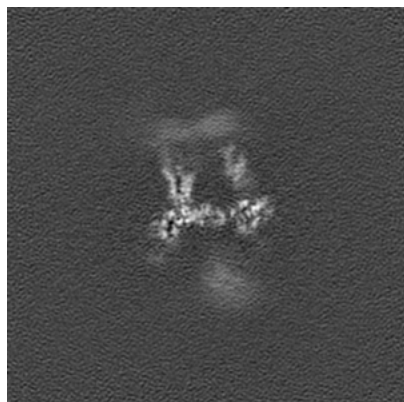


Y Index: 130

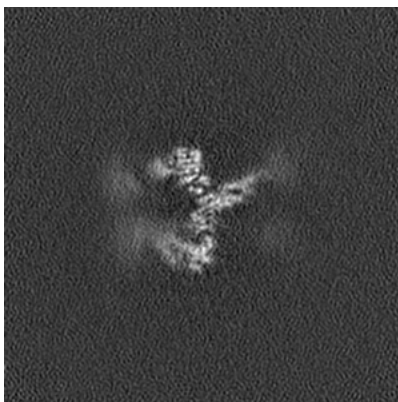


Z Index: 108

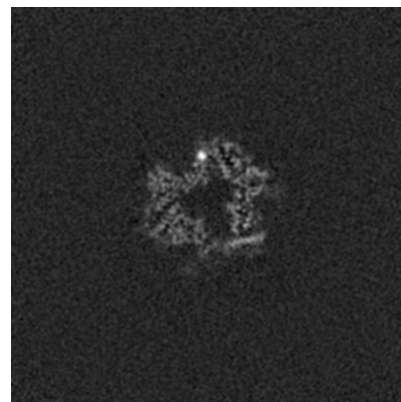
6.3.2 Raw map



X Index: 125



Y Index: 130

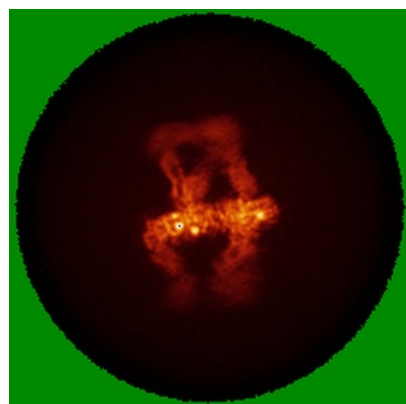


Z Index: 108

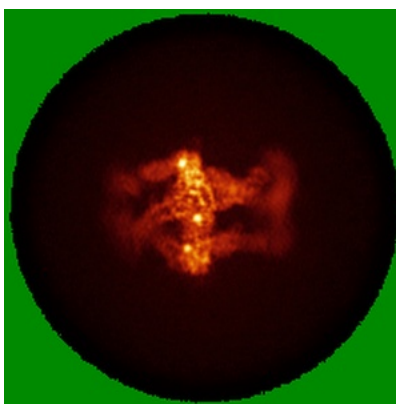
The images above show the largest variance slices of the map in three orthogonal directions.

