



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:30 AM UTC

PDB ID : 6GSR / pdb_00006gsr
EMDB ID : EMD-0046
Title : Single Particle Cryo-EM map of human Transferrin receptor 1 - H-Ferritin complex at 5.5 Angstrom resolution.
Authors : Testi, C.; Montemiglio, L.C.; Vallone, B.; Des Georges, A.; Boffi, A.; Mancina, F.; Baiocco, P.
Deposited on : 2018-06-15
Resolution : 5.50 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:

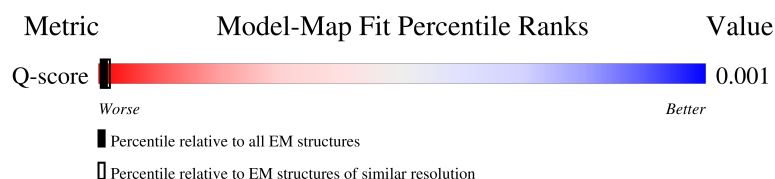
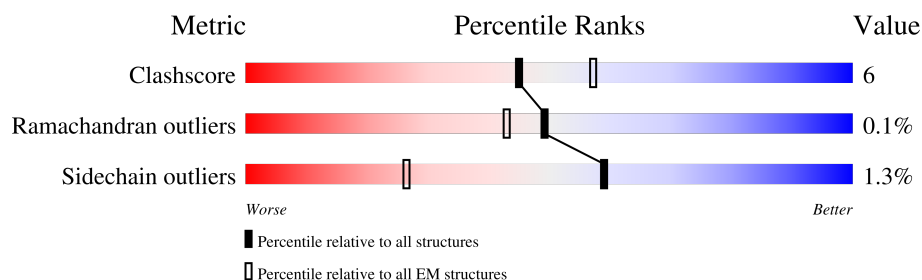
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 5.50 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	520 (5.00 - 6.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	182	
1	Ac	182	
1	Ad	182	
1	Ae	182	

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Mol	Chain	Length	Quality of chain
1	Af	182	95% 90% 5%
1	Ag	182	95% 90% 5%
1	Ah	182	95% 90% 5%
1	Ai	182	95% 90% 5%
1	Aj	182	95% 90% 5%
1	Ak	182	95% 90% 5%
1	Al	182	95% 90% 5%
1	Am	182	95% 90% 5%
1	An	182	95% 90% 5%
1	Ao	182	95% 90% 5%
1	Ap	182	95% 90% 5%
1	Ar	182	95% 90% 5%
1	As	182	95% 90% 5%
1	At	182	95% 90% 5%
1	Au	182	95% 90% 5%
1	Av	182	95% 90% 5%
1	Aw	182	95% 90% 5%
1	Ax	182	95% 90% 5%
1	Ay	182	95% 90% 5%
1	Az	182	95% 90% 5%
2	Ab	640	99% 71% 27% ..
2	Aq	640	99% 72% 25% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 45308 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ac	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ad	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ae	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Af	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ag	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ah	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ai	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Aj	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ak	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Al	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Am	172	Total	C	N	O	S	10	0
			1431	903	244	275	9		
1	An	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ao	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ap	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ar	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	As	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Au	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Av	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Aw	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ax	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Ay	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		
1	Az	172	Total	C	N	O	S	10	0
			1473	931	256	277	9		

- Molecule 2 is a protein called Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	633	Total	C	N	O	S	0	0
			4994	3201	843	936	14		
2	Aq	633	Total	C	N	O	S	0	0
			5004	3210	843	937	14		

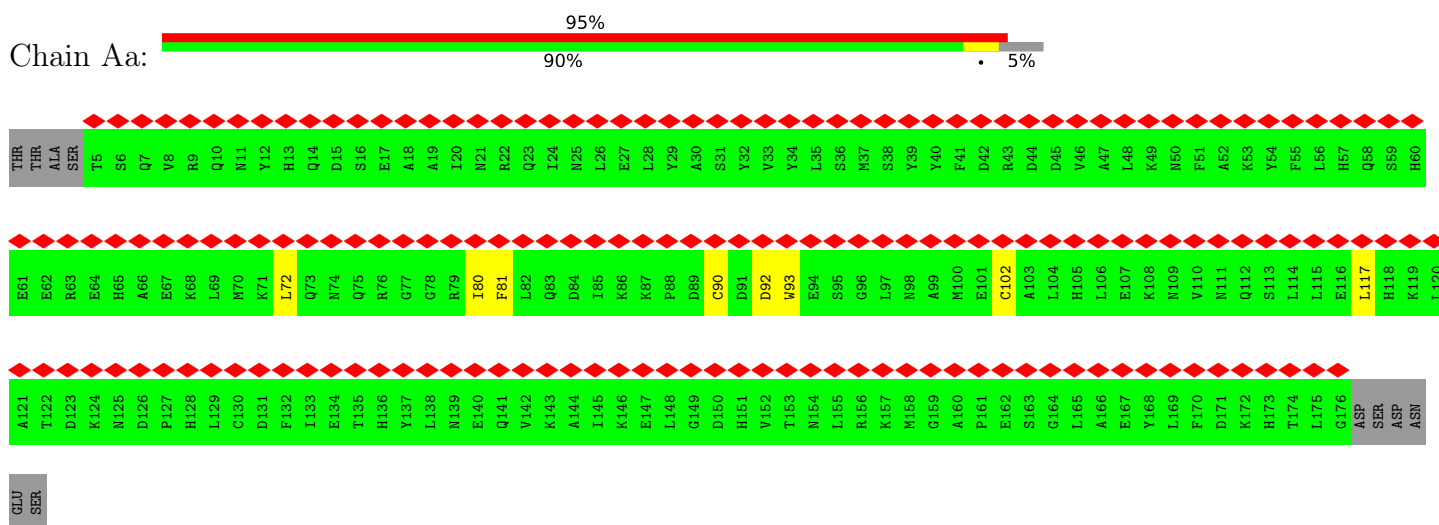
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	142	SER	GLY	conflict	UNP P02786
Aq	142	SER	GLY	conflict	UNP P02786

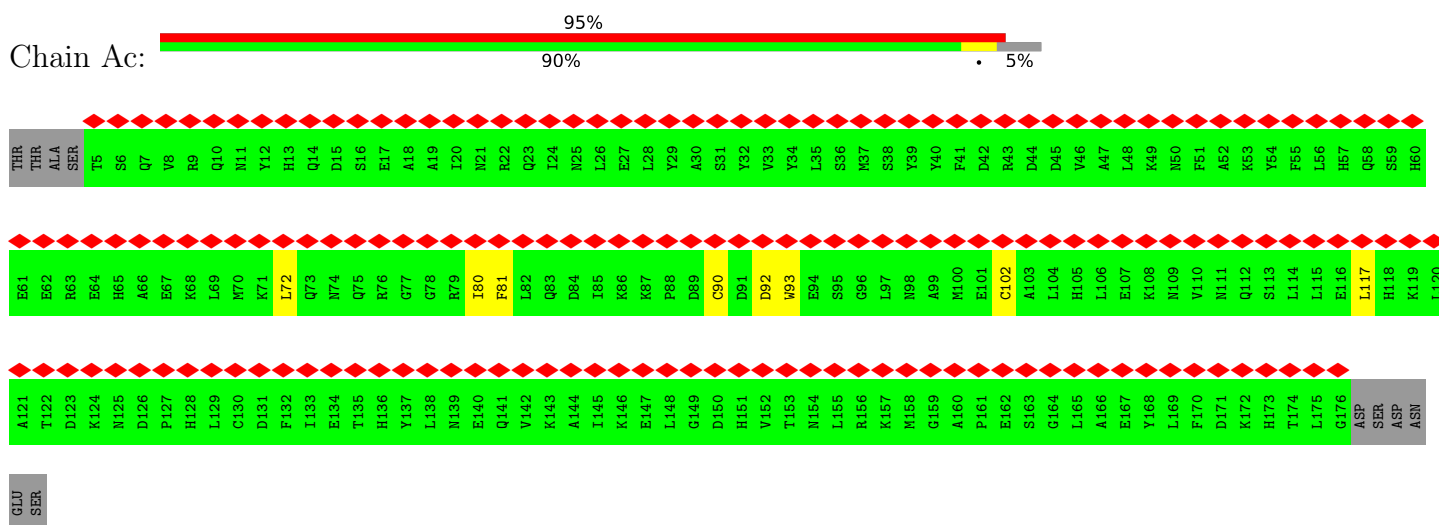
3 Residue-property plots

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.

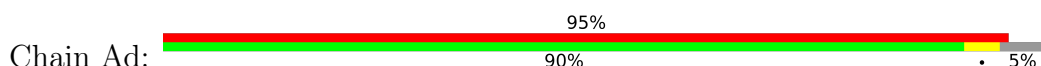
- Molecule 1: Ferritin heavy chain

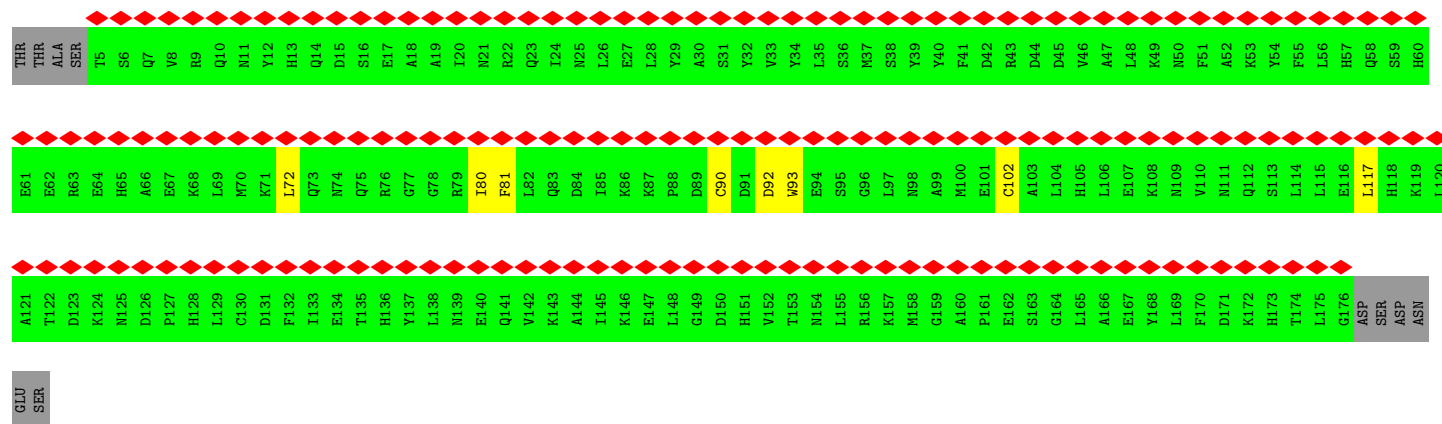


- Molecule 1: Ferritin heavy chain

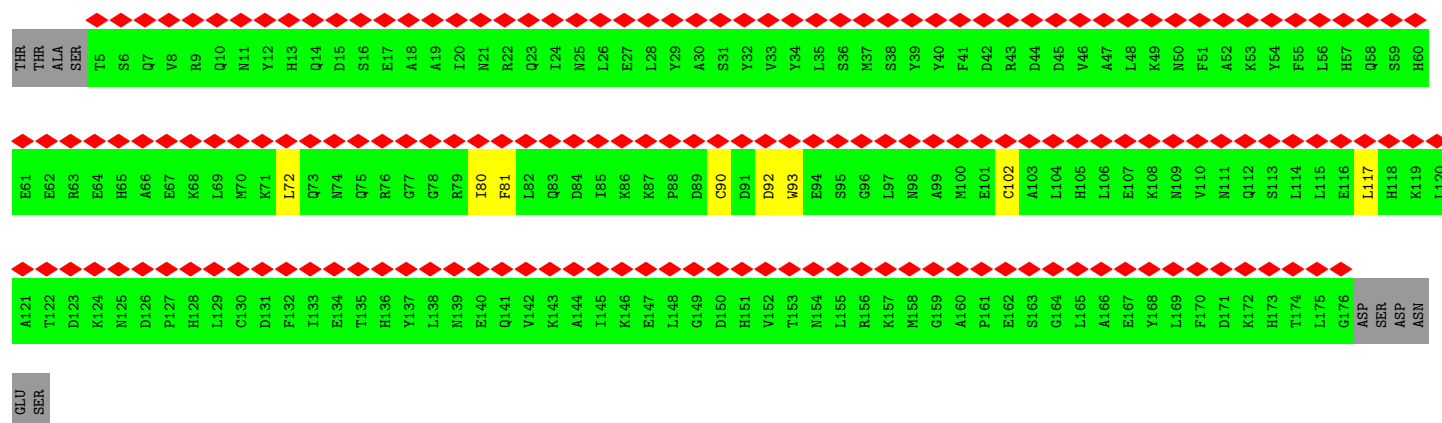
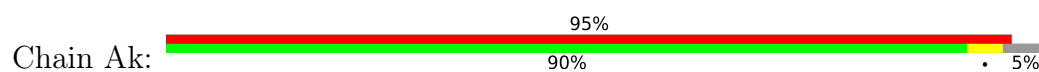


- Molecule 1: Ferritin heavy chain

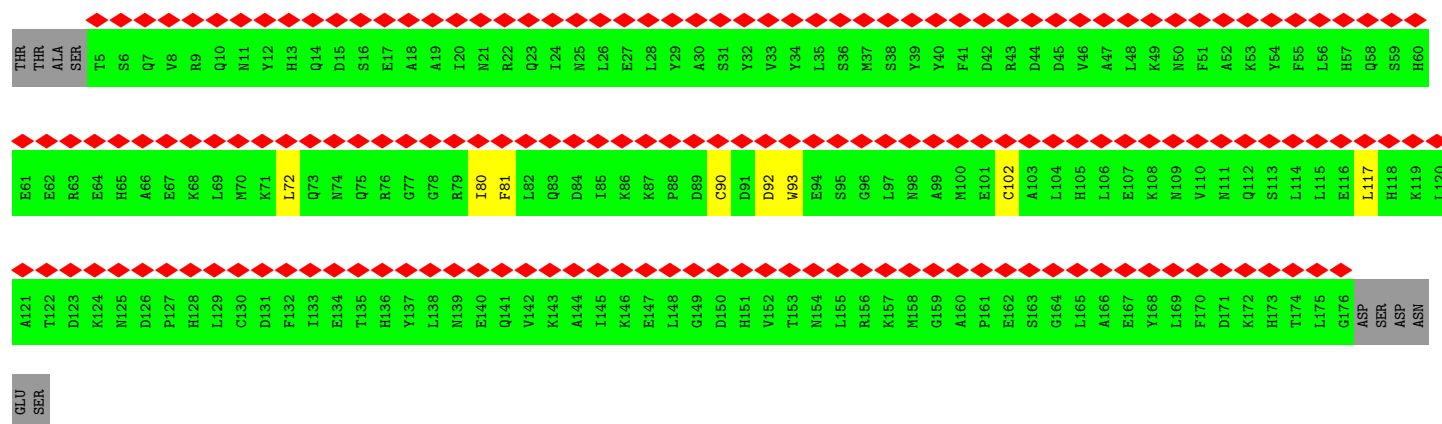
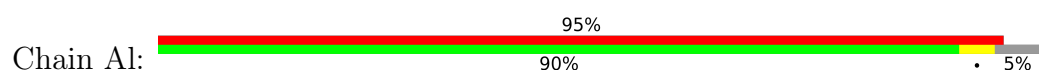




