



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 05:18 PM UTC

PDB ID : 7ZBN / pdb_00007zbn
EMDB ID : EMD-14587
Title : Cryo-EM structure of the human GS-GN complex in the inhibited state
Authors : Marr, L.; Zeqiraj, E.
Deposited on : 2022-03-23
Resolution : 2.62 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:

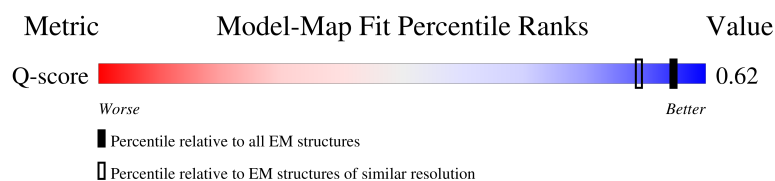
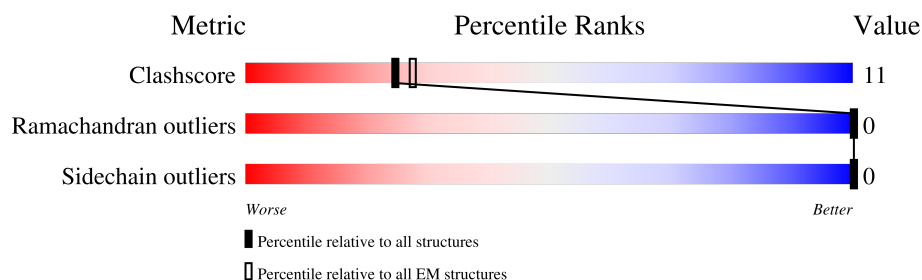
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.62 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	8810 (2.12 - 3.12)

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	737	 66% 18% 16%
1	C	737	 64% 19% 16%
2	B	737	 63% 21% 16%
2	D	737	 63% 21% 16%

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Mol	Chain	Length	Quality of chain
3	E	333	6%8% 90%
3	F	333	6%8% 90%
3	G	333	6%8% 90%
3	H	333	6%8% 90%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41588 atoms, of which 20466 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 Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	617	Total	C	H	N	O	S	0	0
			9830	3202	4842	858	903	25		
1	C	617	Total	C	H	N	O	S	0	0
			9830	3202	4842	858	903	25		

- Molecule 2 is a protein called Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	B	621	Total	C	H	N	O	P	S	0	0
			9896	3218	4879	862	911	1	25		
2	D	621	Total	C	H	N	O	P	S	0	0
			9896	3218	4879	862	911	1	25		

- Molecule 3 is a protein called Isoform GN-1 of Glycogenin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	33	Total	C	H	N	O	S	0	0
			534	170	256	49	58	1		
3	F	33	Total	C	H	N	O	S	0	0
			534	170	256	49	58	1		
3	G	33	Total	C	H	N	O	S	0	0
			534	170	256	49	58	1		
3	H	33	Total	C	H	N	O	S	0	0
			534	170	256	49	58	1		

There are 8 discrepancies between the modelled and reference sequences:

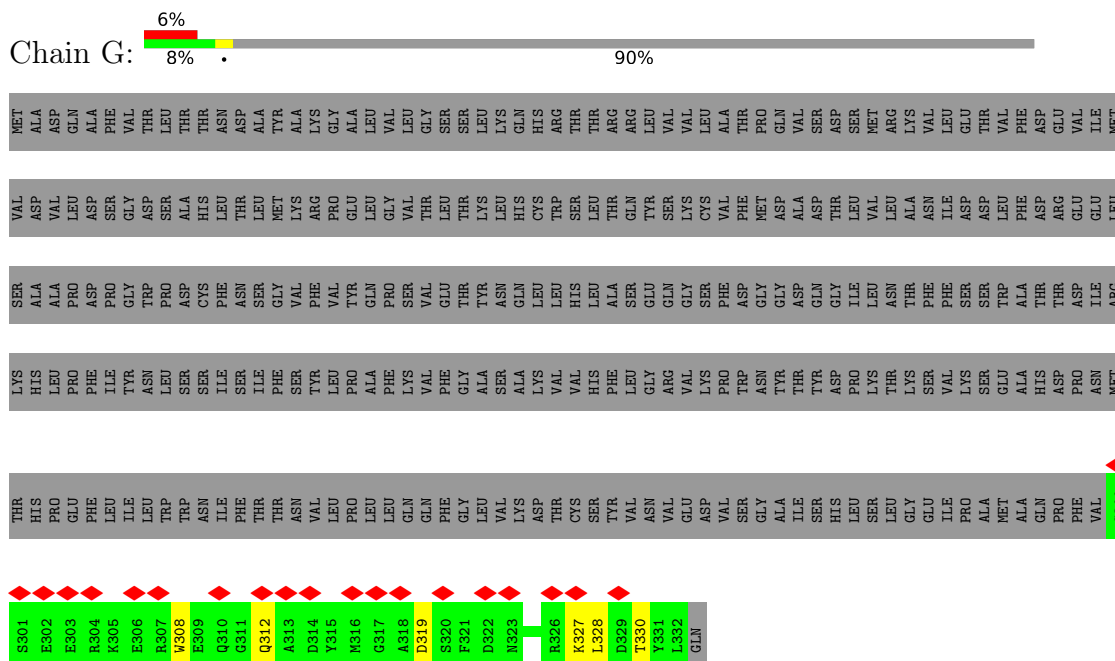
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	THR	conflict	UNP P46976
E	195	PHE	TYR	conflict	UNP P46976
F	2	ALA	THR	conflict	UNP P46976
F	195	PHE	TYR	conflict	UNP P46976
G	2	ALA	THR	conflict	UNP P46976