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

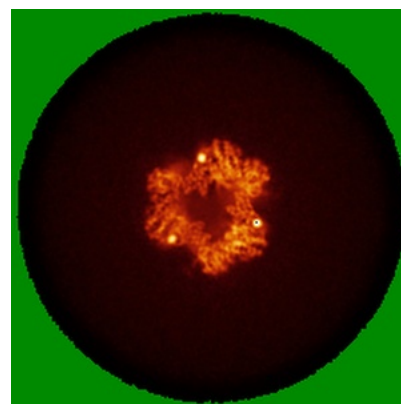
6.4.1 Primary map



X

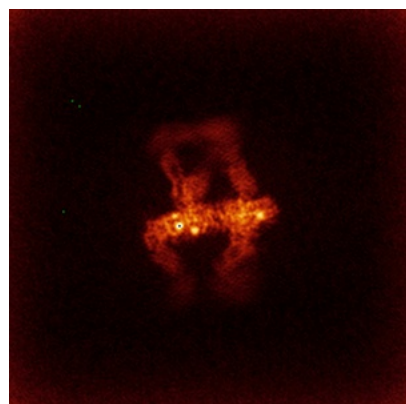


Y

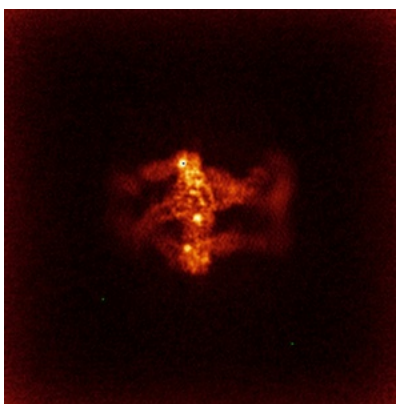


Z

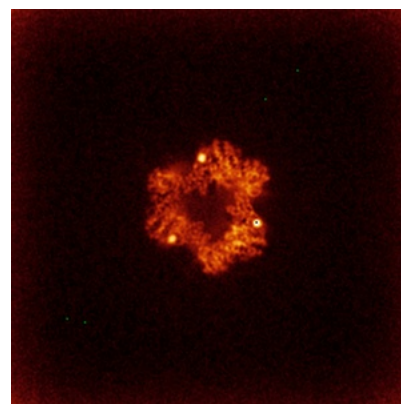
6.4.2 Raw map



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 0.256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

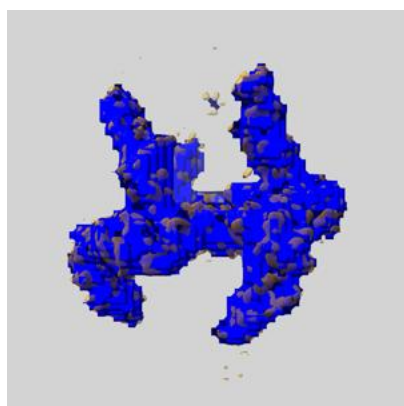
6.6 Mask visualisation [i](#)

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

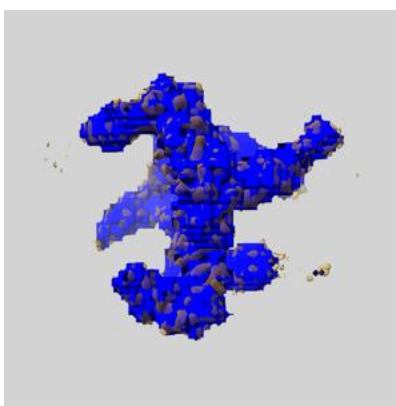
A mask typically either:

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

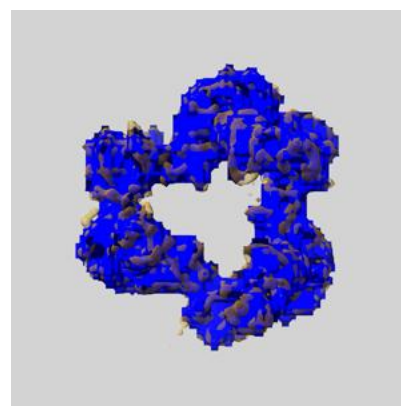
6.6.1 emd_15679_msk_1.map [i](#)