- Molecule 1: Ferritin heavy chain

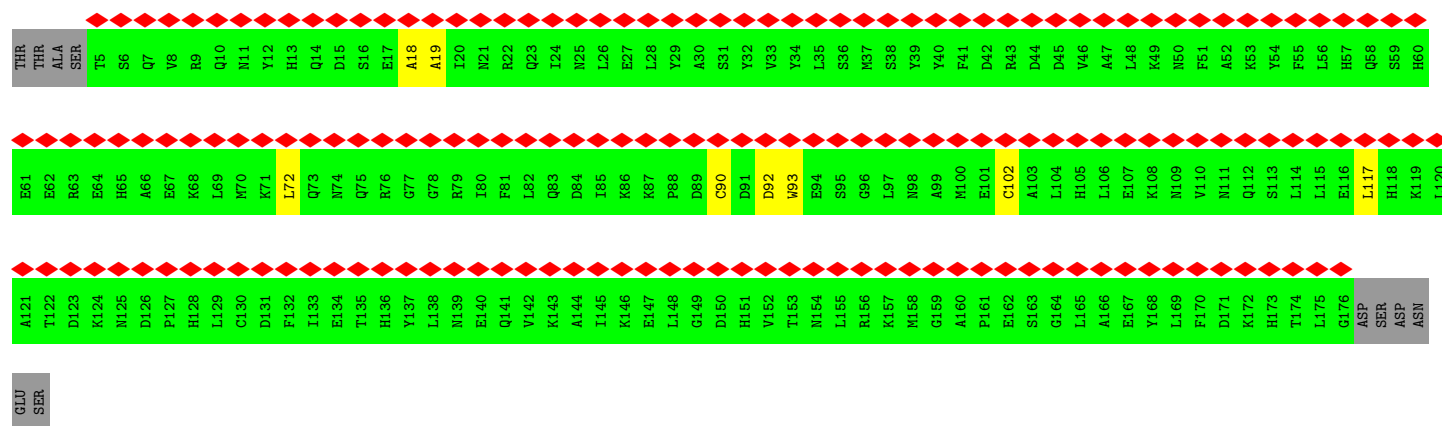


- Molecule 1: Ferritin heavy chain

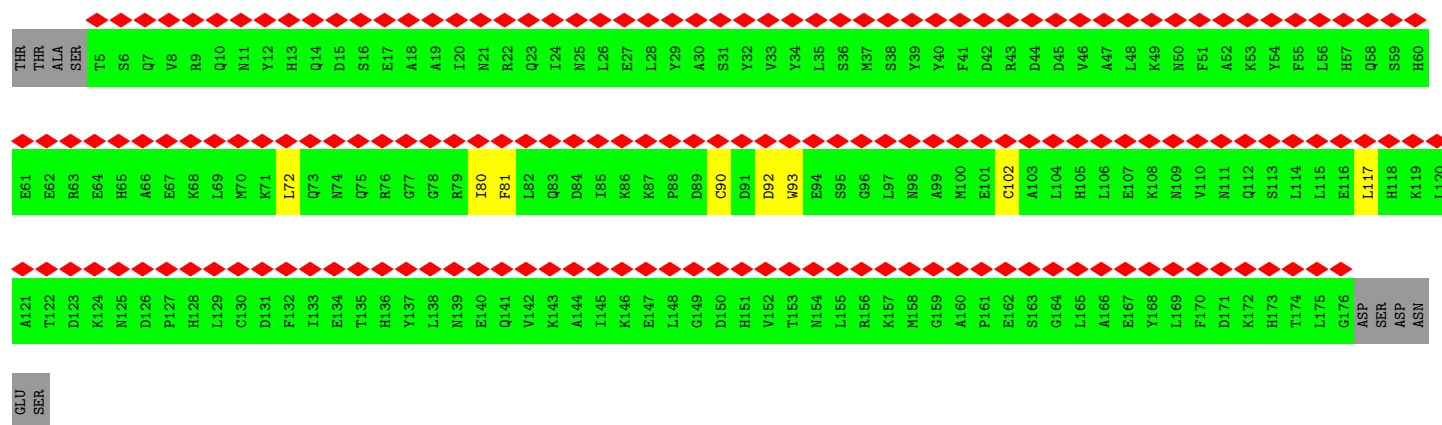
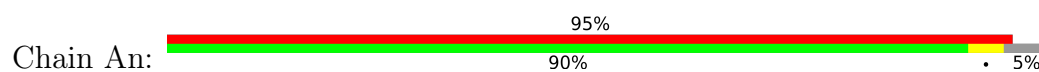


- Molecule 1: Ferritin heavy chain

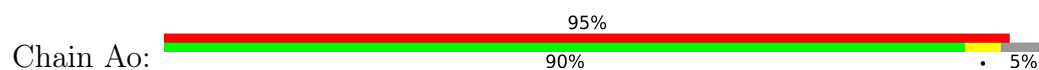




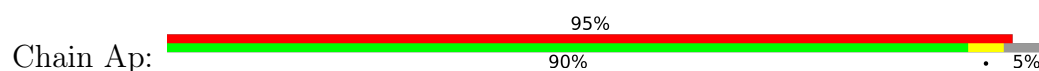
• Molecule 1: Ferritin heavy chain

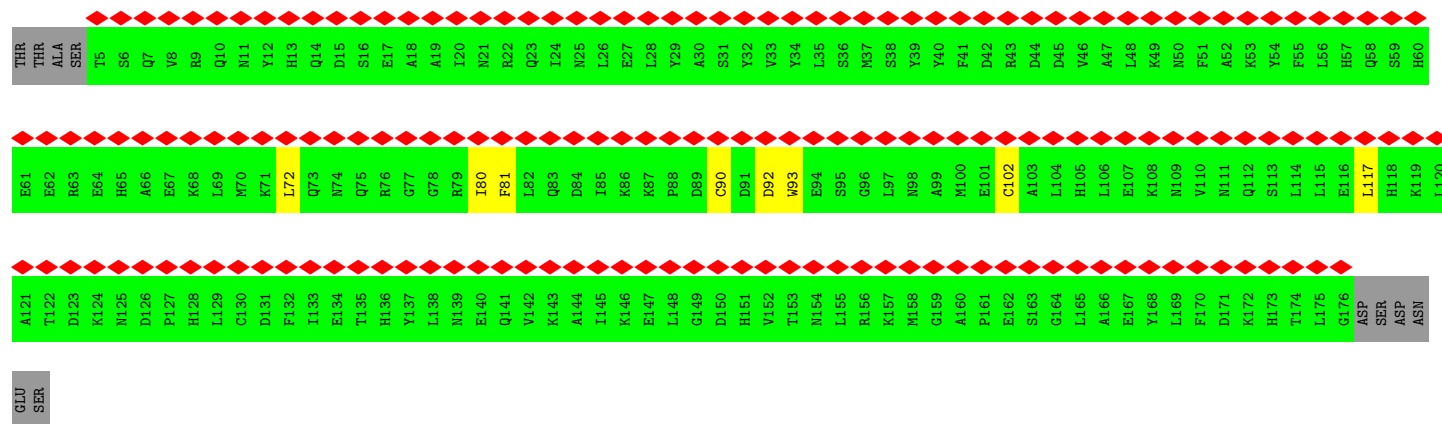


• Molecule 1: Ferritin heavy chain

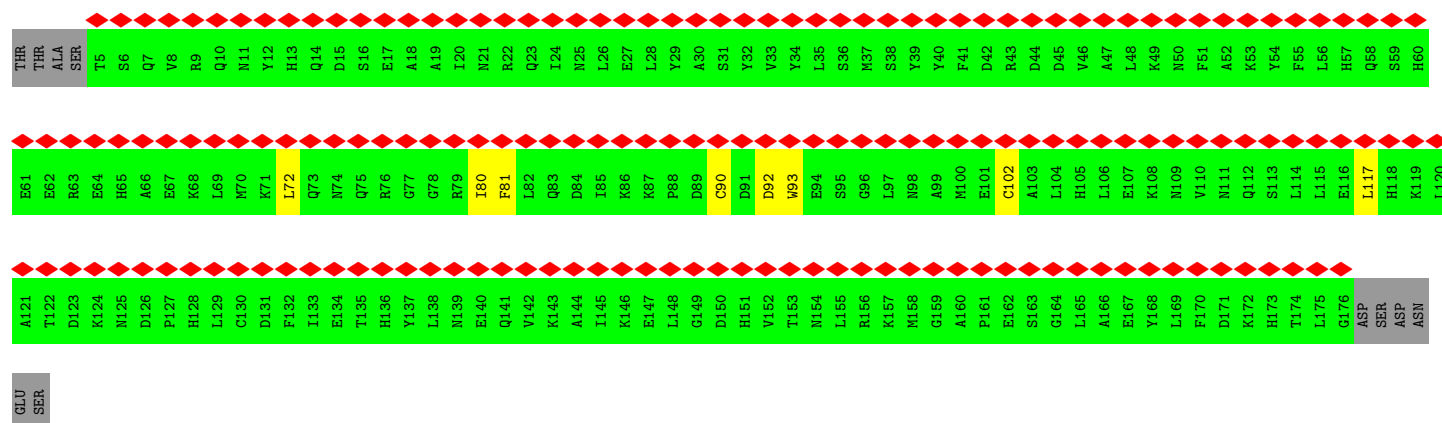
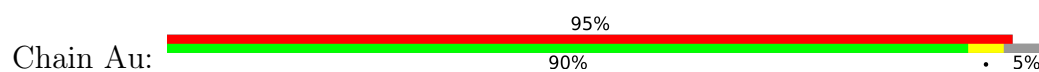


• Molecule 1: Ferritin heavy chain

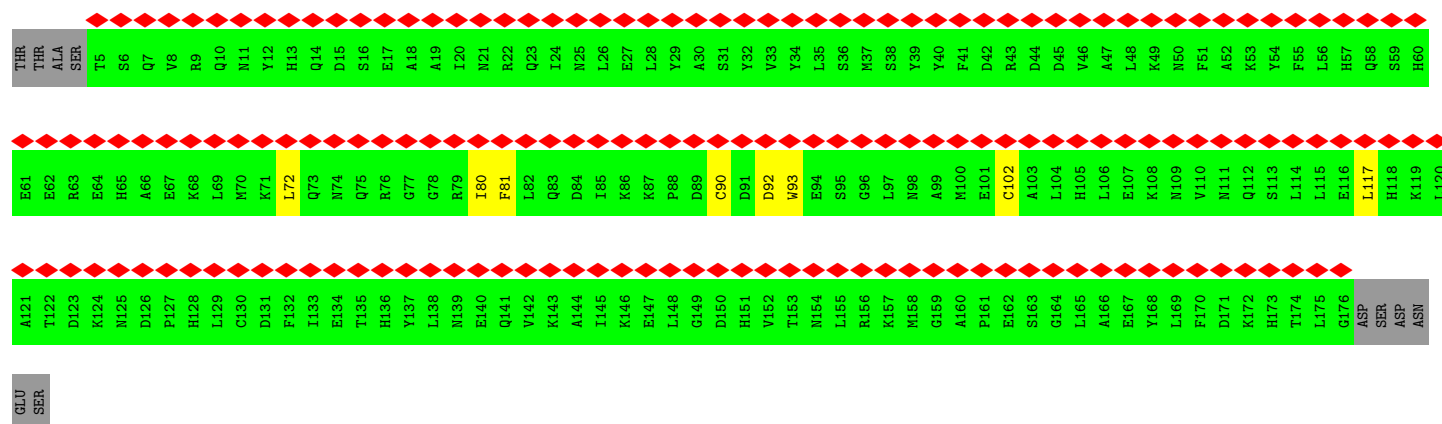




- Molecule 1: Ferritin heavy chain



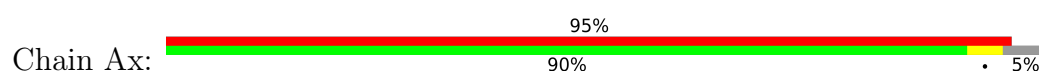
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



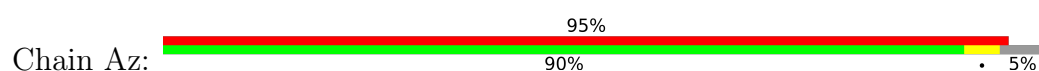
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

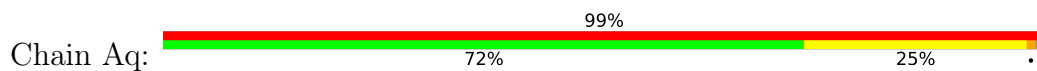


L601	A541	Y481	W421	S361	A301	K241	V181	R121
T602	F542	I482	G422	T362	H302	D242	W182	L122
M603	F543	M483	T423	C363	L303	F243	R183	Y123
D604	F544	L484	A424	R364	G304	E244	D184	W124
V605	L545	D485	L425	M365	T305	D245	Q185	D125
E606	A546	K486	L426	V366	G306	L246	H186	D126
L607	Y547	A487	L427	T367	D307	Y247	F187	L127
M608	S548	V488	K428	S368	P308	T248	V188	K128
G609	G549	L489	L429	E369	Y309	P249	H189	R129
D610	I550	G490	A430	S370	T310	V250	I190	K130
E611	P551	T491	Q431	K371	P311	M251	Q191	L131
B612	A552	G492	M432	N372	G312	G252	V192	S132
M613	V553	F433	F433	V373	F313	S253	K193	E133
Y614	S554	F494	S434	K374	P314	T254	D194	K134
M615	F555	D435	W436	L375	S315	V255	S195	L135
S616	C556	V496	M436	T376	PHE	T256	A196	D136
Q617	F557	A497	W437	V377	ASN	V257	Q197	S137
L618	C558	A498	L438	S378	HIS	R258	N198	T138
L619	L619	S499	K439	N379	T319	K259	S199	D139
S620	D560	P500	D440	V380	Q320	G260	F200	F140
F621	T561	L501	G441	L381	F321	K261	V201	T141
W622	D562	L502	F442	K382	P322	T262	T202	S142
R623	F563	Y503	Q443	E383	S324	T263	W203	T143
D624	P564	T504	P444	L384	R325	F264	D204	I144
L625	V565	L505	S445	K385	R326	K265	K205	K145
N626	L566	I506	R446	L386	S327	E266	W206	L146
Q627	G507	E507	S447	L387	G328	K267	G207	L147
Y628	T568	K508	T448	N388	L329	V268	R208	N148
R629	T569	T509	T449	L389	P330	A269	L209	E149
M630	M570	M510	F450	F390	N331	N270	V210	N150
D631	D571	Q511	A451	G391	I332	A271	Y211	S151
T632	T572	M512	S452	V392	P333	E272	L212	Y152
K633	Y573	V513	W453	L393	V334	S273	V213	V153
E634	K574	K514	S454	K394	Q335	L274	E214	P154
M635	H515	H515	G395	G395	T336	N275	N215	R155
G636	V516	P516	G456	F396	I337	A276	A157	E156
L637	V517	V517	D457	V397	S338	L277	G217	A157
S638	E578	T518	F458	E398	R339	G278	G218	G158
R639	R579	G519	A459	P399	A340	V279	Y219	S159
Q640	T580	Q520	S460	D400	A341	L280	V220	Q160
W641	P581	F521	W461	H401	A342	L281	A221	K161
L642	E582	L522	G462	Y402	E343	Y282	Y222	D162
V643	L583	Y523	A463	V403	K344	M283	S223	E163
S644	M584	Q524	T464	V404	L345	D284	K224	N164
A645	D625	D625	W465	V405	F346	Q285	A225	L165
R646	V586	S526	W466	G406	G347	T286	A226	A166
G647	A587	N527	L467	A407	N348	K287	T227	L167
D648	R588	W528	E468	Q408	K349	F288	V228	V168
F649	A589	A529	A469	R409	E350	P289	T229	V169
P650	A590	S530	Y470	D410	G351	T290	G230	E170
R651	A591	K531	L471	A411	D352	V291	K231	N171
A652	E592	V532	S472	W412	C353	N292	L232	Q172
T653	V593	E533	F473	G413	P354	K293	V233	F173
S654	K594	K594	L474	P414	S355	E294	H234	R174
R655	G595	L535	H475	G415	D356	L295	A235	E175
L656	Q596	T536	L476	A416	P357	S296	W236	F176
F657	V597	L537	K477	A417	K358	F297	F237	K177
T658	D598	D598	A478	K418	T359	F298	G238	L178
D659	Y599	N539	F479	K419	D360	G299	T239	S179
P660	K600	A540	T480	G420		H300	D140	K180

G661	N662	A663	E664	K665	K666	D667	R668	F669	V670	M671	K672	K673	K674	N675	D676	R677	V678	M679	R680	V681	E682	Y683	H684	F685	L686	S687	P688	Y689	V690	S691	P692	K693	E694	S695	P696	F697	R698	H699	V700	F701	W702	G703	S704	G705	S706	H707	T708	L709	P710	A711	L712	L713	E714	N715	L716	K717	L718	R719	K720
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Q721	N722	N723	G724	A725	F726	N727	E728	T729	L730	F731	R732	N733	Q734	L735	A736	L737	A738	T739	W740	T741	I742	Q743	G744	A745	A746	N747	A748	L749	S750	G751	D752	V753	W754	D755	I756	ASP	ASN	GLU	PHE
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• Molecule 2: Transferrin receptor protein 1