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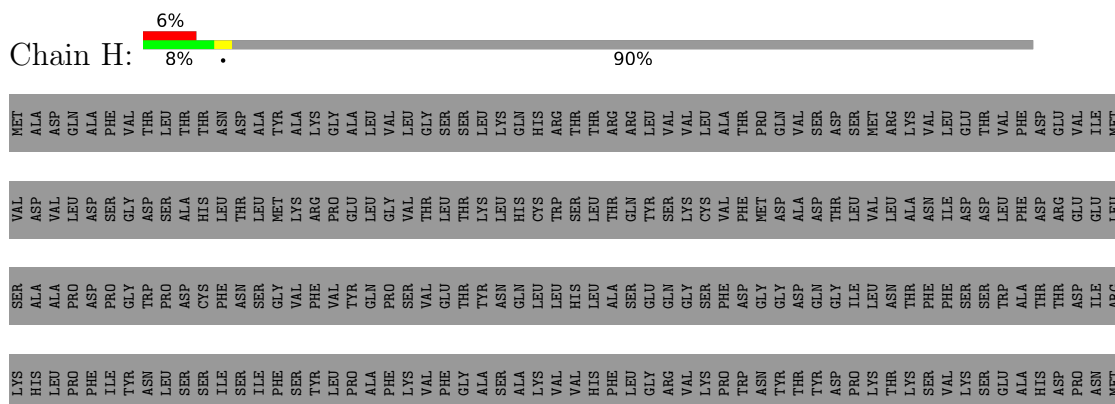
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Chain	Residue	Modelled	Actual	Comment	Reference
G	195	PHE	TYR	conflict	UNP P46976
H	2	ALA	THR	conflict	UNP P46976
H	195	PHE	TYR	conflict	UNP P46976

- Molecule 3: Isoform GN-1 of Glycogenin-1



- Molecule 3: Isoform GN-1 of Glycogenin-1



S301	S302	E303	R304	K305	E306	R307	W308	E309	Q310	G311	Q312	A313	D314	Y315	M316	G317	A318	D319	S320	F321	D322	M323		R326	K327	L328	D329	T330	Y331	L332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000
THR	HIS	PRO	GLU	PHE	LEU	ILE	LEU	TRP	TRP	ASN	ASN	ILE	PHE	THR	THR	ASN	VAL	LEU	PRO	LEU	LEU	GLN	GLN	PHE	GLY	LEU	VAL	VAL	LYS	ASP	THR	CYS	SER	TYR	VAL	ASN	VAL	VAL	GLU	ASP	VAL	VAL	SER	GLY	ALA	ILE	SER	HIS	LEU	SER	SER	LEU	GLY	LEU	ILE	PRO	ALA	MET	ALA	GLN	PRO	PHE	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	739232	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 ($e^-/\text{\AA}^2$)	34.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.313	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	204.48, 204.48, 204.48	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/5121	0.31	0/6942
1	C	0.25	0/5121	0.31	0/6942
2	B	0.25	0/5140	0.32	0/6968
2	D	0.25	0/5140	0.32	0/6968
3	E	0.12	0/282	0.26	0/375
3	F	0.11	0/282	0.23	0/375
3	G	0.11	0/282	0.26	0/375
3	H	0.11	0/282	0.24	0/375
All	All	0.25	0/21650	0.31	0/29320

There are no bond length outliers.

There are no bond angle outliers.

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	A	4988	4842	4854	105	0
1	C	4988	4842	4854	112	0
2	B	5017	4879	4879	116	0
2	D	5017	4879	4878	119	0
3	E	278	256	256	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	278	256	256	3	0
3	G	278	256	256	4	0
3	H	278	256	256	3	0
All	All	21122	20466	20489	440	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 11.