X



Y

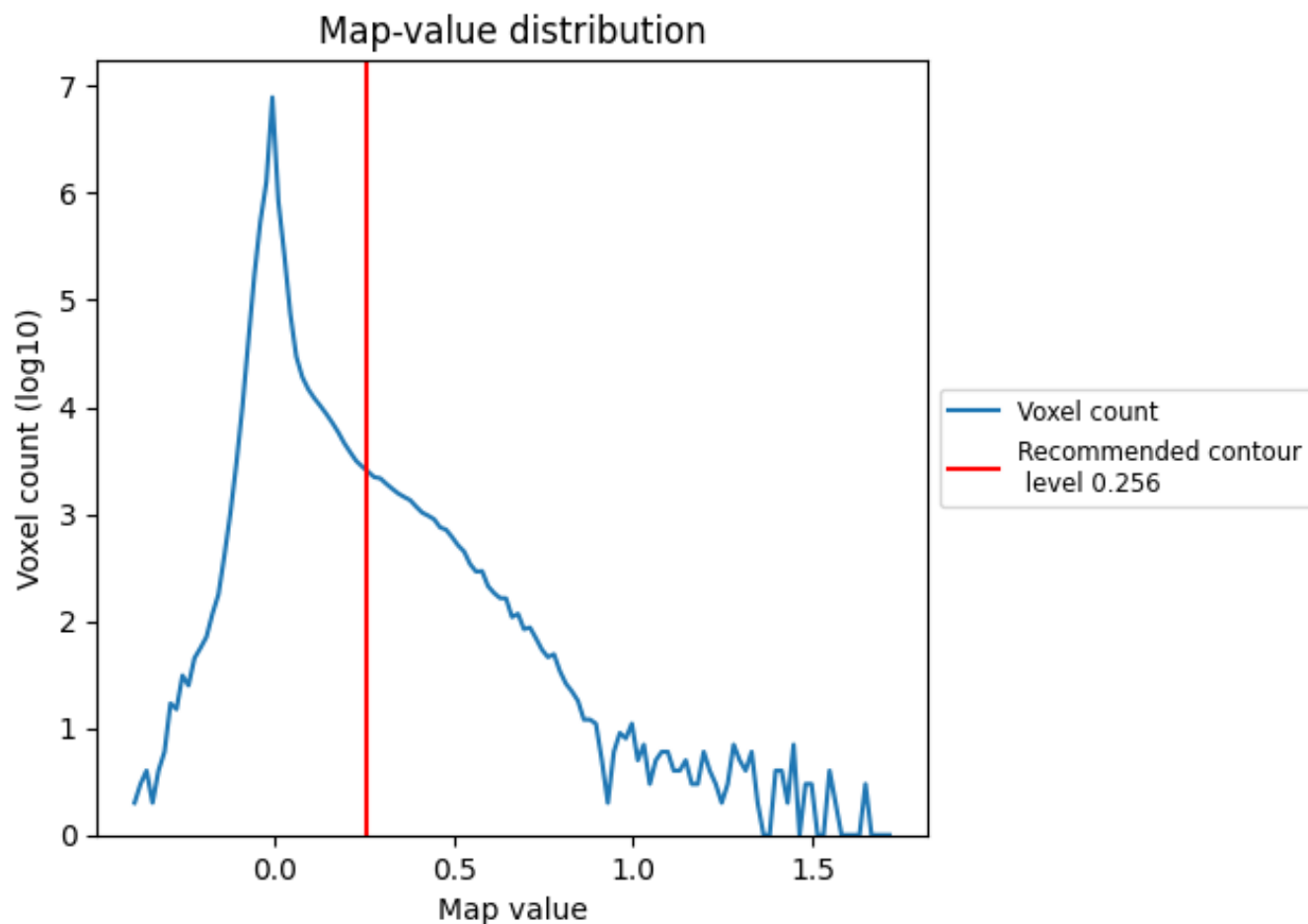


Z

7 Map analysis [i](#)

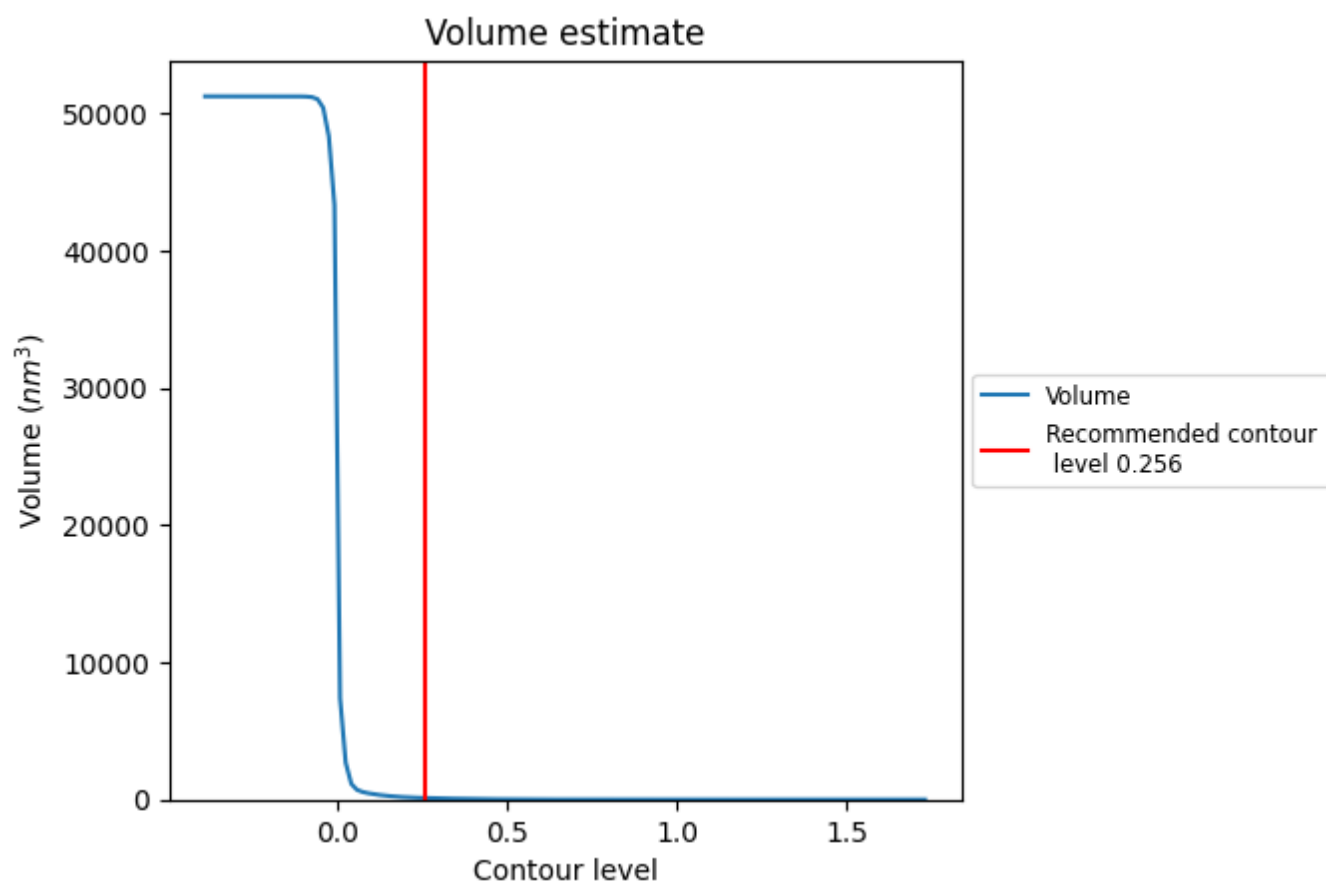
This section contains the results of statistical analysis of the map.

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.