R121	L122	Y123	W124	D125	D126	L127	K128	R129	K130	L131	S132	E133	K134	L135	D136	S137	T138	D139	F140	T141	S142	T143	I144	K145	L146	L147	N148	E149	N150	S151	Y152	V153	P154	R155	E156	A157	S158	Q160	D162	E163	L164	A165	A166	L167	Y168	V169	K170	N171	Q172	R173	H174	E175	F176	K177	G178	S179	K180
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Y181	W182	R183	D184	Q185	H186	F187	V188	K189	I190	Q191	V192	K193	D194	S195	A196	Q197	N198	S199	V200	I201	S202	V203	D204	K205	N206	G207	R208	L209	V210	Y211	L212	V213	E214	N215	P216	G217	Y218	Y219	V220	A221	Y222	S223	K224	A225	A226	T227	V228	T229	K230	K231	L232	V233	H234	A235	N236	F237	G238	T239	K240
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K241	D242	F243	E244	D245	L246	Y247	T248	P249	V250	N251	G252	S253	L254	V255	L256	V257	R258	A259	G260	K261	L262	T263	F264	A265	E266	K267	V268	A269	N270	A271	E272	S273	L274	N275	A276	I277	G278	V279	L280	L281	Y282	M283	D284	Q285	T286	K287	F288	P289	L290	V291	N292	A293	E294	L295	S296	F297	F298	G299	H300
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A301	H302	L303	G304	T305	D307	P308	Y309	T310	P311	G312	F313	P314	S315	PHE	ASN	HIS	T319	Q320	F321	P322	P323	S324	R325	S326	S327	G328	L329	P330	N331	L332	P333	V334	Q335	G336	I337	S338	R339	A340	A341	A342	E343	K344	L345	F346	G347	N348	M349	E350	G351	L352	C353	P354	S355	L356	W357	K358	T359	D360
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S361	T362	C363	R364	K365	V366	T367	S368	S369	S370	K371	N372	V373	K374	L375	T376	V377	S378	N379	V380	L381	K382	E383	L384	K385	L386	L387	N388	L389	F390	G391	V392	L393	K394	G395	F396	V397	F398	P399	D400	H401	Y402	V403	V404	V405	G406	A407	Q408	R409	D410	A411	W412	G413	P414	G415	A416	A417	K418	S419	G420
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V421	G422	T423	A424	L425	L426	L427	K428	L429	A430	Q431	H432	F433	S434	D435	M436	V437	L438	K439	D440	G441	Q442	Q443	P444	S445	R446	S447	L448	L449	F450	A451	S452	W453	K454	A455	G456	D457	F458	G459	S460	V461	O462	A463	T464	E465	V466	L467	E468	G469	W470	L471	S472	S473	L474	H475	L476	K477	A478	F479	T480
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Y481	L482	H483	L484	D485	K486	A487	V488	G489	C490	T491	S492	H493	F494	K495	V496	S497	A498	S499	P500	L501	L502	Y503	T504	L505	I506	E507	K508	T509	M510	Q511	N512	W513	K514	H515	P516	V517	T518	G519	O520	F521	L522	Y523	O524	D525	V526	N527	W528	A529	L530	K531	V532	E533	K534	L535	T536	L537	D538	N539	A540
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A541	F542	P543	F544	L545	A546	Y547	S548	G549	T550	P551	A552	S553	S554	F555	C556	F557	C558	E559	D560	T561	D562	Y563	P564	Y565	L566	G567	T568	T569	M570	D571	T572	Y573	E574	E575	L576	I577	E578	R579	I580	P581	E582	L583	N584	K585	V586	A587	R588	A589	F590	R591	E592	V593	A594	G595	O596	F597	V598	I599	K600
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L601	T602	H603	D604	V605	E606	L607	H608	L609	D610	Y611	E612	R613	L614	N615	S616	Q617	L618	L619	S620	F621	V622	R623	D624	L625	N626	G627	V628	R629	A630	D631	L632	K633	E634	M635	G636	L637	S638	L639	Q640	W641	L642	T643	S644	A645	R646	G647	D648	F649	R650	R651	A652	T653	S654	G655	L656	T657	T658	D659	F660
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G661	N662	A663	E664	K665	K666	D667	R668	F669	V670	M671	K672	K673	K674	N675	D676	R677	V678	M679	R680	V681	E682	Y683	H684	F685	L686	S687	P688	Y689	V690	S691	P692	K693	E694	S695	P696	F697	R698	H699	V700	F701	W702	G703	S704	G705	S706	H707	T708	L709	P710	A711	L712	L713	E714	N715	L716	K717	L718	R719	K720
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Q721	N722	N723	G724	A725	F726	N727	E728	T729	L730	F731	R732	N733	Q734	L735	A736	L737	A738	T739	W740	T741	I742	Q743	G744	A745	A746	N747	A748	L749	S750	G751	D752	V753	W754	D755	I756	ASP	ASN	GLU	PHE
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	Aa	0.35	0/1530	0.59	0/2057
1	Ac	0.35	0/1530	0.59	0/2057
1	Ad	0.35	0/1530	0.59	0/2057
1	Ae	0.35	0/1530	0.59	0/2057
1	Af	0.35	0/1530	0.59	0/2057
1	Ag	0.35	0/1530	0.59	0/2057
1	Ah	0.35	0/1530	0.59	0/2057
1	Ai	0.35	0/1530	0.59	0/2057
1	Aj	0.35	0/1530	0.59	0/2057
1	Ak	0.35	0/1530	0.59	0/2057
1	Al	0.35	0/1530	0.59	0/2057
1	Am	0.36	0/1486	0.59	0/2004
1	An	0.35	0/1530	0.59	0/2057
1	Ao	0.35	0/1530	0.59	0/2057
1	Ap	0.35	0/1530	0.59	0/2057
1	Ar	0.35	0/1530	0.59	0/2057
1	As	0.35	0/1530	0.59	0/2057
1	At	0.35	0/1530	0.59	0/2057
1	Au	0.35	0/1530	0.59	0/2057
1	Av	0.35	0/1530	0.59	0/2057
1	Aw	0.35	0/1530	0.59	0/2057
1	Ax	0.35	0/1530	0.59	0/2057
1	Ay	0.35	0/1530	0.59	0/2057
1	Az	0.35	0/1530	0.59	0/2057
2	Ab	0.43	0/5110	0.79	3/6927 (0.0%)
2	Aq	0.43	0/5121	0.79	3/6942 (0.0%)
All	All	0.37	0/46907	0.64	6/63184 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Ab	403	VAL	CB-CA-C	-6.10	103.34	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Aq	403	VAL	CB-CA-C	-6.09	103.35	110.91
2	Ab	515	HIS	CA-C-N	5.16	124.96	119.28
2	Ab	515	HIS	C-N-CA	5.16	124.96	119.28
2	Aq	515	HIS	CA-C-N	5.13	124.93	119.28
2	Aq	515	HIS	C-N-CA	5.13	124.93	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1473	0	1447	6	0
1	Ac	1473	0	1447	5	0
1	Ad	1473	0	1447	5	0
1	Ae	1473	0	1447	5	0
1	Af	1473	0	1447	6	0
1	Ag	1473	0	1447	5	0
1	Ah	1473	0	1447	6	0
1	Ai	1473	0	1447	5	0
1	Aj	1473	0	1447	6	0
1	Ak	1473	0	1447	6	0
1	Al	1473	0	1447	5	0
1	Am	1431	0	1377	11	0
1	An	1473	0	1447	5	0
1	Ao	1473	0	1447	6	0
1	Ap	1473	0	1447	5	0
1	Ar	1473	0	1447	6	0
1	As	1473	0	1447	6	0
1	At	1473	0	1447	5	0
1	Au	1473	0	1447	6	0
1	Av	1473	0	1447	5	0
1	Aw	1473	0	1447	5	0
1	Ax	1473	0	1447	5	0
1	Ay	1473	0	1447	5	0
1	Az	1473	0	1447	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ab	4994	0	4937	322	0
2	Aq	5004	0	4957	315	0
All	All	45308	0	44552	563	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 6.