All (440) 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:D:497:VAL:HG12	2:D:524:ILE:HD13	1.64	0.79
2:B:497:VAL:HG12	2:B:524:ILE:HD13	1.64	0.79
2:D:379:THR:HG22	2:D:488:LEU:HD11	1.68	0.76
2:B:379:THR:HG22	2:B:488:LEU:HD11	1.69	0.74
1:A:259:SER:HG	1:A:262:THR:HG1	1.35	0.74
1:C:259:SER:HG	1:C:262:THR:HG1	1.35	0.74
2:D:31:GLU:HB3	2:D:64:LEU:HD23	1.69	0.73
2:B:31:GLU:HB3	2:B:64:LEU:HD23	1.69	0.73
2:D:259:SER:HG	2:D:262:THR:HG1	1.36	0.72
2:B:259:SER:HG	2:B:262:THR:HG1	1.35	0.72
1:A:251:CYS:SG	3:E:328:LEU:HD22	2.31	0.70
1:A:307:PHE:HE2	1:A:476:ILE:HD13	1.56	0.70
1:C:251:CYS:SG	3:G:328:LEU:HD22	2.31	0.70
1:C:307:PHE:HE2	1:C:476:ILE:HD13	1.57	0.70
1:C:519:CYS:SG	1:C:524:ILE:HG23	2.31	0.69
2:D:307:PHE:HE2	2:D:476:ILE:HD13	1.56	0.69
1:A:519:CYS:SG	1:A:524:ILE:HG23	2.31	0.69
2:B:307:PHE:HE2	2:B:476:ILE:HD13	1.57	0.69
1:C:638:ARG:HG2	2:D:640:ALA:O	1.93	0.68
1:A:234:GLY:O	3:E:312:GLN:NE2	2.27	0.68
2:B:251:CYS:SG	3:F:328:LEU:HD22	2.35	0.66
2:D:251:CYS:SG	3:H:328:LEU:HD22	2.35	0.66
2:D:229:VAL:HG11	2:D:269:LEU:HA	1.78	0.66
2:B:506:PRO:O	2:B:555:ARG:NH1	2.29	0.65
2:D:506:PRO:O	2:D:555:ARG:NH1	2.29	0.65
2:D:145:ASP:O	2:D:149:ASN:ND2	2.29	0.65
2:B:145:ASP:O	2:B:149:ASN:ND2	2.29	0.65
1:A:229:VAL:HG11	1:A:269:LEU:HA	1.77	0.65
1:C:234:GLY:O	3:G:312:GLN:NE2	2.30	0.64
2:B:229:VAL:HG11	2:B:269:LEU:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG22	1:A:488:LEU:HD11	1.79	0.64
1:C:282:LEU:HD23	1:C:521:VAL:HG21	1.79	0.64
1:A:600:TYR:HH	1:A:604:TYR:HH	1.38	0.63
2:B:28:VAL:CG1	2:B:175:VAL:HG22	2.30	0.62
1:A:506:PRO:O	1:A:555:ARG:NH1	2.30	0.62
2:D:28:VAL:CG1	2:D:175:VAL:HG22	2.30	0.62
1:A:379:THR:HG22	1:A:488:LEU:CD1	2.30	0.62
1:A:420:LEU:HD23	1:A:428:MET:HE1	1.82	0.62
1:C:420:LEU:HD23	1:C:428:MET:HE1	1.82	0.62
1:C:379:THR:HG22	1:C:488:LEU:HD11	1.81	0.61
1:C:379:THR:HG22	1:C:488:LEU:CD1	2.31	0.61
2:B:103:PHE:HZ	2:B:113:LEU:HD13	1.65	0.61
2:B:327:PHE:CZ	2:B:497:VAL:HG13	2.36	0.61
1:A:282:LEU:HD23	1:A:521:VAL:HG21	1.82	0.60
1:C:506:PRO:O	1:C:555:ARG:NH1	2.33	0.60
2:D:103:PHE:HZ	2:D:113:LEU:HD13	1.66	0.60
2:D:600:TYR:OH	2:D:604:TYR:OH	2.12	0.60
2:D:327:PHE:CZ	2:D:497:VAL:HG13	2.37	0.60
2:B:600:TYR:OH	2:B:604:TYR:OH	2.12	0.60
1:A:19:GLU:OE1	1:A:610:HIS:ND1	2.35	0.59
1:A:591:ARG:NH2	2:B:641:SEP:O1P	2.32	0.59
2:B:420:LEU:HD23	2:B:428:MET:HE1	1.83	0.59
1:C:28:VAL:CG1	1:C:175:VAL:HG22	2.32	0.59
1:C:591:ARG:NH2	2:D:641:SEP:O2P	2.33	0.59