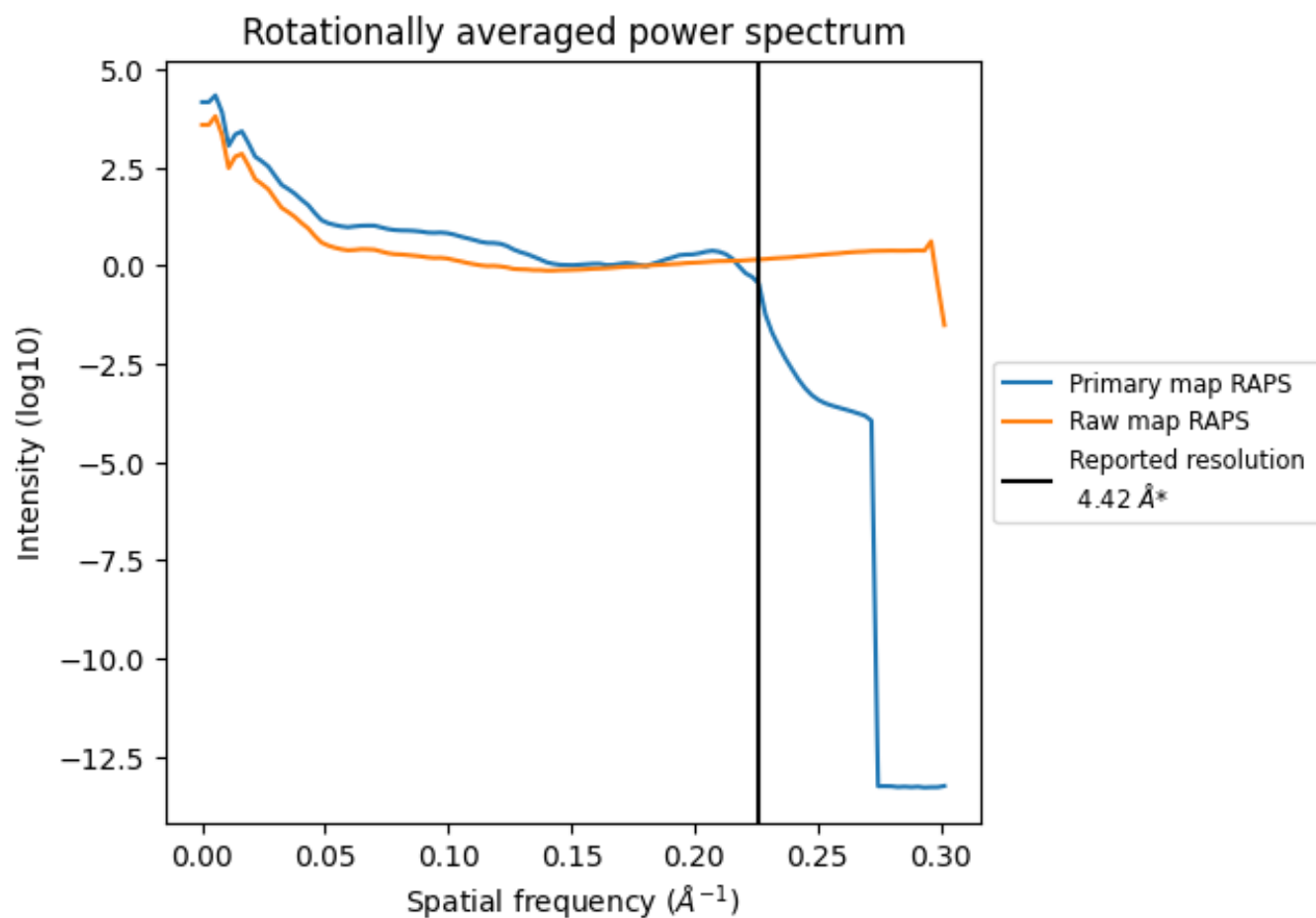
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm^3 ; this corresponds to an approximate mass of 104 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 ⓘ