All (563) 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)
2:Ab:753:VAL:HG13	2:Aq:402:TYR:CZ	1.53	1.44
2:Ab:732:ARG:CB	2:Aq:313:PHE:CD1	1.78	1.43
2:Ab:753:VAL:CG2	2:Aq:449:ILE:HD11	1.47	1.41
2:Ab:753:VAL:HG21	2:Aq:449:ILE:CD1	1.47	1.41
2:Ab:315:SER:HA	2:Aq:732:ARG:NH2	1.11	1.39
2:Ab:673:LYS:NZ	2:Aq:400:ASP:OD2	1.59	1.33
2:Ab:753:VAL:HG13	2:Aq:402:TYR:OH	1.25	1.31
2:Ab:315:SER:CA	2:Aq:732:ARG:NH2	1.95	1.29
2:Ab:669:PHE:HD1	2:Aq:669:PHE:CA	1.32	1.28
2:Ab:313:PHE:HB3	2:Aq:732:ARG:O	1.18	1.27
2:Ab:400:ASP:CA	2:Aq:752:ASP:OD1	1.82	1.26
2:Ab:402:TYR:OH	2:Aq:753:VAL:CG1	1.85	1.25
2:Ab:669:PHE:CD1	2:Aq:669:PHE:CA	1.99	1.25
2:Ab:754:TRP:CE2	2:Aq:394:LYS:HG2	1.72	1.23
2:Ab:754:TRP:CH2	2:Aq:399:PRO:O	1.89	1.22
2:Ab:315:SER:CA	2:Aq:732:ARG:HH21	1.46	1.21
2:Ab:669:PHE:CA	2:Aq:669:PHE:CD1	2.10	1.20
2:Ab:754:TRP:CB	2:Aq:392:VAL:HG11	1.73	1.17
2:Ab:747:ASN:HB3	2:Aq:470:TYR:CE1	1.80	1.15
2:Ab:669:PHE:CD1	2:Aq:669:PHE:HA	1.40	1.15
2:Ab:400:ASP:CB	2:Aq:752:ASP:OD1	1.95	1.14
2:Ab:402:TYR:OH	2:Aq:753:VAL:HG13	0.97	1.14
2:Ab:673:LYS:NZ	2:Aq:400:ASP:CG	2.06	1.13
2:Ab:688:PRO:CB	2:Aq:471:LEU:HD23	1.81	1.11
2:Ab:402:TYR:CZ	2:Aq:753:VAL:HG13	1.85	1.10
2:Ab:732:ARG:HB3	2:Aq:313:PHE:CD1	1.31	1.10
2:Ab:399:PRO:HB2	2:Aq:754:TRP:CZ2	1.87	1.10
2:Ab:400:ASP:HB3	2:Aq:752:ASP:OD1	1.51	1.10
2:Ab:637:LEU:CD2	2:Aq:314:PRO:O	2.00	1.10
2:Ab:669:PHE:HA	2:Aq:669:PHE:CD1	1.71	1.09
2:Ab:753:VAL:CG1	2:Aq:402:TYR:CZ	2.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:399:PRO:CB	2:Aq:754:TRP:CH2	2.37	1.07
2:Ab:400:ASP:HA	2:Aq:752:ASP:OD1	1.48	1.07
2:Ab:754:TRP:HB3	2:Aq:392:VAL:HG11	1.26	1.07
2:Ab:668:ARG:HG3	2:Aq:669:PHE:CG	1.89	1.07
2:Ab:313:PHE:HB3	2:Aq:732:ARG:C	1.80	1.06
2:Ab:732:ARG:HB2	2:Aq:313:PHE:CE1	1.89	1.06
2:Ab:399:PRO:CB	2:Aq:754:TRP:CZ2	2.40	1.04
2:Ab:732:ARG:HB2	2:Aq:313:PHE:CD1	1.57	1.02
2:Ab:313:PHE:HB2	2:Aq:732:ARG:HB3	1.38	1.00
2:Ab:669:PHE:CZ	2:Aq:672:LYS:HB2	1.96	1.00
2:Ab:753:VAL:HG22	2:Aq:402:TYR:CE1	1.96	1.00
2:Ab:688:PRO:HB3	2:Aq:471:LEU:HD23	1.40	1.00
2:Ab:747:ASN:HB3	2:Aq:470:TYR:HE1	1.10	0.99
2:Ab:753:VAL:CG2	2:Aq:449:ILE:CD1	2.21	0.99
2:Ab:754:TRP:HZ2	2:Aq:399:PRO:CB	1.75	0.99
2:Ab:637:LEU:HD22	2:Aq:314:PRO:O	1.63	0.98
2:Ab:313:PHE:CB	2:Aq:732:ARG:HB3	1.94	0.96
2:Ab:733:ASN:HB2	2:Aq:313:PHE:CE2	2.00	0.96
2:Ab:753:VAL:HG13	2:Aq:402:TYR:CE2	2.01	0.95
2:Ab:402:TYR:CZ	2:Aq:753:VAL:CG1	2.46	0.95
2:Ab:753:VAL:CG1	2:Aq:402:TYR:CE2	2.51	0.94
2:Ab:740:TRP:CZ3	2:Aq:312:GLY:HA2	2.01	0.94
2:Ab:753:VAL:HG21	2:Aq:449:ILE:HD11	0.95	0.93
2:Ab:637:LEU:HD21	2:Aq:314:PRO:O	1.66	0.93
2:Ab:212:LEU:N	1:Am:18:ALA:HB1	1.83	0.93
2:Ab:669:PHE:CA	2:Aq:669:PHE:HD1	1.54	0.92
2:Ab:753:VAL:CG1	2:Aq:402:TYR:OH	2.18	0.92
2:Ab:733:ASN:HB2	2:Aq:313:PHE:HE2	1.32	0.91
2:Ab:754:TRP:CZ2	2:Aq:399:PRO:CB	2.54	0.90
2:Ab:313:PHE:CB	2:Aq:732:ARG:O	2.15	0.90
2:Ab:315:SER:C	2:Aq:732:ARG:HH22	1.79	0.90
2:Ab:754:TRP:HH2	2:Aq:399:PRO:O	1.48	0.90
2:Ab:754:TRP:CE3	2:Aq:392:VAL:HG21	2.07	0.90
2:Ab:447:SER:OG	2:Aq:754:TRP:CZ3	2.26	0.89
2:Ab:688:PRO:HB2	2:Aq:471:LEU:HD23	1.53	0.89
2:Ab:399:PRO:CA	2:Aq:754:TRP:HH2	1.87	0.88
2:Ab:637:LEU:HD22	2:Aq:314:PRO:C	1.99	0.88
2:Ab:471:LEU:HD23	2:Aq:688:PRO:HB2	1.55	0.88
2:Ab:754:TRP:HB2	2:Aq:392:VAL:HG11	1.55	0.87
2:Ab:637:LEU:CD2	2:Aq:314:PRO:C	2.47	0.86
2:Ab:733:ASN:CB	2:Aq:313:PHE:HE2	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:733:ASN:CB	2:Aq:313:PHE:CE2	2.51	0.86
2:Ab:399:PRO:CB	2:Aq:754:TRP:HH2	1.83	0.85
2:Ab:688:PRO:HB2	2:Aq:471:LEU:CD2	2.06	0.85
2:Ab:399:PRO:HB2	2:Aq:754:TRP:CH2	2.09	0.85
2:Ab:399:PRO:HB3	2:Aq:754:TRP:CZ2	2.11	0.85
2:Ab:402:TYR:CE1	2:Aq:753:VAL:HG22	2.12	0.85
2:Ab:668:ARG:HG3	2:Aq:669:PHE:CD2	2.11	0.84
2:Ab:399:PRO:HB3	2:Aq:754:TRP:CH2	2.12	0.83
2:Ab:394:LYS:HG2	2:Aq:754:TRP:CD2	2.13	0.83
2:Ab:399:PRO:HB2	2:Aq:754:TRP:HZ2	1.41	0.83
2:Ab:471:LEU:HD23	2:Aq:688:PRO:CB	2.08	0.83
2:Ab:635:MET:O	2:Aq:315:SER:O	1.96	0.82
2:Ab:754:TRP:HZ2	2:Aq:399:PRO:HB3	1.42	0.82
2:Ab:315:SER:HA	2:Aq:732:ARG:HH22	1.45	0.82
2:Ab:394:LYS:HG2	2:Aq:754:TRP:CE2	2.15	0.82
2:Ab:313:PHE:CG	2:Aq:732:ARG:HB3	2.15	0.82
2:Ab:688:PRO:CB	2:Aq:471:LEU:CD2	2.59	0.81
2:Ab:735:LEU:HD23	2:Aq:314:PRO:HD2	1.60	0.81
2:Ab:399:PRO:CB	2:Aq:754:TRP:HZ2	1.92	0.80
2:Ab:449:ILE:HD11	2:Aq:753:VAL:HG21	1.62	0.80
2:Aq:230:GLY:O	2:Aq:372:ASN:HB2	1.81	0.80
2:Ab:669:PHE:CZ	2:Aq:672:LYS:CB	2.64	0.80
2:Ab:315:SER:C	2:Aq:732:ARG:NH2	2.39	0.80
2:Ab:732:ARG:HB3	2:Aq:313:PHE:HD1	0.99	0.79
2:Ab:154:PRO:HD2	2:Ab:161:LYS:HD2	1.63	0.79
2:Aq:154:PRO:HD2	2:Aq:161:LYS:HD2	1.63	0.79
2:Ab:230:GLY:O	2:Ab:372:ASN:HB2	1.81	0.79
2:Ab:754:TRP:CH2	2:Aq:399:PRO:C	2.59	0.79
2:Aq:401:HIS:CE1	2:Aq:679:MET:HE1	2.18	0.79
2:Ab:754:TRP:CZ2	2:Aq:399:PRO:HB3	2.18	0.78
2:Ab:313:PHE:HD2	2:Aq:733:ASN:HA	1.49	0.78
2:Ab:401:HIS:CE1	2:Ab:679:MET:HE1	2.18	0.78
2:Ab:668:ARG:HB2	2:Aq:669:PHE:CZ	2.19	0.78
2:Ab:402:TYR:HH	2:Aq:753:VAL:HG13	0.98	0.78
2:Ab:753:VAL:HG23	2:Aq:449:ILE:HD11	1.64	0.78
2:Ab:673:LYS:CE	2:Aq:400:ASP:CG	2.57	0.77
2:Aq:518:THR:HG22	2:Aq:520:GLN:H	1.48	0.77
2:Ab:312:GLY:HA2	2:Aq:740:TRP:CH2	2.20	0.77
2:Ab:754:TRP:HZ2	2:Aq:399:PRO:HB2	1.48	0.77
2:Ab:313:PHE:CG	2:Aq:732:ARG:CB	2.67	0.76
2:Ab:394:LYS:CD	2:Aq:754:TRP:CE2	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:754:TRP:CE2	2:Aq:394:LYS:CG	2.63	0.76
2:Ab:399:PRO:O	2:Aq:754:TRP:CH2	2.38	0.76
2:Ab:668:ARG:HG3	2:Aq:669:PHE:CD1	2.20	0.76
2:Ab:518:THR:HG22	2:Ab:520:GLN:H	1.49	0.76
2:Ab:754:TRP:NE1	2:Aq:394:LYS:HG2	1.89	0.75
2:Ab:313:PHE:CB	2:Aq:732:ARG:C	2.58	0.75
2:Ab:754:TRP:HB3	2:Aq:392:VAL:CG1	2.14	0.75
2:Ab:400:ASP:OD2	2:Aq:673:LYS:NZ	2.17	0.74
2:Ab:149:GLU:C	2:Ab:153:VAL:HG23	2.13	0.74
2:Ab:753:VAL:HG11	2:Aq:402:TYR:CE2	2.23	0.74
2:Aq:149:GLU:C	2:Aq:153:VAL:HG23	2.13	0.74
2:Ab:400:ASP:CG	2:Aq:673:LYS:HZ3	1.95	0.73
2:Ab:447:SER:OG	2:Aq:754:TRP:CH2	2.41	0.73
2:Ab:740:TRP:CH2	2:Aq:312:GLY:HA2	2.22	0.73
2:Aq:626:ASN:O	2:Aq:629:ARG:HG3	1.89	0.73
2:Ab:637:LEU:HD23	2:Aq:315:SER:C	2.12	0.72
2:Ab:626:ASN:O	2:Ab:629:ARG:HG3	1.89	0.72
2:Ab:669:PHE:CB	2:Aq:669:PHE:HD1	2.02	0.71
2:Ab:399:PRO:C	2:Aq:754:TRP:CH2	2.69	0.71
2:Ab:669:PHE:CG	2:Aq:668:ARG:HG3	2.26	0.71
2:Ab:399:PRO:C	2:Aq:754:TRP:HH2	1.99	0.71
2:Ab:400:ASP:N	2:Aq:752:ASP:OD1	2.23	0.70
2:Ab:735:LEU:HD23	2:Aq:314:PRO:CD	2.21	0.70
2:Ab:754:TRP:O	2:Aq:180:LYS:HD3	1.90	0.70
2:Aq:635:MET:HE3	2:Aq:728:GLU:HG3	1.74	0.70
2:Ab:754:TRP:CD2	2:Aq:394:LYS:HG2	2.26	0.69
2:Ab:747:ASN:CB	2:Aq:470:TYR:CE1	2.70	0.69
2:Ab:754:TRP:CZ2	2:Aq:399:PRO:HB2	2.25	0.69
2:Ab:635:MET:HE3	2:Ab:728:GLU:HG3	1.74	0.69
2:Ab:669:PHE:HD1	2:Aq:669:PHE:CB	2.05	0.69
2:Ab:753:VAL:HG22	2:Aq:402:TYR:CD1	2.28	0.69
2:Aq:518:THR:CG2	2:Aq:520:GLN:H	2.06	0.68
2:Ab:664:GLU:CD	2:Ab:664:GLU:H	2.02	0.68
2:Ab:754:TRP:HH2	2:Aq:399:PRO:C	2.00	0.68
2:Ab:313:PHE:CB	2:Aq:732:ARG:CB	2.72	0.67
2:Ab:518:THR:CG2	2:Ab:520:GLN:H	2.06	0.67
2:Aq:664:GLU:CD	2:Aq:664:GLU:H	2.02	0.67
2:Ab:673:LYS:HE2	2:Aq:400:ASP:CG	2.19	0.67
2:Ab:668:ARG:CB	2:Aq:669:PHE:CZ	2.75	0.67
2:Ab:754:TRP:NE1	2:Aq:394:LYS:CG	2.43	0.67
2:Ab:153:VAL:HB	2:Ab:154:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:673:LYS:NZ	2:Aq:400:ASP:CB	2.58	0.67
2:Ab:754:TRP:HE3	2:Aq:392:VAL:HG21	1.59	0.67
2:Aq:153:VAL:HB	2:Aq:154:PRO:HD3	1.76	0.67
2:Ab:313:PHE:HD2	2:Aq:733:ASN:CA	2.07	0.66
2:Ab:669:PHE:CE1	2:Aq:672:LYS:HB3	2.29	0.66
2:Ab:155:ARG:HD2	2:Ab:409:ARG:O	1.95	0.66
2:Aq:272:GLU:OE1	2:Aq:331:ASN:HB2	1.96	0.66
2:Ab:315:SER:CA	2:Aq:732:ARG:HH22	1.92	0.66
1:As:93:TRP:HZ3	1:As:102[B]:CYS:HG	1.42	0.66
2:Ab:272:GLU:OE1	2:Ab:331:ASN:HB2	1.96	0.66
1:Ah:93:TRP:HZ3	1:Ah:102[B]:CYS:HG	1.42	0.66
2:Ab:134:LYS:HZ1	2:Ab:435:ASP:HB3	1.61	0.66
2:Ab:394:LYS:CG	2:Aq:754:TRP:CE2	2.78	0.65
2:Ab:753:VAL:HG22	2:Aq:402:TYR:CZ	2.31	0.65
2:Aq:155:ARG:HD2	2:Aq:409:ARG:O	1.95	0.65
2:Ab:748:ALA:HA	2:Aq:477:LYS:NZ	2.11	0.65
2:Aq:297:PHE:O	2:Aq:336:THR:HG21	1.97	0.65
2:Ab:297:PHE:O	2:Ab:336:THR:HG21	1.97	0.65
1:Ak:93:TRP:HZ3	1:Ak:102[B]:CYS:HG	1.45	0.64
1:An:93:TRP:HZ3	1:An:102[B]:CYS:SG	2.21	0.64
1:Ap:93:TRP:HZ3	1:Ap:102[B]:CYS:SG	2.21	0.64
1:Ax:93:TRP:HZ3	1:Ax:102[B]:CYS:SG	2.21	0.64
1:Ac:93:TRP:HZ3	1:Ac:102[B]:CYS:SG	2.21	0.64
1:As:93:TRP:HZ3	1:As:102[B]:CYS:SG	2.21	0.64
1:Ay:93:TRP:HZ3	1:Ay:102[B]:CYS:SG	2.21	0.64
1:Ar:93:TRP:HZ3	1:Ar:102[B]:CYS:SG	2.21	0.64
1:Aa:93:TRP:HZ3	1:Aa:102[B]:CYS:SG	2.21	0.64
1:Ag:93:TRP:HZ3	1:Ag:102[B]:CYS:SG	2.21	0.64
1:At:93:TRP:HZ3	1:At:102[B]:CYS:SG	2.21	0.64
2:Ab:402:TYR:CZ	2:Aq:753:VAL:HG11	2.33	0.64
1:Ai:93:TRP:HZ3	1:Ai:102[B]:CYS:SG	2.21	0.64
1:Av:93:TRP:HZ3	1:Av:102[B]:CYS:SG	2.21	0.64
1:Ae:93:TRP:HZ3	1:Ae:102[B]:CYS:SG	2.21	0.64
1:Af:93:TRP:HZ3	1:Af:102[B]:CYS:SG	2.21	0.63
1:Al:93:TRP:HZ3	1:Al:102[B]:CYS:SG	2.21	0.63
1:Au:93:TRP:HZ3	1:Au:102[B]:CYS:SG	2.21	0.63
1:Aj:93:TRP:HZ3	1:Aj:102[B]:CYS:SG	2.21	0.63
1:Ak:93:TRP:HZ3	1:Ak:102[B]:CYS:SG	2.21	0.63
2:Aq:149:GLU:O	2:Aq:153:VAL:HG23	1.98	0.63
2:Ab:149:GLU:O	2:Ab:153:VAL:HG23	1.98	0.63
1:Ah:93:TRP:HZ3	1:Ah:102[B]:CYS:SG	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:93:TRP:HZ3	1:Ao:102[B]:CYS:SG	2.21	0.63
1:Az:93:TRP:HZ3	1:Az:102[B]:CYS:SG	2.21	0.63
1:Aw:93:TRP:HZ3	1:Aw:102[B]:CYS:SG	2.21	0.63
2:Ab:732:ARG:HB3	2:Aq:313:PHE:HB2	1.80	0.63
1:Am:93:TRP:HZ3	1:Am:102[B]:CYS:SG	2.21	0.63
2:Ab:400:ASP:CG	2:Aq:673:LYS:NZ	2.57	0.62
1:Ad:93:TRP:HZ3	1:Ad:102[B]:CYS:SG	2.21	0.62
1:Af:93:TRP:HZ3	1:Af:102[B]:CYS:HG	1.42	0.62
1:Aj:93:TRP:HZ3	1:Aj:102[B]:CYS:HG	1.47	0.62
2:Aq:345:LEU:O	2:Aq:349:MET:HG3	2.00	0.62
2:Ab:721:GLN:NE2	2:Ab:725:ALA:HB3	2.14	0.62
2:Ab:394:LYS:HD3	2:Aq:754:TRP:CE2	2.33	0.62
2:Ab:211:TYR:C	1:Am:18:ALA:HB1	2.24	0.62
2:Ab:754:TRP:HH2	2:Aq:399:PRO:CA	2.13	0.62
1:Ad:93:TRP:CZ3	1:Ad:102[B]:CYS:SG	2.93	0.62
1:Am:93:TRP:CZ3	1:Am:102[B]:CYS:SG	2.93	0.62
1:Af:93:TRP:CZ3	1:Af:102[B]:CYS:SG	2.93	0.61
1:Ai:93:TRP:CZ3	1:Ai:102[B]:CYS:SG	2.93	0.61
1:Ao:93:TRP:CZ3	1:Ao:102[B]:CYS:SG	2.93	0.61
2:Aq:721:GLN:NE2	2:Aq:725:ALA:HB3	2.14	0.61
1:Au:93:TRP:CZ3	1:Au:102[B]:CYS:SG	2.93	0.61
1:Ao:93:TRP:HZ3	1:Ao:102[B]:CYS:HG	1.47	0.61
1:At:93:TRP:CZ3	1:At:102[B]:CYS:SG	2.93	0.61
1:Au:93:TRP:HZ3	1:Au:102[B]:CYS:HG	1.43	0.61
1:An:93:TRP:CZ3	1:An:102[B]:CYS:SG	2.93	0.61
1:Ax:93:TRP:CZ3	1:Ax:102[B]:CYS:SG	2.93	0.61
1:Ak:93:TRP:CZ3	1:Ak:102[B]:CYS:SG	2.93	0.61
1:Aw:93:TRP:CZ3	1:Aw:102[B]:CYS:SG	2.93	0.61
2:Ab:753:VAL:HG21	2:Aq:449:ILE:HD13	1.73	0.61
1:Aj:93:TRP:CZ3	1:Aj:102[B]:CYS:SG	2.93	0.61
1:Az:93:TRP:CZ3	1:Az:102[B]:CYS:SG	2.93	0.61
2:Ab:346:PHE:HD2	2:Ab:362:THR:HG22	1.65	0.60
2:Ab:754:TRP:CZ3	2:Aq:399:PRO:O	2.53	0.60
2:Ab:313:PHE:CD2	2:Aq:733:ASN:N	2.70	0.60
2:Ab:345:LEU:O	2:Ab:349:MET:HG3	1.99	0.60
2:Aq:251:ASN:C	2:Aq:251:ASN:OD1	2.45	0.60
1:As:93:TRP:CZ3	1:As:102[B]:CYS:SG	2.93	0.60
1:Ac:93:TRP:CZ3	1:Ac:102[B]:CYS:SG	2.93	0.60
2:Aq:134:LYS:NZ	2:Aq:435:ASP:HB3	2.17	0.60
2:Aq:190:ILE:HD13	2:Aq:384:ILE:HD13	1.84	0.59
2:Ab:251:ASN:OD1	2:Ab:251:ASN:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:312:GLY:HA2	2:Aq:740:TRP:CZ3	2.38	0.59
2:Ab:754:TRP:CH2	2:Aq:399:PRO:CA	2.85	0.59
2:Aq:230:GLY:C	2:Aq:372:ASN:HB2	2.26	0.59
2:Ab:190:ILE:HD13	2:Ab:384:ILE:HD13	1.84	0.59
2:Ab:297:PHE:CE1	2:Ab:336:THR:OG1	2.56	0.59
2:Ab:230:GLY:C	2:Ab:372:ASN:HB2	2.26	0.59
2:Aq:297:PHE:CE1	2:Aq:336:THR:OG1	2.56	0.59
2:Aq:346:PHE:HD2	2:Aq:362:THR:HG22	1.65	0.59
2:Ab:471:LEU:HD23	2:Aq:688:PRO:HB3	1.85	0.59
2:Aq:387:LEU:O	2:Aq:409:ARG:NH2	2.36	0.59
2:Ab:387:LEU:O	2:Ab:409:ARG:NH2	2.36	0.59
2:Aq:193:LYS:HE2	2:Aq:217:GLY:O	2.03	0.59
2:Ab:134:LYS:NZ	2:Ab:435:ASP:HB3	2.17	0.58
2:Aq:635:MET:HE3	2:Aq:728:GLU:CG	2.33	0.58
2:Ab:635:MET:HE3	2:Ab:728:GLU:CG	2.33	0.58
2:Ab:203:VAL:HG22	2:Ab:210:VAL:HG12	1.86	0.58
2:Aq:203:VAL:HG22	2:Aq:210:VAL:HG12	1.86	0.58
2:Aq:506:ILE:O	2:Aq:510:MET:HG3	2.04	0.58
2:Ab:732:ARG:CB	2:Aq:313:PHE:HB2	2.29	0.58
2:Aq:300:HIS:HD2	2:Aq:302:HIS:H	1.52	0.58
2:Ab:300:HIS:HD2	2:Ab:302:HIS:H	1.51	0.57
2:Ab:193:LYS:HE2	2:Ab:217:GLY:O	2.03	0.57
1:Ap:93:TRP:CZ3	1:Ap:102[B]:CYS:SG	2.93	0.57
2:Ab:399:PRO:O	2:Aq:754:TRP:CZ3	2.57	0.57
2:Ab:313:PHE:CD2	2:Aq:733:ASN:CA	2.87	0.57
1:Ay:93:TRP:CZ3	1:Ay:102[B]:CYS:SG	2.93	0.57
2:Ab:290:ILE:O	2:Ab:339:ARG:NH2	2.37	0.57
1:Ar:93:TRP:CZ3	1:Ar:102[B]:CYS:SG	2.93	0.57
2:Ab:637:LEU:CD2	2:Aq:315:SER:C	2.78	0.57
1:Aa:93:TRP:CZ3	1:Aa:102[B]:CYS:SG	2.93	0.57
1:Ae:93:TRP:CZ3	1:Ae:102[B]:CYS:SG	2.93	0.57
1:Al:93:TRP:CZ3	1:Al:102[B]:CYS:SG	2.93	0.57
2:Aq:290:ILE:O	2:Aq:339:ARG:NH2	2.37	0.57
2:Ab:313:PHE:CD1	2:Aq:732:ARG:HB3	2.40	0.56
2:Ab:753:VAL:CG2	2:Aq:449:ILE:HD13	2.28	0.56
2:Ab:506:ILE:O	2:Ab:510:MET:HG3	2.04	0.56
2:Aq:540:ALA:O	2:Aq:543:PRO:HD2	2.06	0.56
2:Ab:312:GLY:HA2	2:Aq:740:TRP:HH2	1.71	0.56
2:Ab:540:ALA:O	2:Ab:543:PRO:HD2	2.06	0.56
2:Ab:154:PRO:HD2	2:Ab:161:LYS:CD	2.36	0.56
2:Ab:447:SER:OG	2:Aq:754:TRP:HZ3	1.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:668:ARG:HB2	2:Aq:669:PHE:CE2	2.40	0.55
2:Ab:313:PHE:CD1	2:Aq:732:ARG:CB	2.90	0.55
2:Ab:258:ARG:HD2	2:Ab:284:ASP:OD1	2.07	0.55
2:Ab:688:PRO:HB3	2:Aq:471:LEU:CD2	2.25	0.55
2:Ab:402:TYR:CE1	2:Aq:753:VAL:CG2	2.88	0.55
2:Ab:753:VAL:HG23	2:Aq:449:ILE:CD1	2.24	0.55
2:Ab:718:LEU:O	2:Ab:726:PHE:HB2	2.08	0.54
2:Ab:748:ALA:HA	2:Aq:477:LYS:HZ1	1.70	0.54
2:Aq:258:ARG:HD2	2:Aq:284:ASP:OD1	2.07	0.54
2:Ab:669:PHE:CE1	2:Aq:672:LYS:CB	2.88	0.54
1:Ag:93:TRP:CZ3	1:Ag:102[B]:CYS:SG	2.93	0.54
2:Aq:637:LEU:HD11	2:Aq:732:ARG:HG2	1.90	0.54
2:Ab:313:PHE:CG	2:Aq:732:ARG:HB2	2.41	0.54
1:Ah:93:TRP:CZ3	1:Ah:102[B]:CYS:SG	2.93	0.54
2:Aq:154:PRO:HD2	2:Aq:161:LYS:CD	2.36	0.54
2:Ab:637:LEU:HD11	2:Ab:732:ARG:HG2	1.90	0.54
2:Aq:721:GLN:NE2	2:Aq:723:ASN:HB3	2.23	0.54
1:Ar:93:TRP:HZ3	1:Ar:102[B]:CYS:HG	1.42	0.54
1:Av:93:TRP:CZ3	1:Av:102[B]:CYS:SG	2.93	0.54
2:Ab:221:ALA:O	2:Ab:222:TYR:HB2	2.08	0.53