2:D:529:THR:HG22	2:D:553:LEU:HB3	1.85	0.59
2:B:19:GLU:OE1	2:B:610:HIS:ND1	2.35	0.59
1:A:28:VAL:CG1	1:A:175:VAL:HG22	2.33	0.59
2:B:529:THR:HG22	2:B:553:LEU:HB3	1.85	0.59
2:D:420:LEU:HD23	2:D:428:MET:HE1	1.84	0.59
2:D:249:ALA:O	2:D:272:ARG:NH1	2.34	0.58
1:C:103:PHE:HZ	1:C:113:LEU:HD13	1.68	0.58
1:A:103:PHE:HZ	1:A:113:LEU:HD13	1.68	0.58
2:B:249:ALA:O	2:B:272:ARG:NH1	2.34	0.58
2:D:332:TYR:OH	2:D:454:ASP:OD1	2.16	0.58
3:H:327:LYS:O	3:H:330:THR:HG22	2.04	0.58
2:D:379:THR:HG22	2:D:488:LEU:CD1	2.32	0.58
2:B:404:LEU:HD11	2:D:428:MET:SD	2.44	0.58
1:C:19:GLU:OE1	1:C:610:HIS:ND1	2.37	0.58
1:C:229:VAL:HG11	1:C:269:LEU:HA	1.86	0.58
3:F:327:LYS:O	3:F:330:THR:HG22	2.04	0.58
1:A:249:ALA:O	1:A:272:ARG:NH1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:THR:HG22	2:B:488:LEU:CD1	2.33	0.57
2:B:428:MET:SD	2:D:404:LEU:HD11	2.44	0.57
1:C:249:ALA:O	1:C:272:ARG:NH1	2.34	0.57
2:D:586:ARG:HA	2:D:589:THR:HG22	1.86	0.57
2:B:400:PHE:HE2	2:B:416:MET:HE1	1.69	0.57
1:C:232:GLU:O	1:C:236:ARG:NH1	2.37	0.57
1:A:232:GLU:O	1:A:236:ARG:NH1	2.37	0.57
1:A:63:PHE:CZ	1:A:87:LEU:HD11	2.40	0.57
1:C:63:PHE:CZ	1:C:87:LEU:HD11	2.40	0.57
2:D:19:GLU:OE1	2:D:610:HIS:ND1	2.37	0.57
2:D:400:PHE:HE2	2:D:416:MET:HE1	1.69	0.57
1:A:404:LEU:HD11	1:C:428:MET:SD	2.44	0.56
1:A:428:MET:SD	1:C:404:LEU:HD11	2.45	0.56
2:B:586:ARG:HA	2:B:589:THR:HG22	1.87	0.56
2:B:332:TYR:OH	2:B:454:ASP:OD1	2.18	0.56
1:C:529:THR:HG22	1:C:553:LEU:HB3	1.88	0.56
2:D:443:VAL:HG11	2:D:460:ILE:HG21	1.87	0.56
1:A:115:VAL:HG21	1:A:161:PHE:CZ	2.40	0.56
1:A:529:THR:HG22	1:A:553:LEU:HB3	1.88	0.56
1:C:400:PHE:HE2	1:C:416:MET:HE1	1.70	0.56
1:A:400:PHE:HE2	1:A:416:MET:HE1	1.70	0.56
1:C:115:VAL:HG21	1:C:161:PHE:CZ	2.40	0.56
1:C:204:THR:CG2	1:C:257:THR:HG22	2.36	0.56
1:A:148:ALA:HB1	1:A:244:MET:HE1	1.88	0.56
1:C:148:ALA:HB1	1:C:244:MET:HE1	1.88	0.55
2:D:204:THR:CG2	2:D:257:THR:HG22	2.36	0.55
2:D:231:LYS:O	2:D:235:GLU:OE1	2.23	0.55
2:B:63:PHE:CZ	2:B:87:LEU:HD11	2.41	0.55
2:B:231:LYS:O	2:B:235:GLU:OE1	2.23	0.55
1:A:55:GLY:O	1:A:59:GLY:N	2.39	0.55
1:A:204:THR:CG2	1:A:257:THR:HG22	2.36	0.55
2:B:204:THR:CG2	2:B:257:THR:HG22	2.37	0.55
2:D:63:PHE:CZ	2:D:87:LEU:HD11	2.41	0.55
1:A:443:VAL:CG1	1:A:460:ILE:HD13	2.37	0.55
2:B:55:GLY:O	2:B:59:GLY:N	2.40	0.55
2:B:443:VAL:HG11	2:B:460:ILE:HG21	1.89	0.55
1:C:204:THR:HG22	1:C:257:THR:HG22	1.89	0.54
1:C:443:VAL:CG1	1:C:460:ILE:HD13	2.37	0.54
2:D:443:VAL:CG1	2:D:460:ILE:HD13	2.38	0.54
1:C:55:GLY:O	1:C:59:GLY:N	2.39	0.54