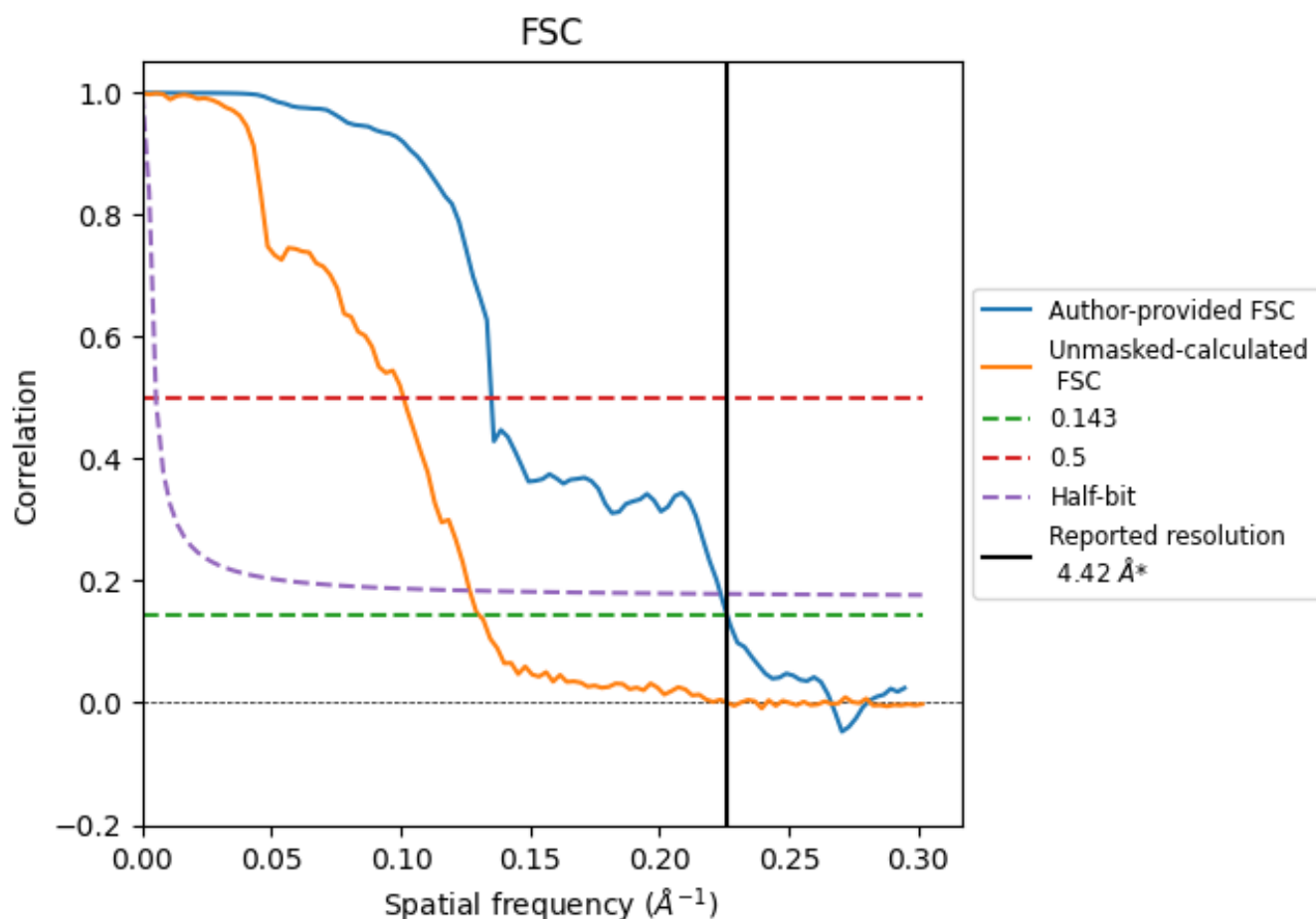


*Reported resolution corresponds to spatial frequency of 0.226 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.226 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