1:Aa:93:TRP:HZ3	1:Aa:102[B]:CYS:HG	1.42	0.53
2:Aq:241:LYS:HE2	2:Aq:245:ASP:OD2	2.09	0.53
2:Aq:718:LEU:O	2:Aq:726:PHE:HB2	2.08	0.53
2:Ab:241:LYS:HE2	2:Ab:245:ASP:OD2	2.09	0.53
2:Ab:343:GLU:CD	2:Ab:362:THR:HG21	2.34	0.53
2:Ab:668:ARG:CG	2:Aq:669:PHE:CD2	2.90	0.53
2:Ab:673:LYS:CE	2:Aq:400:ASP:OD2	2.52	0.53
2:Ab:721:GLN:NE2	2:Ab:723:ASN:HB3	2.23	0.52
2:Ab:753:VAL:CG2	2:Aq:402:TYR:CZ	2.91	0.52
2:Aq:251:ASN:OD1	2:Aq:251:ASN:O	2.28	0.52
2:Aq:343:GLU:CD	2:Aq:362:THR:HG21	2.34	0.52
2:Ab:313:PHE:CD2	2:Aq:732:ARG:C	2.88	0.52
2:Aq:401:HIS:ND1	2:Aq:679:MET:HE1	2.24	0.52
2:Ab:224:LYS:HD3	2:Ab:331:ASN:O	2.10	0.52
2:Aq:153:VAL:CB	2:Aq:154:PRO:HD3	2.40	0.52
2:Aq:221:ALA:O	2:Aq:222:TYR:HB2	2.08	0.52
2:Ab:392:VAL:HG11	2:Aq:754:TRP:HB3	1.91	0.52
2:Aq:184:ASP:HB3	2:Aq:388:ASN:HB2	1.92	0.52
2:Aq:243:PHE:HB3	2:Aq:274:LEU:HD11	1.91	0.52
2:Ab:243:PHE:HB3	2:Ab:274:LEU:HD11	1.91	0.52
1:Ai:80:ILE:O	1:Ai:81[B]:PHE:HD1	1.94	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:80:ILE:O	1:An:81[B]:PHE:HD1	1.94	0.52
2:Aq:224:LYS:HD3	2:Aq:331:ASN:O	2.10	0.52
1:Ax:80:ILE:O	1:Ax:81[B]:PHE:HD1	1.94	0.52
1:Ah:80:ILE:O	1:Ah:81[B]:PHE:HD1	1.94	0.51
1:Ao:80:ILE:O	1:Ao:81[B]:PHE:HD1	1.94	0.51
2:Aq:209:LEU:HD12	2:Aq:209:LEU:N	2.25	0.51
1:Ar:80:ILE:O	1:Ar:81[B]:PHE:HD1	1.94	0.51
1:At:80:ILE:O	1:At:81[B]:PHE:HD1	1.94	0.51
1:Aa:80:ILE:O	1:Aa:81[B]:PHE:HD1	1.94	0.51
2:Ab:184:ASP:HB3	2:Ab:388:ASN:HB2	1.92	0.51
2:Ab:251:ASN:OD1	2:Ab:251:ASN:O	2.28	0.51
2:Ab:642:LEU:HA	2:Ab:739:THR:HG23	1.92	0.51
1:Af:80:ILE:O	1:Af:81[B]:PHE:HD1	1.94	0.51
1:Au:80:ILE:O	1:Au:81[B]:PHE:HD1	1.94	0.51
1:Ag:80:ILE:O	1:Ag:81[B]:PHE:HD1	1.94	0.51
2:Aq:134:LYS:HZ1	2:Aq:435:ASP:HB3	1.74	0.51
1:Av:80:ILE:O	1:Av:81[B]:PHE:HD1	1.94	0.51
2:Ab:153:VAL:CB	2:Ab:154:PRO:HD3	2.40	0.51
2:Ab:401:HIS:ND1	2:Ab:679:MET:HE1	2.24	0.51
2:Ab:680:ARG:HD3	2:Aq:476:LEU:HD13	1.91	0.51
1:Ad:80:ILE:O	1:Ad:81[B]:PHE:HD1	1.94	0.51
2:Aq:642:LEU:HA	2:Aq:739:THR:HG23	1.92	0.51
1:Aj:80:ILE:O	1:Aj:81[B]:PHE:HD1	1.94	0.51
1:Ak:80:ILE:O	1:Ak:81[B]:PHE:HD1	1.94	0.51
1:Ae:80:ILE:O	1:Ae:81[B]:PHE:HD1	1.94	0.51
1:Ac:80:ILE:O	1:Ac:81[B]:PHE:HD1	1.94	0.51
1:Al:80:ILE:O	1:Al:81[B]:PHE:HD1	1.94	0.51
2:Aq:226:ALA:HB3	2:Aq:333:PRO:HG3	1.93	0.51
2:Aq:470:TYR:HB2	2:Aq:474:LEU:HB2	1.93	0.51
2:Ab:470:TYR:HB2	2:Ab:474:LEU:HB2	1.93	0.51
2:Ab:667:ASP:HB3	2:Ab:670:VAL:HG12	1.93	0.51
2:Aq:709:LEU:HB2	2:Aq:710:PRO:HD3	1.93	0.50
1:As:80:ILE:O	1:As:81[B]:PHE:HD1	1.94	0.50
1:Az:80:ILE:O	1:Az:81[B]:PHE:HD1	1.94	0.50
2:Ab:394:LYS:CG	2:Aq:754:TRP:CD2	2.91	0.50
1:Aw:80:ILE:O	1:Aw:81[B]:PHE:HD1	1.94	0.50
2:Ab:226:ALA:HB3	2:Ab:333:PRO:HG3	1.93	0.50
2:Ab:343:GLU:CG	2:Ab:362:THR:HG21	2.42	0.50
2:Aq:162:ASP:OD1	2:Aq:409:ARG:NH1	2.44	0.50
1:Ay:80:ILE:O	1:Ay:81[B]:PHE:HD1	1.94	0.50
2:Ab:471:LEU:CD2	2:Aq:688:PRO:HB2	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ab:753:VAL:HG21	2:Aq:449:ILE:HD12	1.73	0.50
1:Ap:80:ILE:O	1:Ap:81[B]:PHE:HD1	1.94	0.50
2:Aq:343:GLU:CG	2:Aq:362:THR:HG21	2.41	0.50
2:Ab:162:ASP:OD1	2:Ab:409:ARG:NH1	2.44	0.50
2:Ab:699:HIS:CE1	2:Ab:701:PHE:HB2	2.47	0.50
2:Ab:733:ASN:ND2	2:Aq:313:PHE:CE2	2.78	0.50
2:Ab:493:ASN:O	2:Ab:557:PHE:HA	2.12	0.50
2:Ab:709:LEU:HB2	2:Ab:710:PRO:HD3	1.93	0.50
2:Aq:635:MET:CE	2:Aq:728:GLU:HG3	2.42	0.50
2:Ab:304:GLY:O	2:Ab:537:LEU:HD21	2.12	0.50
2:Ab:449:ILE:CD1	2:Aq:753:VAL:HG21	2.35	0.50
2:Aq:699:HIS:CE1	2:Aq:701:PHE:HB2	2.47	0.50
2:Ab:313:PHE:CG	2:Aq:732:ARG:C	2.90	0.49
2:Aq:493:ASN:O	2:Aq:557:PHE:HA	2.12	0.49
2:Aq:667:ASP:HB3	2:Aq:670:VAL:HG12	1.93	0.49
2:Ab:635:MET:CE	2:Ab:728:GLU:HG3	2.42	0.49
2:Aq:304:GLY:O	2:Aq:537:LEU:HD21	2.12	0.49
2:Ab:543:PRO:O	2:Ab:547:TYR:HB3	2.13	0.49
2:Aq:403:VAL:HG22	2:Aq:479:PHE:CE1	2.48	0.48
2:Aq:543:PRO:O	2:Aq:547:TYR:HB3	2.13	0.48
2:Aq:346:PHE:CD2	2:Aq:362:THR:HG22	2.46	0.48
2:Ab:192:VAL:HG12	2:Ab:193:LYS:N	2.28	0.48
2:Ab:153:VAL:O	2:Ab:414:PRO:HA	2.14	0.48
2:Aq:192:VAL:HG12	2:Aq:193:LYS:N	2.28	0.48
2:Aq:283:MET:HE2	2:Aq:297:PHE:CD1	2.49	0.48
2:Ab:283:MET:HE2	2:Ab:297:PHE:CD1	2.49	0.48
2:Ab:542:PHE:HB3	2:Ab:543:PRO:HD3	1.96	0.48
2:Ab:673:LYS:HE2	2:Aq:400:ASP:OD1	2.14	0.48
2:Aq:561:THR:HG22	2:Aq:562:ASP:O	2.14	0.48
2:Ab:346:PHE:CD2	2:Ab:362:THR:HG22	2.46	0.47
2:Ab:403:VAL:HG22	2:Ab:479:PHE:CE1	2.48	0.47
2:Aq:542:PHE:HB3	2:Aq:543:PRO:HD3	1.96	0.47
2:Aq:619:LEU:HD21	2:Aq:623:ARG:HH21	1.80	0.47
2:Ab:310:THR:HG22	2:Ab:310:THR:O	2.14	0.47
2:Ab:394:LYS:HG2	2:Aq:754:TRP:CE3	2.50	0.47
2:Ab:619:LEU:HD21	2:Ab:623:ARG:HH21	1.80	0.47
2:Aq:325:ARG:HB3	2:Aq:326:SER:H	1.47	0.47
2:Aq:153:VAL:O	2:Aq:414:PRO:HA	2.14	0.47
2:Ab:561:THR:HG22	2:Ab:562:ASP:O	2.14	0.47
2:Aq:288:PHE:O	2:Aq:290:ILE:N	2.45	0.47
2:Ab:147:LEU:CD2	2:Ab:165:LEU:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Aq:243:PHE:HB3	2:Aq:274:LEU:CD1	2.45	0.46
2:Ab:325:ARG:HB3	2:Ab:326:SER:H	1.47	0.46
2:Ab:754:TRP:CZ2	2:Aq:394:LYS:HG2	2.42	0.46
2:Aq:146:LEU:C	2:Aq:146:LEU:HD23	2.41	0.46
2:Aq:258:ARG:HH11	2:Aq:284:ASP:CG	2.24	0.46
2:Aq:715:ASN:O	2:Aq:726:PHE:HD1	1.99	0.46
2:Aq:310:THR:O	2:Aq:310:THR:HG22	2.14	0.46
2:Ab:258:ARG:HH11	2:Ab:284:ASP:CG	2.24	0.46
2:Ab:628:TYR:O	2:Ab:632:ILE:HG12	2.16	0.46
2:Ab:146:LEU:HD23	2:Ab:146:LEU:C	2.41	0.46
2:Ab:629:ARG:O	2:Ab:633:LYS:HG2	2.16	0.46
2:Aq:146:LEU:HD23	2:Aq:146:LEU:O	2.15	0.46
2:Aq:147:LEU:CD2	2:Aq:165:LEU:HD11	2.45	0.46
2:Ab:194:ASP:HB2	2:Ab:378:SER:O	2.15	0.46
2:Aq:559:GLU:C	2:Aq:561:THR:H	2.24	0.46
2:Aq:628:TYR:O	2:Aq:632:ILE:HG12	2.16	0.46
2:Ab:146:LEU:HD23	2:Ab:146:LEU:O	2.15	0.46
2:Ab:212:LEU:HB3	1:Am:19:ALA:HA	1.97	0.46
2:Ab:243:PHE:HB3	2:Ab:274:LEU:CD1	2.45	0.46
2:Aq:194:ASP:HB2	2:Aq:378:SER:O	2.15	0.46
2:Ab:632:ILE:HG22	2:Ab:637:LEU:O	2.16	0.45
2:Ab:637:LEU:HD21	2:Aq:315:SER:CA	2.46	0.45
2:Ab:721:GLN:O	2:Ab:721:GLN:HG3	2.16	0.45
1:Ae:90[B]:CYS:SG	1:Ae:92:ASP:O	2.74	0.45
1:Al:90[B]:CYS:SG	1:Al:92:ASP:O	2.74	0.45
2:Aq:667:ASP:HB3	2:Aq:670:VAL:CG1	2.46	0.45
2:Ab:667:ASP:HB3	2:Ab:670:VAL:CG1	2.46	0.45
2:Ab:715:ASN:O	2:Ab:726:PHE:HD1	1.99	0.45
2:Aq:632:ILE:HG22	2:Aq:637:LEU:O	2.16	0.45
1:Aa:90[B]:CYS:SG	1:Aa:92:ASP:O	2.74	0.45
1:Ad:90[B]:CYS:SG	1:Ad:92:ASP:O	2.74	0.45
1:Am:90[B]:CYS:SG	1:Am:92:ASP:O	2.74	0.45
1:Ar:90[B]:CYS:SG	1:Ar:92:ASP:O	2.74	0.45
2:Aq:346:PHE:HD1	2:Aq:349:MET:HE2	1.81	0.45
2:Aq:652:ALA:HB1	2:Aq:749:LEU:HB3	1.99	0.45
2:Ab:754:TRP:HH2	2:Aq:399:PRO:HA	1.80	0.45
2:Ab:211:TYR:HA	1:Am:18:ALA:HA	1.98	0.45
2:Ab:490:GLY:HA3	2:Ab:559:GLU:OE1	2.17	0.45
2:Aq:518:THR:HG23	2:Aq:520:GLN:CG	2.47	0.45
1:Ay:90[B]:CYS:SG	1:Ay:92:ASP:O	2.74	0.45
2:Ab:470:TYR:O	2:Ab:471:LEU:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ap:90[B]:CYS:SG	1:Ap:92:ASP:O	2.74	0.45
2:Ab:288:PHE:O	2:Ab:290:ILE:N	2.45	0.45
2:Ab:652:ALA:HB1	2:Ab:749:LEU:HB3	1.99	0.45
2:Aq:629:ARG:O	2:Aq:633:LYS:HG2	2.16	0.45
2:Ab:324:SER:HB3	2:Ab:327:SER:HB3	1.99	0.44
2:Aq:490:GLY:HA3	2:Aq:559:GLU:OE1	2.17	0.44
1:Ac:90[B]:CYS:SG	1:Ac:92:ASP:O	2.74	0.44
2:Aq:324:SER:HB3	2:Aq:327:SER:HB3	1.99	0.44
2:Ab:212:LEU:H	1:Am:18:ALA:C	2.24	0.44
2:Ab:637:LEU:HD21	2:Aq:315:SER:HA	2.00	0.44
1:Af:90[B]:CYS:SG	1:Af:92:ASP:O	2.74	0.44
1:Ap:72:LEU:C	1:Ap:72:LEU:HD13	2.43	0.44
2:Aq:470:TYR:O	2:Aq:471:LEU:C	2.60	0.44
1:As:90[B]:CYS:SG	1:As:92:ASP:O	2.74	0.44
1:Ay:72:LEU:HD13	1:Ay:72:LEU:C	2.43	0.44
1:Af:72:LEU:HD13	1:Af:72:LEU:C	2.43	0.44
2:Aq:721:GLN:HG3	2:Aq:721:GLN:O	2.16	0.44
1:Au:90[B]:CYS:SG	1:Au:92:ASP:O	2.74	0.44
1:Aa:72:LEU:HD13	1:Aa:72:LEU:C	2.43	0.44
2:Ab:672:LYS:HB2	2:Aq:669:PHE:CZ	2.53	0.44
2:Ab:754:TRP:CH2	2:Aq:399:PRO:CB	3.00	0.44
1:Aj:90[B]:CYS:SG	1:Aj:92:ASP:O	2.74	0.44
1:Ak:90[B]:CYS:SG	1:Ak:92:ASP:O	2.74	0.44
1:Au:72:LEU:HD13	1:Au:72:LEU:C	2.43	0.44
2:Ab:135:LEU:HD21	2:Ab:432:MET:HE1	2.00	0.44
2:Ab:212:LEU:HD22	1:Am:19:ALA:HB2	1.99	0.44
1:Ag:72:LEU:C	1:Ag:72:LEU:HD13	2.43	0.44
1:Ag:90[B]:CYS:SG	1:Ag:92:ASP:O	2.74	0.44
1:An:72:LEU:HD13	1:An:72:LEU:C	2.43	0.44
1:Av:72:LEU:HD13	1:Av:72:LEU:C	2.43	0.44
1:Av:90[B]:CYS:SG	1:Av:92:ASP:O	2.74	0.44
1:Ax:72:LEU:C	1:Ax:72:LEU:HD13	2.43	0.44
2:Ab:346:PHE:HD1	2:Ab:349:MET:HE2	1.82	0.44
2:Ab:633:LYS:C	2:Ab:635:MET:H	2.26	0.44
2:Ab:753:VAL:CB	2:Aq:402:TYR:CZ	3.00	0.44
1:Ar:72:LEU:HD13	1:Ar:72:LEU:C	2.43	0.44
1:As:72:LEU:C	1:As:72:LEU:HD13	2.43	0.44
2:Ab:313:PHE:CD1	2:Aq:732:ARG:HB2	2.51	0.44
2:Ab:559:GLU:C	2:Ab:561:THR:H	2.25	0.44
1:Ac:72:LEU:C	1:Ac:72:LEU:HD13	2.43	0.44
1:Ae:72:LEU:HD13	1:Ae:72:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Aq:135:LEU:HD21	2:Aq:432:MET:HE1	2.00	0.44
2:Aq:166:ALA:HB2	2:Aq:409:ARG:NH1	2.33	0.44
2:Aq:621:PHE:CZ	2:Aq:709:LEU:HD22	2.53	0.44
1:Aw:90[B]:CYS:SG	1:Aw:92:ASP:O	2.74	0.44
1:Az:72:LEU:HD13	1:Az:72:LEU:C	2.43	0.44
2:Ab:518:THR:HG23	2:Ab:520:GLN:CG	2.47	0.44
1:Al:72:LEU:C	1:Al:72:LEU:HD13	2.43	0.44
1:Ao:90[B]:CYS:SG	1:Ao:92:ASP:O	2.74	0.44
1:Aw:72:LEU:C	1:Aw:72:LEU:HD13	2.43	0.44
1:Az:90[B]:CYS:SG	1:Az:92:ASP:O	2.74	0.44
2:Ab:621:PHE:CZ	2:Ab:709:LEU:HD22	2.53	0.43
1:Ah:72:LEU:C	1:Ah:72:LEU:HD13	2.43	0.43
1:Ai:72:LEU:HD13	1:Ai:72:LEU:C	2.43	0.43
1:Ao:72:LEU:C	1:Ao:72:LEU:HD13	2.43	0.43
1:At:72:LEU:C	1:At:72:LEU:HD13	2.43	0.43
2:Ab:637:LEU:CD2	2:Aq:315:SER:CA	2.96	0.43
2:Ab:713:LEU:HA	2:Ab:713:LEU:HD23	1.76	0.43
1:Ah:90[B]:CYS:SG	1:Ah:92:ASP:O	2.74	0.43
1:Ai:90[B]:CYS:SG	1:Ai:92:ASP:O	2.74	0.43
1:Aj:72:LEU:HD13	1:Aj:72:LEU:C	2.43	0.43
1:Ak:72:LEU:C	1:Ak:72:LEU:HD13	2.43	0.43
1:At:90[B]:CYS:SG	1:At:92:ASP:O	2.74	0.43
2:Ab:166:ALA:HB2	2:Ab:409:ARG:NH1	2.34	0.43
2:Ab:695:SER:HA	2:Ab:696:PRO:HD3	1.84	0.43
2:Ab:740:TRP:CZ3	2:Aq:312:GLY:CA	2.89	0.43
1:Ad:72:LEU:C	1:Ad:72:LEU:HD13	2.43	0.43
1:Am:72:LEU:HD13	1:Am:72:LEU:C	2.43	0.43
2:Aq:403:VAL:HG22	2:Aq:479:PHE:CZ	2.53	0.43
2:Aq:645:ALA:HB2	2:Aq:743:GLN:HG2	2.01	0.43
2:Ab:403:VAL:HG22	2:Ab:479:PHE:CZ	2.53	0.43
2:Ab:192:VAL:HG12	2:Ab:193:LYS:H	1.84	0.43
2:Aq:633:LYS:C	2:Aq:635:MET:H	2.26	0.43
2:Ab:304:GLY:HA2	2:Ab:537:LEU:HD11	2.01	0.42
2:Ab:314:PRO:O	2:Aq:732:ARG:NH2	2.51	0.42
2:Aq:699:HIS:CE1	2:Aq:702:TRP:CD1	3.07	0.42
2:Ab:165:LEU:HD12	2:Ab:165:LEU:HA	1.82	0.42
1:Ax:90[B]:CYS:SG	1:Ax:92:ASP:O	2.74	0.42
2:Aq:304:GLY:HA2	2:Aq:537:LEU:HD11	2.01	0.42
2:Aq:433:PHE:O	2:Aq:437:VAL:HG23	2.19	0.42
2:Ab:433:PHE:O	2:Ab:437:VAL:HG23	2.20	0.42
2:Ab:645:ALA:HB2	2:Ab:743:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:90[B]:CYS:SG	1:An:92:ASP:O	2.74	0.42
2:Ab:699:HIS:CE1	2:Ab:702:TRP:CD1	3.07	0.42
2:Aq:214:GLU:OE2	2:Aq:341:ALA:HB2	2.20	0.42
2:Ab:748:ALA:HA	2:Aq:477:LYS:HZ2	1.81	0.42
2:Ab:262:ILE:HB	2:Ab:266:GLU:OE1	2.19	0.42
2:Ab:297:PHE:CD1	2:Ab:336:THR:OG1	2.73	0.41
2:Ab:733:ASN:ND2	2:Aq:313:PHE:HE2	2.19	0.41
2:Ab:752:ASP:CG	2:Aq:399:PRO:C	2.87	0.41
2:Aq:262:ILE:HB	2:Aq:266:GLU:OE1	2.19	0.41
2:Aq:322:PRO:HA	2:Aq:323:PRO:HD3	1.95	0.41
2:Ab:214:GLU:OE2	2:Ab:341:ALA:HB2	2.20	0.41
2:Ab:393:ILE:HG21	2:Ab:437:VAL:HG21	2.02	0.41
2:Aq:192:VAL:HG12	2:Aq:193:LYS:H	1.84	0.41
2:Ab:402:TYR:CE2	2:Aq:753:VAL:HG11	2.55	0.41
2:Aq:339:ARG:O	2:Aq:343:GLU:HG3	2.21	0.41
2:Aq:515:HIS:HA	2:Aq:516:PRO:HD3	1.82	0.41
2:Aq:628:TYR:C	2:Aq:630:ALA:N	2.78	0.41
2:Ab:339:ARG:O	2:Ab:343:GLU:HG3	2.21	0.41
2:Ab:755:ASP:O	2:Ab:756:ILE:HG13	2.20	0.41
2:Aq:755:ASP:O	2:Aq:756:ILE:HG13	2.20	0.41
2:Ab:210:VAL:HG23	1:Am:18:ALA:HB2	2.01	0.41
2:Ab:283:MET:HE2	2:Ab:297:PHE:CG	2.56	0.41
2:Ab:433:PHE:HA	2:Ab:436:MET:HE3	2.02	0.41
2:Ab:628:TYR:C	2:Ab:630:ALA:N	2.78	0.41
2:Ab:680:ARG:HD3	2:Aq:476:LEU:CD1	2.51	0.41
2:Aq:148:ASN:HD22	2:Aq:148:ASN:HA	1.76	0.41
2:Aq:297:PHE:CD1	2:Aq:336:THR:OG1	2.74	0.41
2:Ab:394:LYS:HG2	2:Aq:754:TRP:CZ2	2.55	0.40
2:Ab:689:TYR:CE1	2:Aq:693:LYS:HE2	2.56	0.40
2:Ab:599:ILE:O	2:Ab:600:LYS:C	2.64	0.40
2:Aq:231:LYS:HB2	2:Aq:231:LYS:HE3	1.79	0.40
2:Aq:433:PHE:HA	2:Aq:436:MET:HE3	2.02	0.40
2:Aq:283:MET:HE2	2:Aq:297:PHE:CG	2.56	0.40
2:Aq:393:ILE:HG21	2:Aq:437:VAL:HG21	2.02	0.40
2:Ab:459:GLY:O	2:Ab:460:SER:C	2.65	0.40
2:Ab:645:ALA:HB1	2:Ab:742:ILE:HG22	2.04	0.40
2:Ab:689:TYR:CD1	2:Aq:693:LYS:HE2	2.56	0.40
2:Aq:221:ALA:O	2:Aq:222:TYR:CB	2.69	0.40
2:Aq:664:GLU:CD	2:Aq:664:GLU:N	2.75	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	Aa	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ac	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ad	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ae	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Af	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ag	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ah	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ai	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Aj	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ak	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Al	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Am	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	An	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ao	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ap	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ar	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	As	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	At	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Au	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Av	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Aw	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ax	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Ay	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
1	Az	180/182 (99%)	177 (98%)	3 (2%)	0	100	100
2	Ab	629/640 (98%)	604 (96%)	22 (4%)	3 (0%)	24	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Aq	629/640 (98%)	605 (96%)	21 (3%)	3 (0%)	24	64
All	All	5578/5648 (99%)	5457 (98%)	115 (2%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ab	325	ARG
2	Aq	325	ARG
2	Ab	154	PRO
2	Ab	289	PRO
2	Aq	154	PRO
2	Aq	289	PRO