1:C:188:LEU:HD21	1:C:252:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:HB2	1:A:91:LEU:HD12	1.89	0.54
2:B:443:VAL:CG1	2:B:460:ILE:HD13	2.38	0.54
1:C:443:VAL:HG11	1:C:460:ILE:HD13	1.90	0.54
2:D:497:VAL:HG12	2:D:524:ILE:CD1	2.37	0.54
2:B:400:PHE:CE2	2:B:416:MET:HE1	2.42	0.54
2:B:497:VAL:HG12	2:B:524:ILE:CD1	2.37	0.54
1:C:82:ALA:HB2	1:C:91:LEU:HD12	1.89	0.54
1:C:443:VAL:HG11	1:C:460:ILE:HG21	1.90	0.54
2:D:55:GLY:O	2:D:59:GLY:N	2.41	0.54
1:A:126:LEU:HD23	1:A:130:LYS:HD2	1.89	0.54
1:A:204:THR:HG22	1:A:257:THR:HG22	1.90	0.54
1:A:443:VAL:HG11	1:A:460:ILE:HG21	1.90	0.54
1:A:443:VAL:HG11	1:A:460:ILE:HD13	1.90	0.53
2:D:400:PHE:CE2	2:D:416:MET:HE1	2.42	0.53
3:G:308:TRP:NE1	3:G:319:ASP:OD1	2.40	0.53
1:A:188:LEU:HD21	1:A:252:ALA:HB2	1.89	0.53
1:C:209:LEU:HD13	1:C:242:TYR:CD1	2.43	0.53
1:C:586:ARG:HA	1:C:589:THR:HG22	1.89	0.53
1:A:63:PHE:HZ	1:A:87:LEU:HD11	1.74	0.53
1:A:638:ARG:HH11	1:A:638:ARG:C	2.16	0.53
2:D:374:ASN:O	2:D:447:ASN:N	2.41	0.53
1:A:586:ARG:HA	1:A:589:THR:HG22	1.89	0.53
1:C:63:PHE:HZ	1:C:87:LEU:HD11	1.74	0.53
2:D:188:LEU:HD21	2:D:252:ALA:HB2	1.91	0.53
3:H:308:TRP:NE1	3:H:319:ASP:OD1	2.40	0.53
1:C:70:GLU:N	1:C:70:GLU:OE1	2.40	0.53
2:B:188:LEU:HD21	2:B:252:ALA:HB2	1.91	0.53
3:F:308:TRP:NE1	3:F:319:ASP:OD1	2.40	0.53
1:C:400:PHE:CE2	1:C:416:MET:HE1	2.43	0.53
1:A:70:GLU:OE1	1:A:70:GLU:N	2.40	0.53
2:B:374:ASN:O	2:B:447:ASN:N	2.41	0.53
2:D:548:TYR:HB3	2:D:592:LEU:HD11	1.91	0.53
2:B:577:GLN:NE2	2:B:585:GLN:OE1	2.41	0.53
1:C:145:ASP:O	1:C:149:ASN:ND2	2.40	0.52
2:D:40:VAL:HG12	2:D:40:VAL:O	2.10	0.52
1:A:400:PHE:CE2	1:A:416:MET:HE1	2.44	0.52
2:B:204:THR:HG22	2:B:257:THR:HG22	1.91	0.52
2:B:40:VAL:HG12	2:B:40:VAL:O	2.10	0.52
2:B:548:TYR:HB3	2:B:592:LEU:HD11	1.92	0.52
3:E:308:TRP:NE1	3:E:319:ASP:OD1	2.41	0.52
2:B:443:VAL:HG11	2:B:460:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:O	1:A:149:ASN:ND2	2.41	0.52
1:C:312:PHE:HE1	1:C:476:ILE:HD11	1.75	0.52
1:C:638:ARG:HD3	1:C:638:ARG:C	2.35	0.52
2:D:209:LEU:HD11	2:D:233:ALA:HB2	1.92	0.52
2:D:577:GLN:NE2	2:D:585:GLN:OE1	2.38	0.52
1:C:141:VAL:HG22	1:C:244:MET:HE2	1.92	0.51
2:B:188:LEU:CD1	2:B:200:THR:HB	2.41	0.51
1:C:548:TYR:HB3	1:C:592:LEU:HD11	1.92	0.51
2:D:204:THR:HG22	2:D:257:THR:HG22	1.91	0.51
1:A:548:TYR:HB3	1:A:592:LEU:HD11	1.92	0.51
2:B:115:VAL:HG21	2:B:161:PHE:CZ	2.46	0.51
2:B:232:GLU:O	2:B:236:ARG:NH1	2.44	0.51
1:C:547:ALA:CB	1:C:638:ARG:HD2	2.40	0.51