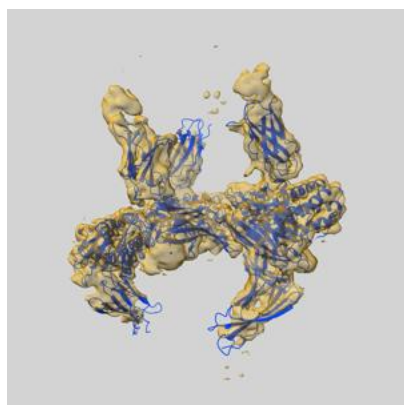
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.42	-	-
Author-provided FSC curve	4.42	7.41	4.47
Unmasked-calculated*	7.66	9.89	7.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.66 differs from the reported value 4.42 by more than 10 %

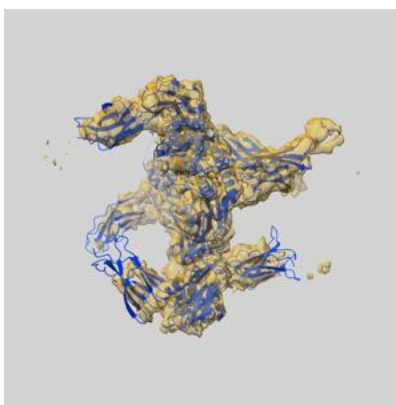
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15679 and PDB model 8AVD. Per-residue inclusion information can be found in section 3 on page 11.

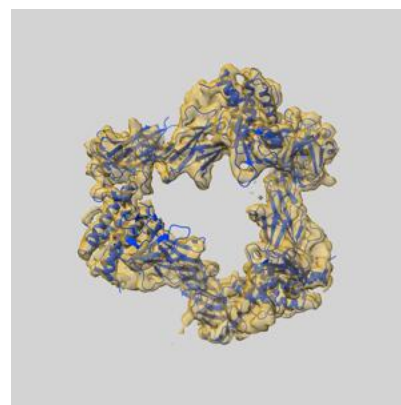
9.1 Map-model overlay [i](#)



X



Y



Z

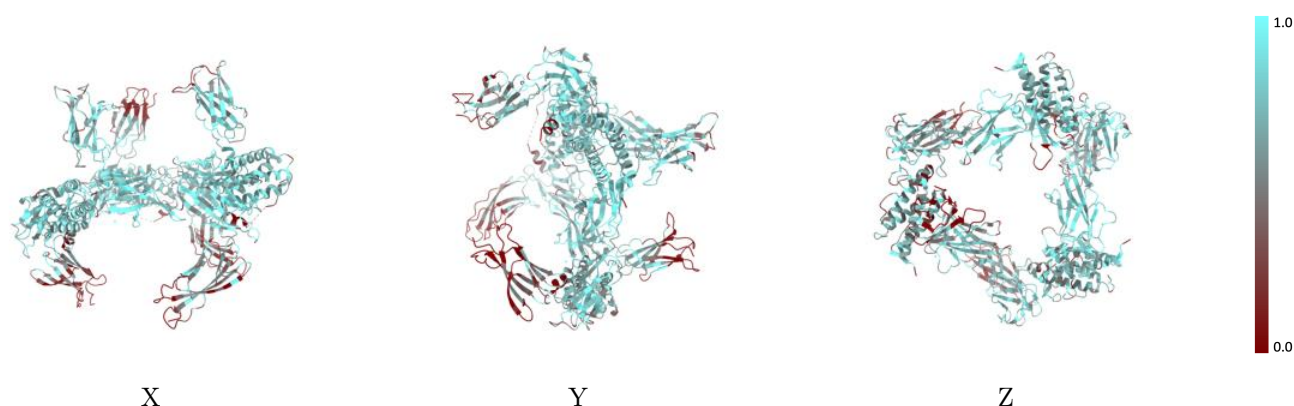
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