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	Aa	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ac	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ad	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ae	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Af	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ag	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ah	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ai	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Aj	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ak	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Al	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Am	155/162 (96%)	154 (99%)	1 (1%)	78	82
1	An	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ao	163/162 (101%)	162 (99%)	1 (1%)	78	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ap	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ar	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	As	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	At	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Au	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Av	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Aw	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ax	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Ay	163/162 (101%)	162 (99%)	1 (1%)	78	82
1	Az	163/162 (101%)	162 (99%)	1 (1%)	78	82
2	Ab	540/549 (98%)	522 (97%)	18 (3%)	33	55
2	Aq	542/549 (99%)	524 (97%)	18 (3%)	33	55
All	All	4986/4986 (100%)	4926 (99%)	60 (1%)	59	74

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	117	LEU
2	Ab	181	VAL
2	Ab	250	VAL
2	Ab	251	ASN
2	Ab	325	ARG
2	Ab	367	THR
2	Ab	383	GLU
2	Ab	398	GLU
2	Ab	402	TYR
2	Ab	446	ARG
2	Ab	457	ASP
2	Ab	491	THR
2	Ab	518	THR
2	Ab	524	GLN
2	Ab	527	ASN
2	Ab	532	VAL
2	Ab	561	THR
2	Ab	593	VAL
2	Ab	664	GLU
1	Ac	117	LEU
1	Ad	117	LEU

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Mol	Chain	Res	Type
1	Ae	117	LEU
1	Af	117	LEU
1	Ag	117	LEU
1	Ah	117	LEU
1	Ai	117	LEU
1	Aj	117	LEU
1	Ak	117	LEU
1	Al	117	LEU
1	Am	117	LEU
1	An	117	LEU
1	Ao	117	LEU
1	Ap	117	LEU
2	Aq	181	VAL
2	Aq	250	VAL
2	Aq	251	ASN
2	Aq	325	ARG
2	Aq	367	THR
2	Aq	383	GLU
2	Aq	398	GLU
2	Aq	402	TYR
2	Aq	446	ARG
2	Aq	457	ASP
2	Aq	491	THR
2	Aq	518	THR
2	Aq	524	GLN
2	Aq	527	ASN
2	Aq	532	VAL
2	Aq	561	THR
2	Aq	593	VAL
2	Aq	664	GLU
1	Ar	117	LEU
1	As	117	LEU
1	At	117	LEU
1	Au	117	LEU
1	Av	117	LEU
1	Aw	117	LEU
1	Ax	117	LEU
1	Ay	117	LEU
1	Az	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	112	GLN
1	Aa	151	HIS
1	Aa	173	HIS
2	Ab	148	ASN
2	Ab	171	ASN
2	Ab	215	ASN
2	Ab	285	GLN
2	Ab	300	HIS
2	Ab	401	HIS
2	Ab	596	GLN
2	Ab	603	HIS
2	Ab	608	ASN
2	Ab	626	ASN
2	Ab	715	ASN
2	Ab	721	GLN
1	Ac	112	GLN
1	Ac	151	HIS
1	Ac	173	HIS
1	Ad	112	GLN
1	Ad	151	HIS
1	Ad	173	HIS
1	Ae	112	GLN
1	Ae	151	HIS
1	Ae	173	HIS
1	Af	112	GLN
1	Af	151	HIS
1	Af	173	HIS
1	Ag	112	GLN
1	Ag	151	HIS
1	Ag	173	HIS
1	Ah	112	GLN
1	Ah	151	HIS
1	Ah	173	HIS
1	Ai	112	GLN
1	Ai	151	HIS
1	Ai	173	HIS
1	Aj	112	GLN
1	Ak	112	GLN
1	Al	112	GLN
1	Al	151	HIS
1	Al	173	HIS
1	Am	112	GLN
1	Am	151	HIS

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Mol	Chain	Res	Type
1	An	112	GLN
1	An	173	HIS
1	Ao	112	GLN
1	Ap	112	GLN
1	Ap	151	HIS
2	Aq	148	ASN
2	Aq	171	ASN
2	Aq	215	ASN
2	Aq	285	GLN
2	Aq	300	HIS
2	Aq	401	HIS
2	Aq	596	GLN
2	Aq	603	HIS
2	Aq	608	ASN
2	Aq	626	ASN
2	Aq	715	ASN
2	Aq	721	GLN
2	Aq	743	GLN
1	Ar	112	GLN
1	Ar	151	HIS
1	As	112	GLN
1	As	151	HIS
1	As	173	HIS
1	At	112	GLN
1	At	151	HIS
1	Au	112	GLN
1	Au	151	HIS
1	Av	112	GLN
1	Av	151	HIS
1	Aw	112	GLN
1	Aw	151	HIS
1	Ax	98	ASN
1	Ax	112	GLN
1	Ay	112	GLN
1	Ay	151	HIS
1	Ay	173	HIS
1	Az	112	GLN
1	Az	151	HIS

5.3.3 RNA ⓘ

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.

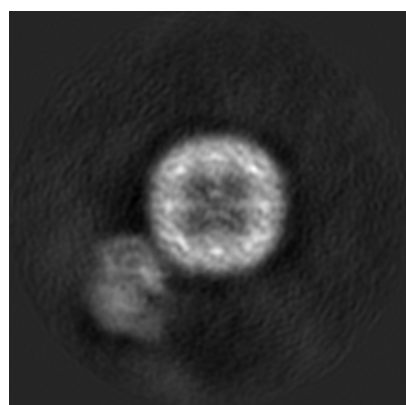
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0046. These allow visual inspection of the internal detail of the map and identification of artifacts.