1:A:141:VAL:HG22	1:A:244:MET:HE2	1.93	0.51
2:D:115:VAL:HG21	2:D:161:PHE:CZ	2.46	0.51
2:D:188:LEU:CD1	2:D:200:THR:HB	2.41	0.51
1:A:519:CYS:O	1:A:524:ILE:HG22	2.11	0.50
1:C:519:CYS:O	1:C:524:ILE:HG22	2.11	0.50
2:D:312:PHE:HE1	2:D:476:ILE:HD11	1.75	0.50
2:D:595:LEU:HD21	2:D:634:TYR:O	2.10	0.50
1:A:82:ALA:HB1	1:A:87:LEU:CB	2.41	0.50
2:B:312:PHE:HE1	2:B:476:ILE:HD11	1.75	0.50
1:A:351:TYR:CE1	1:A:355:VAL:HG11	2.47	0.50
2:B:209:LEU:HD11	2:B:233:ALA:HB2	1.93	0.50
1:C:82:ALA:HB1	1:C:87:LEU:CB	2.41	0.50
1:A:312:PHE:HE1	1:A:476:ILE:HD11	1.76	0.50
2:D:63:PHE:HZ	2:D:87:LEU:HD11	1.76	0.50
2:D:443:VAL:HG11	2:D:460:ILE:HD13	1.92	0.50
2:B:82:ALA:HB2	2:B:91:LEU:HD12	1.94	0.50
2:D:242:TYR:OH	2:D:246:ARG:NH1	2.38	0.50
1:A:638:ARG:HD2	2:B:640:ALA:O	2.11	0.50
2:D:232:GLU:O	2:D:236:ARG:NH1	2.45	0.50
2:D:307:PHE:CE2	2:D:476:ILE:HD13	2.44	0.50
2:D:348:ARG:HB3	2:D:568:THR:HG21	1.94	0.49
2:B:548:TYR:HA	2:B:588:ARG:HB3	1.94	0.49
2:D:306:GLU:OE2	2:D:309:ARG:NH1	2.41	0.49
2:B:63:PHE:HZ	2:B:87:LEU:HD11	1.77	0.49
2:B:307:PHE:CE2	2:B:476:ILE:HD13	2.44	0.49
2:B:306:GLU:OE2	2:B:309:ARG:NH1	2.41	0.49
1:C:351:TYR:CE1	1:C:355:VAL:HG11	2.48	0.49
2:D:82:ALA:HB2	2:D:91:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:MET:HE3	1:A:542:ILE:HD11	1.94	0.49
2:B:348:ARG:HB3	2:B:568:THR:HG21	1.94	0.49
2:D:351:TYR:CE1	2:D:355:VAL:HG11	2.47	0.49
1:C:40:VAL:HG12	1:C:40:VAL:O	2.13	0.48
2:D:191:CYS:HA	2:D:196:LEU:HD21	1.94	0.48
2:D:282:LEU:HD21	2:D:518:GLU:HG3	1.95	0.48
2:B:191:CYS:HA	2:B:196:LEU:HD21	1.94	0.48
2:B:282:LEU:HD21	2:B:518:GLU:HG3	1.95	0.48
2:D:188:LEU:HD11	2:D:200:THR:HB	1.96	0.48
1:A:348:ARG:HB3	1:A:568:THR:HG21	1.95	0.48
1:A:374:ASN:O	1:A:447:ASN:N	2.43	0.48
2:B:62:TYR:OH	2:B:64:LEU:HD21	2.13	0.48
1:C:538:MET:HE3	1:C:542:ILE:HD11	1.94	0.48
2:D:548:TYR:HA	2:D:588:ARG:HB3	1.96	0.48
2:B:549:GLY:HA2	2:B:585:GLN:HE21	1.79	0.48
2:D:62:TYR:OH	2:D:64:LEU:HD21	2.13	0.48
1:C:348:ARG:HB3	1:C:568:THR:HG21	1.95	0.48
2:B:188:LEU:HD11	2:B:200:THR:HB	1.96	0.47
1:C:281:GLY:HA2	1:C:601:LEU:HD12	1.95	0.47
1:C:374:ASN:O	1:C:447:ASN:N	2.43	0.47
2:B:279:PRO:HB2	2:B:601:LEU:HD22	1.96	0.47
2:B:351:TYR:CE1	2:B:355:VAL:HG11	2.49	0.47
2:B:416:MET:HE3	2:D:416:MET:HE3	1.97	0.47
1:C:191:CYS:HA	1:C:196:LEU:HD21	1.96	0.47
1:A:281:GLY:HA2	1:A:601:LEU:HD12	1.95	0.47
2:D:64:LEU:HB2	2:D:114:VAL:HG12	1.96	0.47
1:A:40:VAL:O	1:A:40:VAL:HG12	2.14	0.47
1:A:191:CYS:HA	1:A:196:LEU:HD21	1.96	0.47