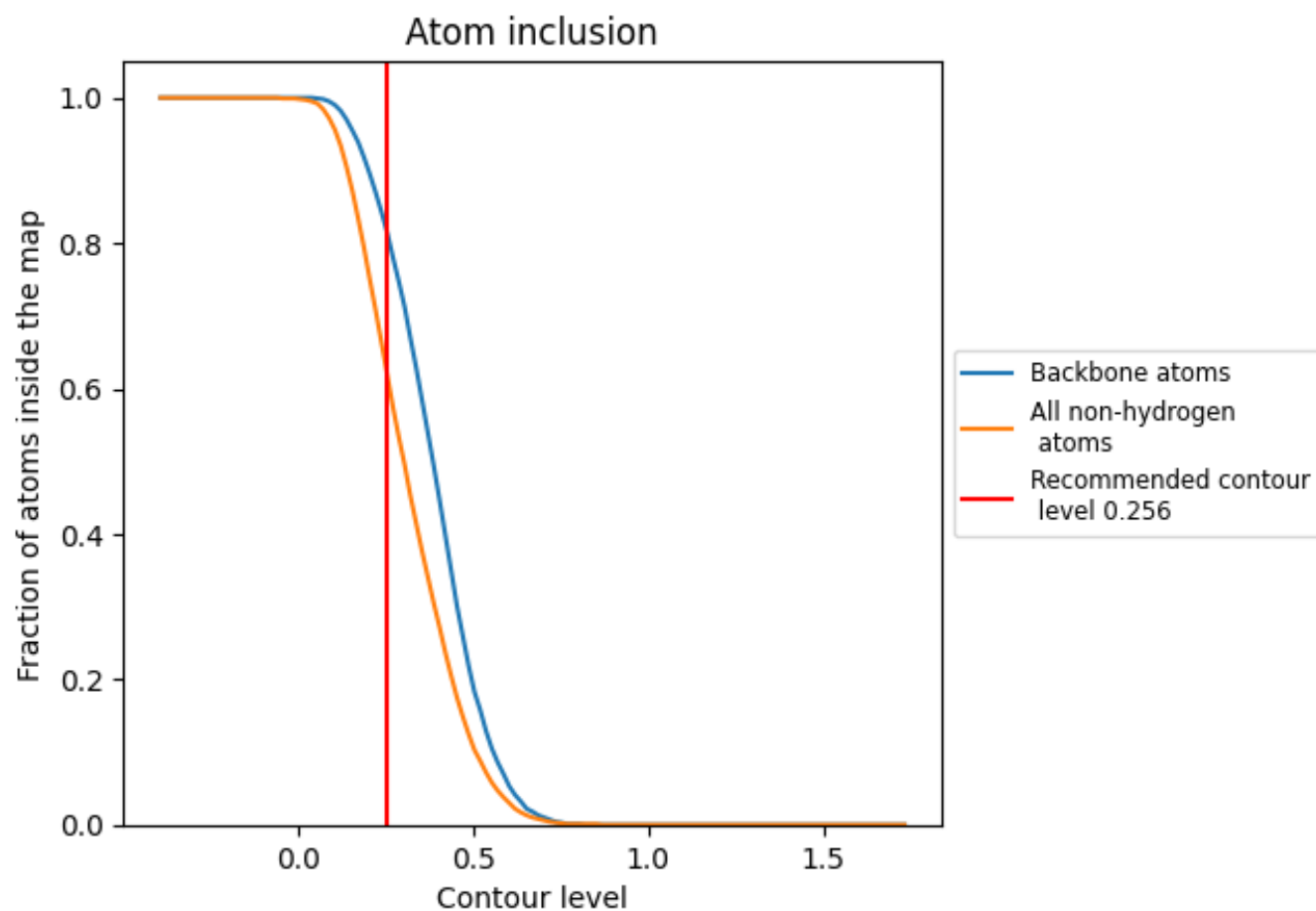
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.256).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 62% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6170	0.2330
A	0.6710	0.2540
B	0.5920	0.2250
C	0.5730	0.2280
D	0.5440	0.2050
E	0.6770	0.2590
F	0.6910	0.2570

1.0

0.0

<0.0