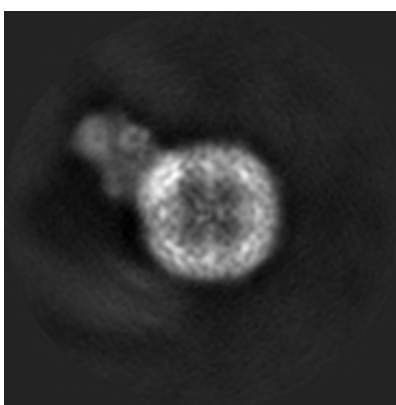
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

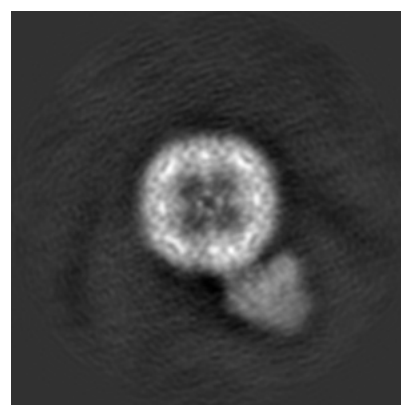
6.1.1 Primary map



X



Y

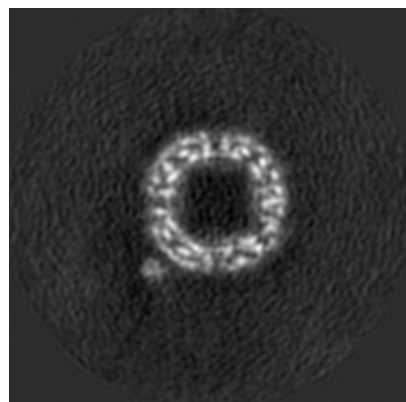


Z

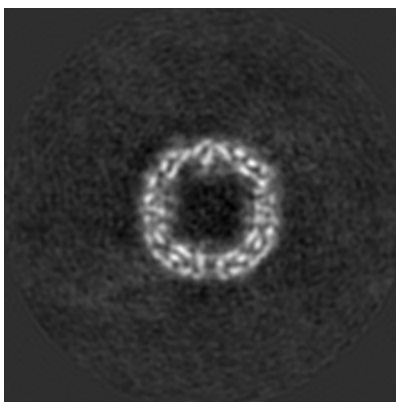
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

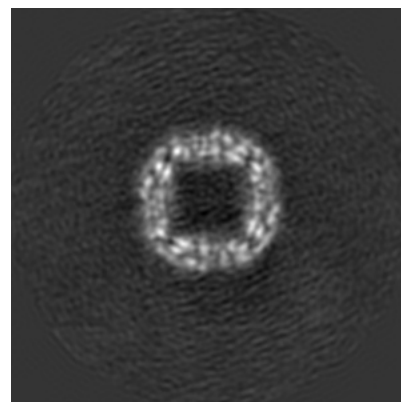
6.2.1 Primary map



X Index: 128



Y Index: 128

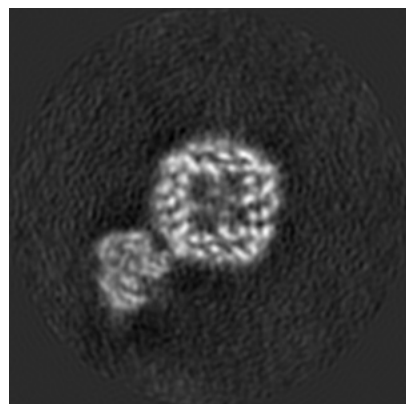


Z Index: 128

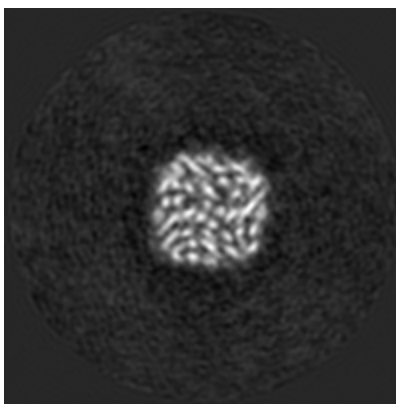
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

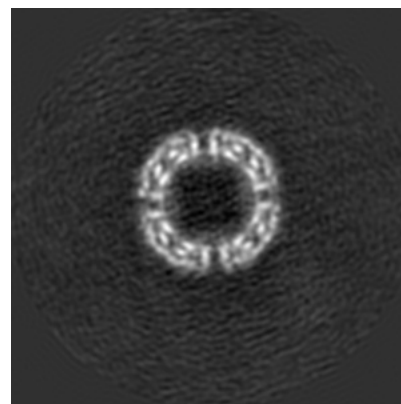
6.3.1 Primary map



X Index: 151



Y Index: 162

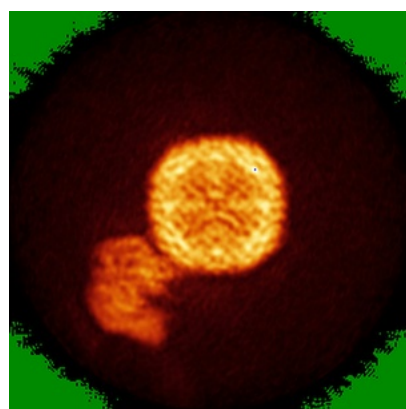


Z Index: 131

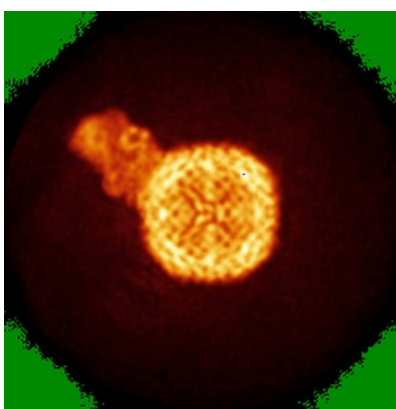
The images above show the largest variance slices of the map in three orthogonal directions.

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

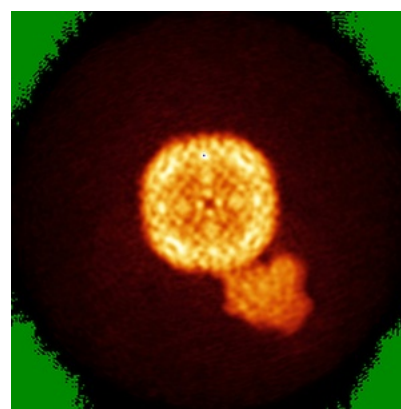
6.4.1 Primary map



X



Y

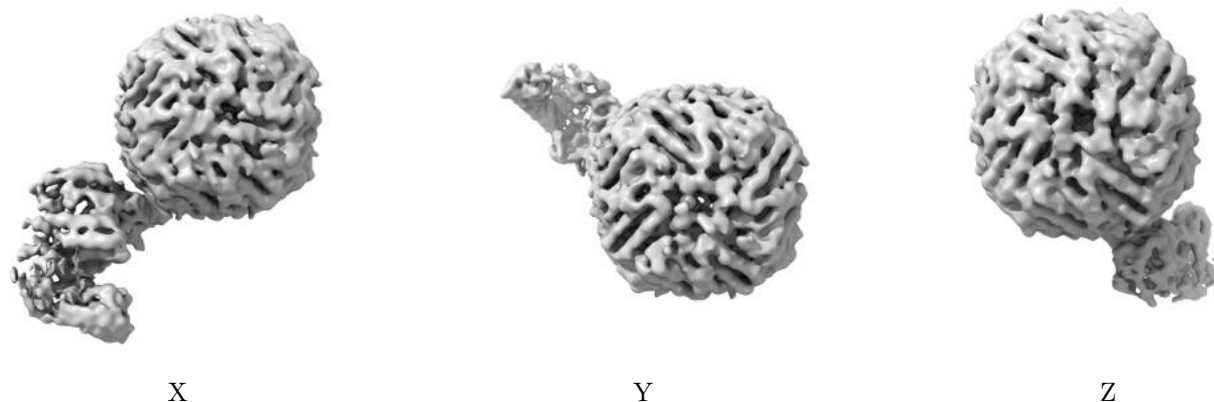


Z

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

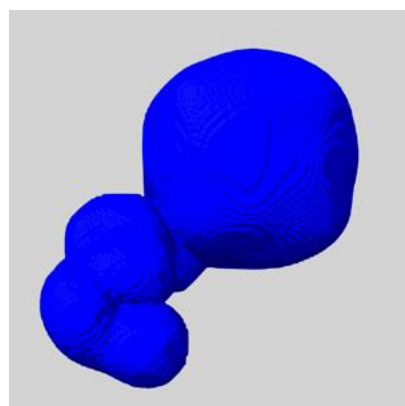
6.6 Mask visualisation [i](#)

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

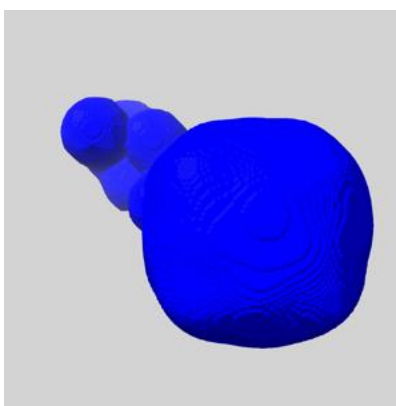
A mask typically either:

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

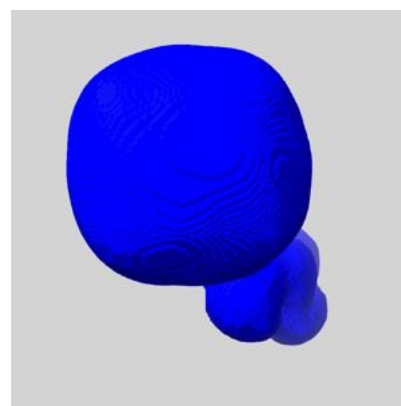
6.6.1 emd_0046_msk_1.map [i](#)



X



Y

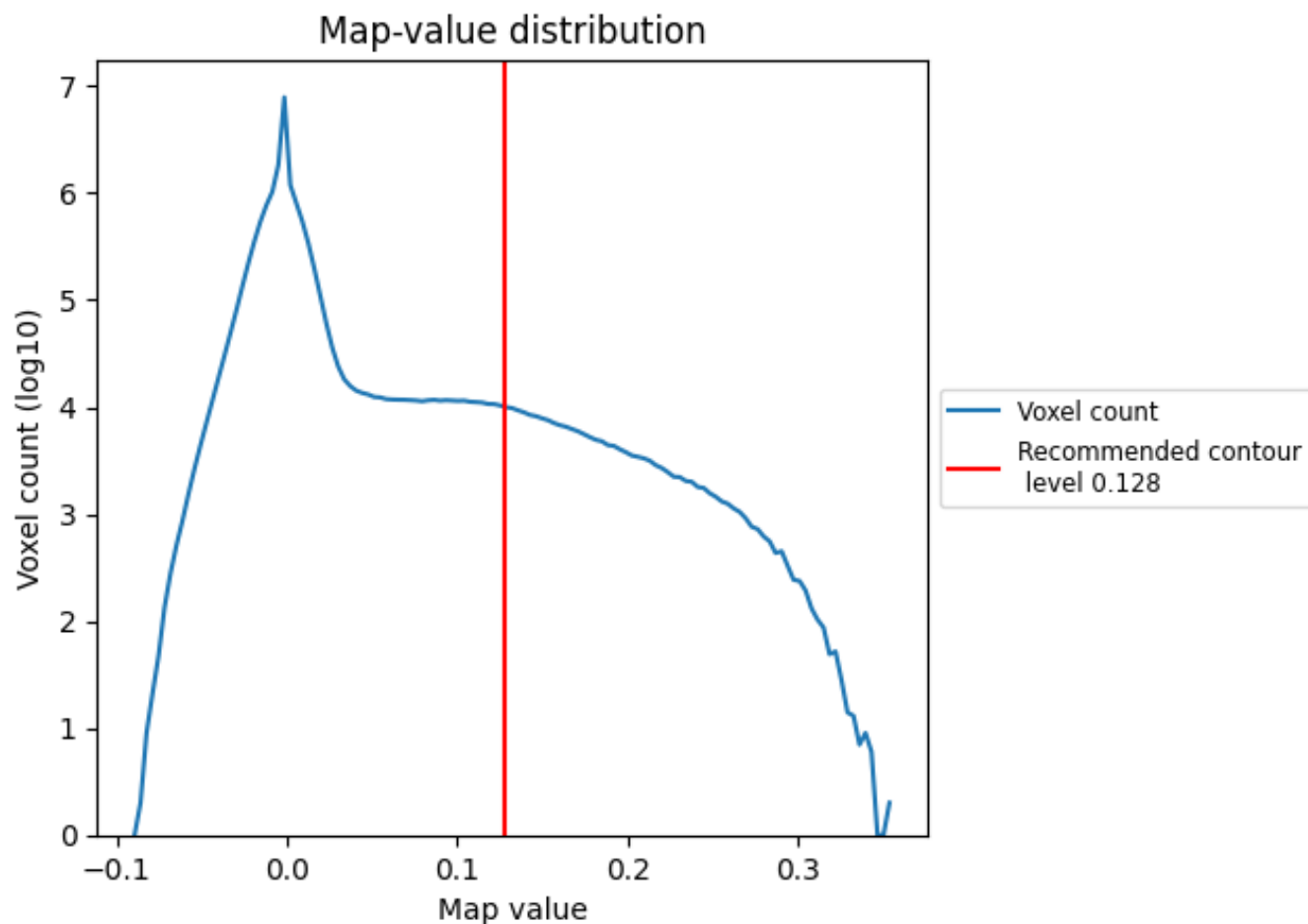


Z

7 Map analysis [i](#)

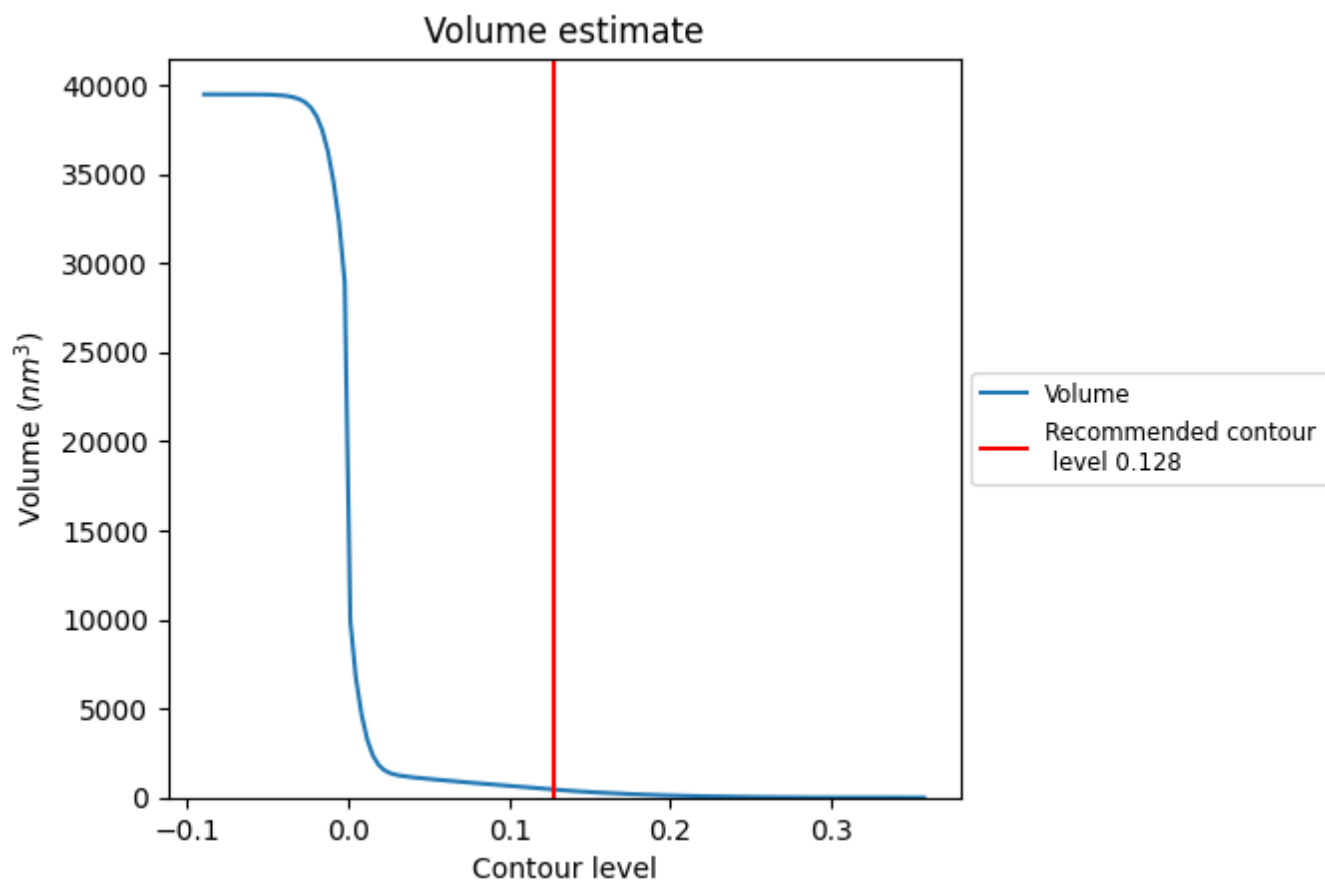
This section contains the results of statistical analysis of the map.

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.