2:B:64:LEU:HB2	2:B:114:VAL:HG12	1.97	0.47
2:B:281:GLY:HA2	2:B:601:LEU:HD12	1.97	0.47
2:D:279:PRO:HB2	2:D:601:LEU:HD22	1.97	0.47
2:D:383:GLN:CG	2:D:488:LEU:HD12	2.45	0.47
1:A:383:GLN:CG	1:A:488:LEU:HD12	2.45	0.47
1:C:638:ARG:HD3	1:C:638:ARG:O	2.15	0.47
2:D:281:GLY:HA2	2:D:601:LEU:HD12	1.97	0.47
2:B:214:CYS:SG	2:B:215:ALA:N	2.87	0.46
2:D:214:CYS:SG	2:D:215:ALA:N	2.88	0.46
2:D:310:GLY:HA2	2:D:386:ARG:HB2	1.96	0.46
1:A:310:GLY:HA2	1:A:386:ARG:HB2	1.98	0.46
1:C:94:MET:HG3	1:C:101:VAL:HG21	1.97	0.46
2:D:506:PRO:HA	2:D:529:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG13	1:A:175:VAL:HG22	1.96	0.46
1:A:94:MET:HG3	1:A:101:VAL:HG21	1.97	0.46
1:A:78:GLU:O	1:A:78:GLU:HG3	2.15	0.46
1:A:416:MET:SD	1:C:420:LEU:HD22	2.55	0.46
1:A:420:LEU:HD22	1:C:416:MET:SD	2.55	0.46
1:C:78:GLU:O	1:C:78:GLU:HG3	2.15	0.46
2:D:497:VAL:CG1	2:D:524:ILE:HD13	2.40	0.46
2:B:310:GLY:HA2	2:B:386:ARG:HB2	1.96	0.46
2:B:506:PRO:HA	2:B:529:THR:HG23	1.98	0.46
1:C:310:GLY:HA2	1:C:386:ARG:HB2	1.98	0.46
1:A:594:ASP:OD2	2:B:580:ARG:NH1	2.49	0.46
2:B:383:GLN:HG2	2:B:488:LEU:HD12	1.98	0.46
1:C:209:LEU:HD11	1:C:233:ALA:HB2	1.97	0.46
2:D:383:GLN:HG2	2:D:488:LEU:HD12	1.98	0.46
2:B:497:VAL:CG1	2:B:524:ILE:HD13	2.40	0.46
1:A:279:PRO:HB2	1:A:601:LEU:HD22	1.98	0.46
1:A:420:LEU:HD23	1:A:428:MET:CE	2.46	0.46
1:C:28:VAL:HG13	1:C:175:VAL:HG22	1.97	0.46
2:B:420:LEU:HD22	2:D:416:MET:SD	2.56	0.45
1:C:279:PRO:HB2	1:C:601:LEU:HD22	1.98	0.45
1:C:420:LEU:HD23	1:C:428:MET:CE	2.46	0.45
1:A:348:ARG:O	1:A:352:LEU:HD23	2.17	0.45
2:B:312:PHE:CD2	2:B:441:PRO:HG2	2.51	0.45
2:B:600:TYR:HB2	2:B:634:TYR:CZ	2.51	0.45
1:C:595:LEU:HD21	1:C:634:TYR:O	2.17	0.45
2:B:383:GLN:CG	2:B:488:LEU:HD12	2.46	0.45
1:C:188:LEU:CD1	1:C:200:THR:HB	2.46	0.45
1:A:188:LEU:CD1	1:A:200:THR:HB	2.46	0.45
2:B:348:ARG:O	2:B:352:LEU:HD23	2.16	0.45
1:C:383:GLN:CG	1:C:488:LEU:HD12	2.47	0.45
1:A:323:THR:HA	1:A:361:THR:O	2.17	0.45
2:B:525:PRO:HD3	2:B:586:ARG:HG2	1.98	0.45
1:C:594:ASP:OD2	2:D:580:ARG:NH1	2.50	0.45
2:D:525:PRO:HD3	2:D:586:ARG:HG2	1.99	0.45
2:B:94:MET:HG3	2:B:101:VAL:HG21	1.99	0.45
2:D:78:GLU:HG3	2:D:78:GLU:O	2.15	0.45
2:D:282:LEU:HD23	2:D:521:VAL:HG21	1.98	0.45
2:D:312:PHE:CD2	2:D:441:PRO:HG2	2.51	0.45
1:A:312:PHE:CD2	1:A:441:PRO:HG2	2.51	0.45
1:C:600:TYR:HB2	1:C:634:TYR:CZ	2.52	0.45
1:A:82:ALA:HB1	1:A:87:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PRO:HA	1:A:529:THR:HG23	1.99	0.45
2:B:351:TYR:CZ	2:B:355:VAL:HG11	2.52	0.45