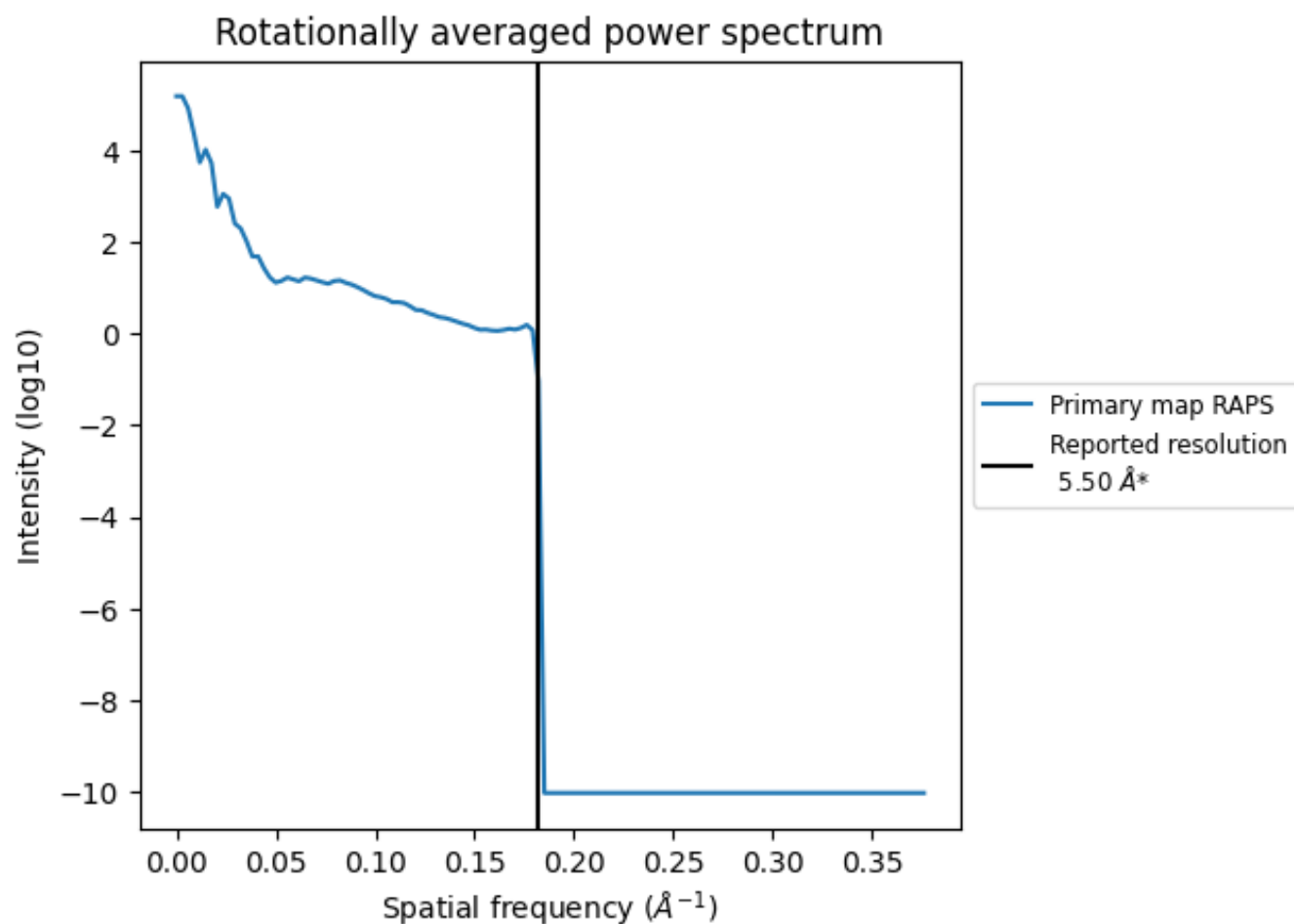
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 444 nm³; this corresponds to an approximate mass of 401 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 ⓘ

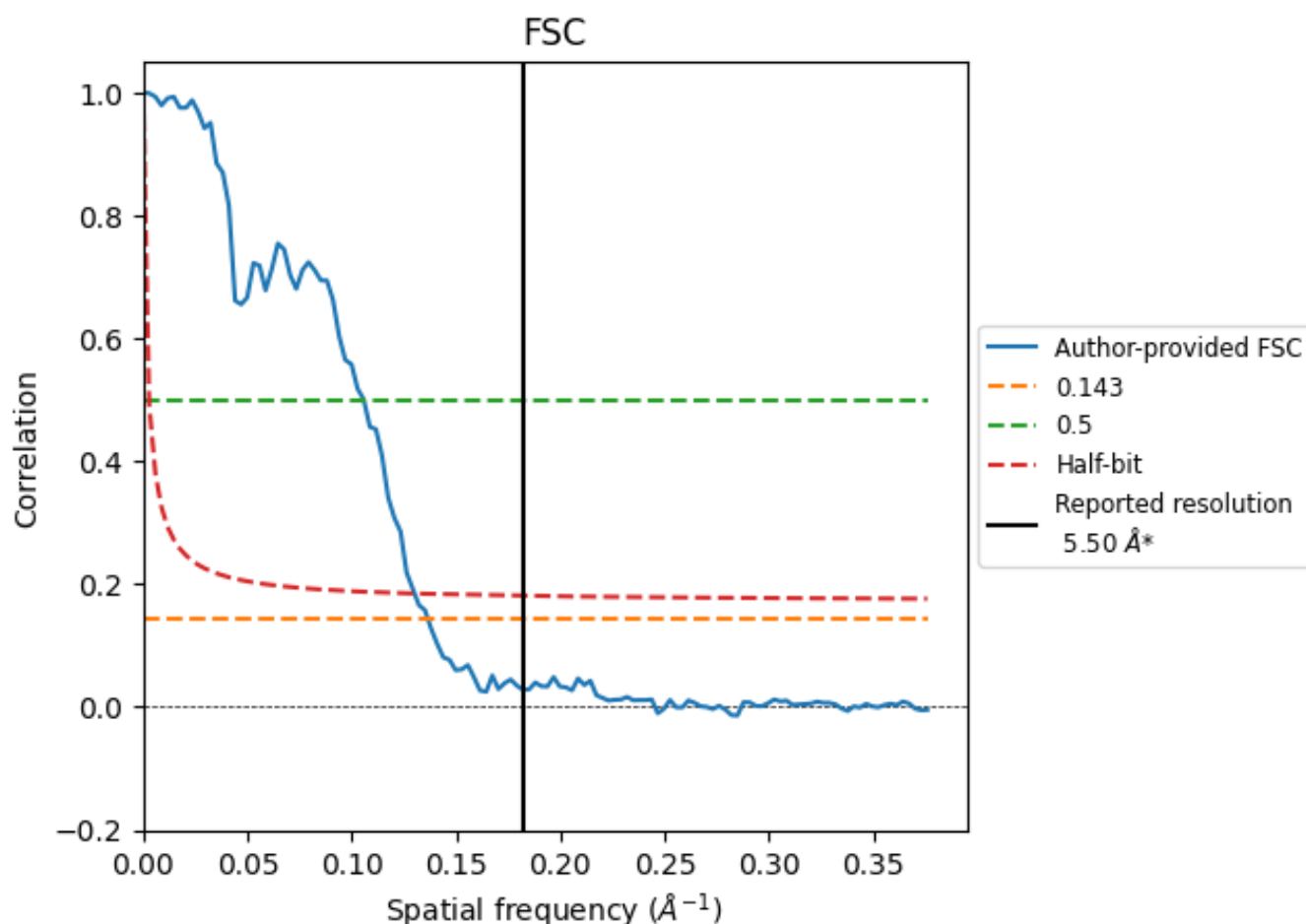


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

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 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

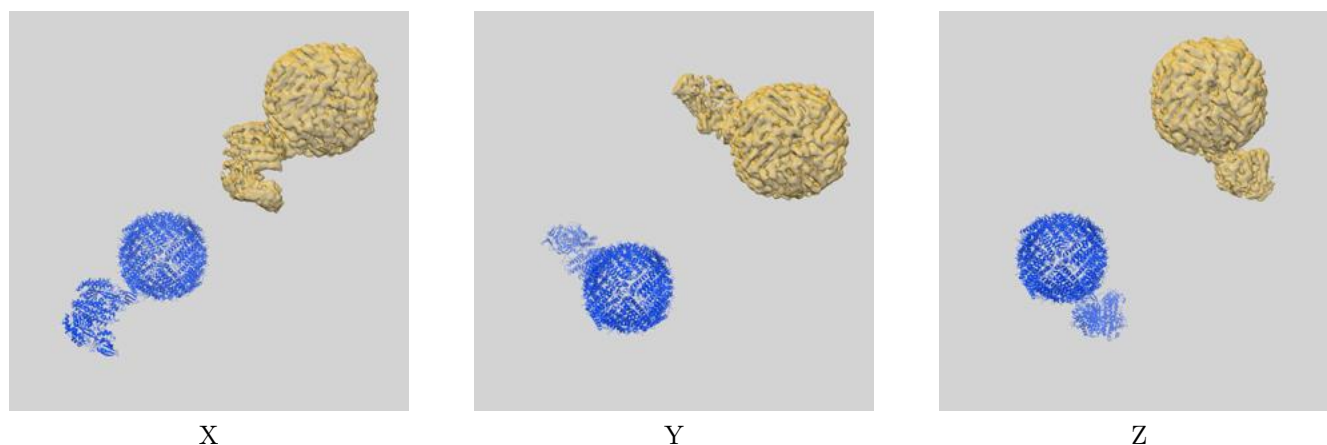
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	7.33	9.45	7.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.33 differs from the reported value 5.5 by more than 10 %

9 Map-model fit [i](#)

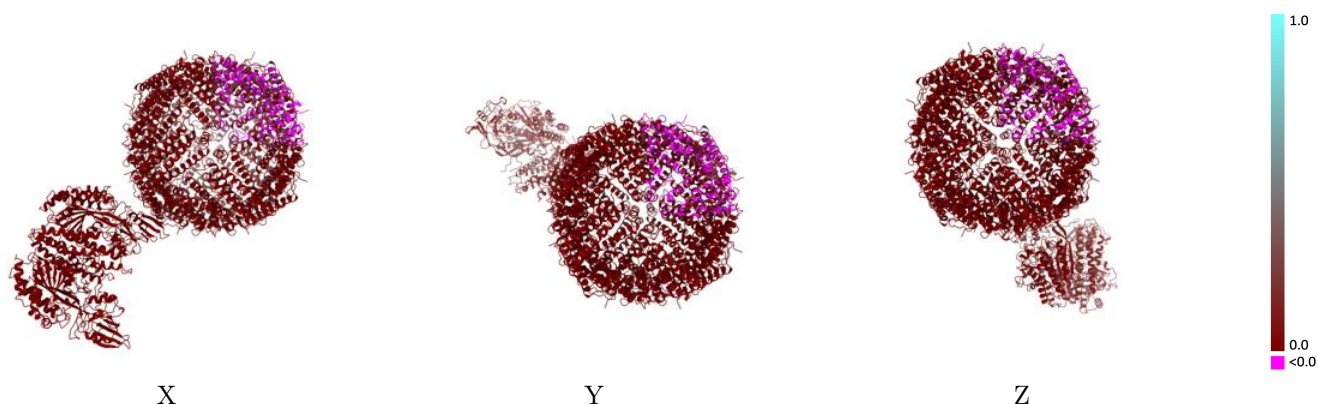
This section contains information regarding the fit between EMDB map EMD-0046 and PDB model 6GSR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



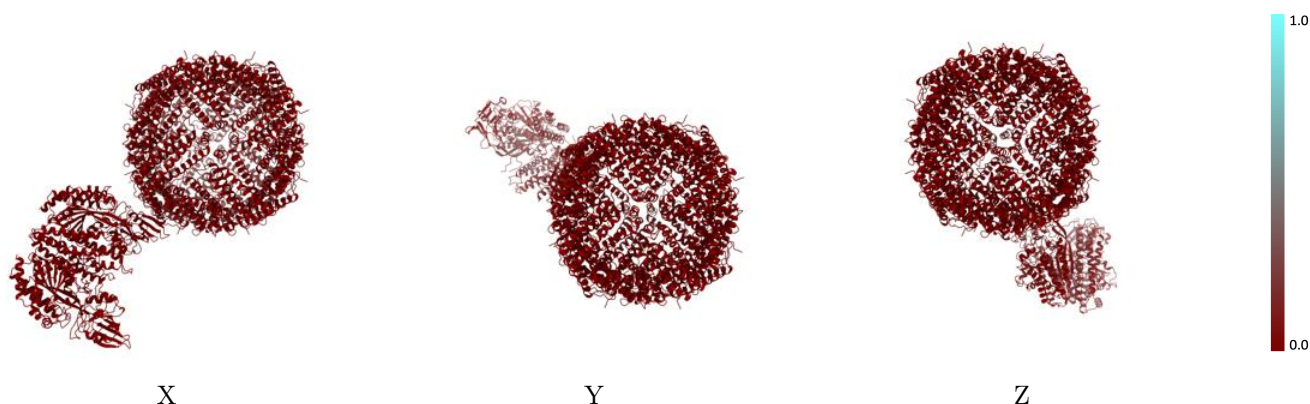
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



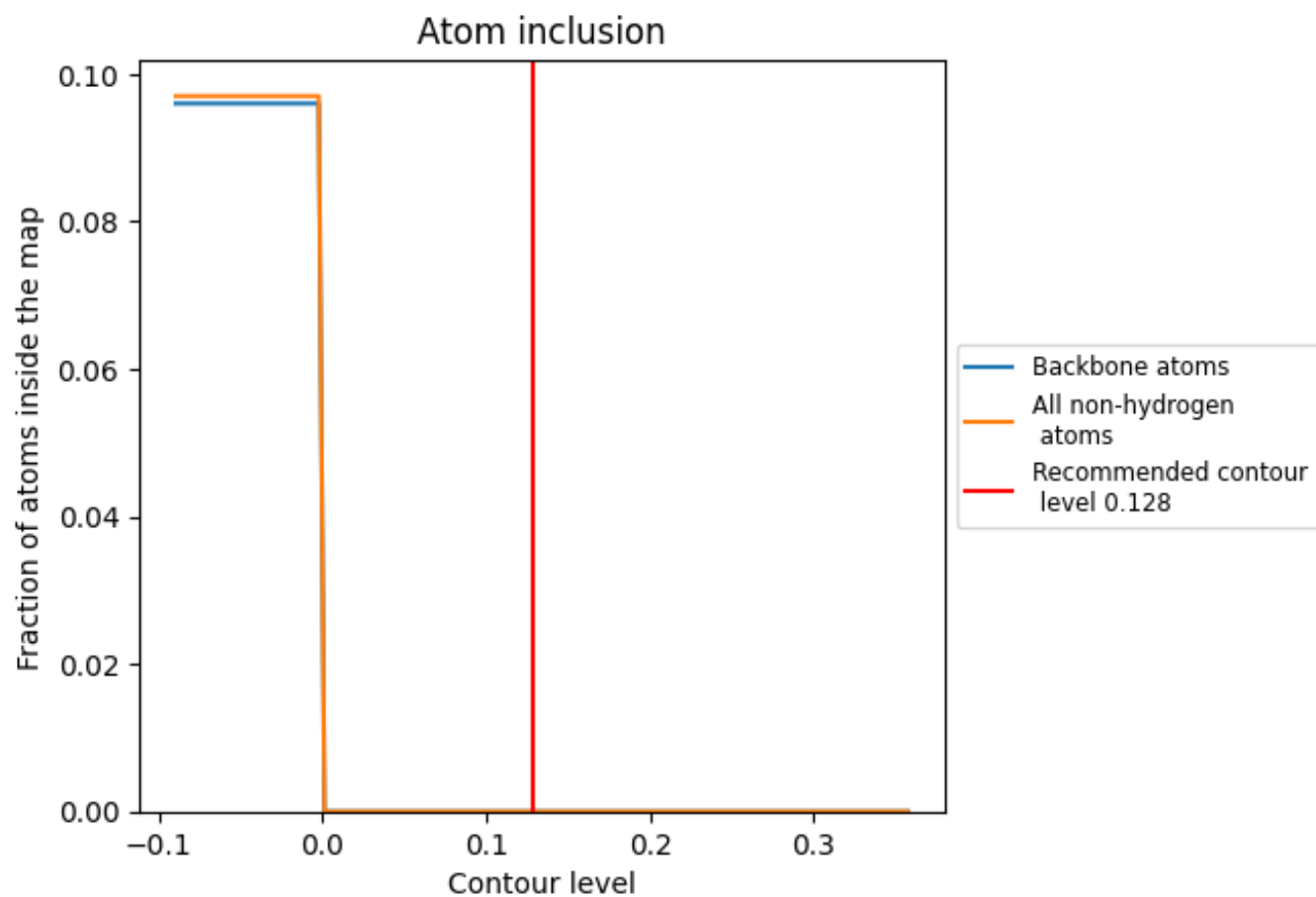
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.128).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 0.0010
Aa	 0.0000	 0.0020
Ab	 0.0000	 0.0000
Ac	 0.0000	 0.0000
Ad	 0.0000	 0.0020
Ae	 0.0000	 0.0060
Af	 0.0000	 0.0000
Ag	 0.0000	 0.0000
Ah	 0.0000	 0.0000
Ai	 0.0000	 0.0000
Aj	 0.0000	 0.0000
Ak	 0.0000	 0.0100
Al	 0.0000	 0.0010
Am	 0.0000	 0.0000
An	 0.0000	 0.0000
Ao	 0.0000	 0.0000
Ap	 0.0000	 -0.0020
Aq	 0.0000	 0.0000
Ar	 0.0000	 0.0000
As	 0.0000	 0.0000
At	 0.0000	 0.0000
Au	 0.0000	 0.0000
Av	 0.0000	 0.0010
Aw	 0.0000	 0.0000
Ax	 0.0000	 0.0090
Ay	 0.0000	 0.0000
Az	 0.0000	 0.0000