1:A:600:TYR:HB2	1:A:634:TYR:CZ	2.52	0.44
2:B:282:LEU:HD23	2:B:521:VAL:HG21	1.98	0.44
1:C:312:PHE:CD2	1:C:441:PRO:HG2	2.51	0.44
1:A:306:GLU:OE2	1:A:309:ARG:NH1	2.41	0.44
1:A:307:PHE:CE2	1:A:476:ILE:HD13	2.44	0.44
1:A:595:LEU:HD21	1:A:634:TYR:O	2.17	0.44
2:B:78:GLU:O	2:B:78:GLU:HG3	2.15	0.44
2:B:416:MET:SD	2:D:420:LEU:HD22	2.57	0.44
1:C:503:GLY:O	1:C:526:SER:HA	2.18	0.44
1:C:537:PHE:CE1	1:C:601:LEU:HD21	2.52	0.44
1:A:503:GLY:O	1:A:526:SER:HA	2.18	0.44
1:C:82:ALA:HB1	1:C:87:LEU:HB2	1.99	0.44
1:C:307:PHE:CE2	1:C:476:ILE:HD13	2.45	0.44
1:A:351:TYR:CZ	1:A:355:VAL:HG11	2.53	0.44
1:A:537:PHE:CE1	1:A:601:LEU:HD21	2.53	0.44
2:B:82:ALA:HB1	2:B:87:LEU:CB	2.47	0.44
1:C:351:TYR:CZ	1:C:355:VAL:HG11	2.53	0.44
1:C:525:PRO:HD3	1:C:586:ARG:HG2	2.00	0.44
2:D:94:MET:HG3	2:D:101:VAL:HG21	1.99	0.44
1:A:433:PHE:HA	1:A:436:GLN:OE1	2.18	0.44
2:D:68:TYR:CE1	2:D:73:VAL:HG21	2.53	0.44
1:C:323:THR:HA	1:C:361:THR:O	2.17	0.44
1:C:348:ARG:O	1:C:352:LEU:HD23	2.18	0.44
1:C:433:PHE:HA	1:C:436:GLN:OE1	2.18	0.44
1:C:506:PRO:HA	1:C:529:THR:HG23	1.99	0.44
1:A:548:TYR:HA	1:A:588:ARG:HB3	1.98	0.44
2:D:145:ASP:OD2	2:D:240:HIS:NE2	2.40	0.44
2:D:351:TYR:CZ	2:D:355:VAL:HG11	2.53	0.44
2:D:600:TYR:HB2	2:D:634:TYR:CZ	2.53	0.44
1:A:334:PHE:CE2	1:A:340:ASP:HB3	2.53	0.44
2:B:639:PRO:O	2:B:642:VAL:HG12	2.18	0.44
1:C:334:PHE:CE2	1:C:340:ASP:HB3	2.53	0.44
1:C:548:TYR:HA	1:C:588:ARG:HB3	1.98	0.44
1:A:43:ILE:HG12	1:A:181:GLU:OE2	2.18	0.44
1:C:68:TYR:CE1	1:C:73:VAL:HG21	2.53	0.44
1:C:152:VAL:HA	1:C:186:VAL:HG11	2.00	0.44
2:D:148:ALA:HB1	2:D:244:MET:HE1	2.00	0.44
1:C:541:HIS:NE2	1:C:600:TYR:OH	2.44	0.43
1:A:525:PRO:HD3	1:A:586:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:444:CYS:HB2	2:B:457:LEU:HD21	2.00	0.43
2:B:145:ASP:OD2	2:B:240:HIS:NE2	2.40	0.43
1:C:43:ILE:HG12	1:C:181:GLU:OE2	2.18	0.43
2:D:348:ARG:O	2:D:352:LEU:HD23	2.18	0.43
2:D:537:PHE:CE1	2:D:601:LEU:HD21	2.53	0.43
1:A:541:HIS:NE2	1:A:600:TYR:OH	2.44	0.43
2:B:30:PHE:CD1	2:B:63:PHE:HB2	2.54	0.43
2:B:99:CYS:SG	2:B:160:TRP:CZ3	3.12	0.43
2:B:323:THR:HA	2:B:361:THR:O	2.18	0.43
1:C:584:ILE:HG12	2:D:591:ARG:HD3	1.99	0.43
2:D:420:LEU:HD23	2:D:428:MET:CE	2.47	0.43
2:D:444:CYS:HB2	2:D:457:LEU:HD21	2.00	0.43
1:A:152:VAL:HA	1:A:186:VAL:HG11	2.01	0.43
2:B:148:ALA:HB1	2:B:244:MET:HE1	2.00	0.43
2:B:185:GLY:HA3	2:B:248:ALA:HB2	2.01	0.43
2:B:257:THR:HG23	2:B:274:PRO:HG3	2.01	0.43
2:B:537:PHE:CE1	2:B:601:LEU:HD21	2.53	0.43
2:B:541:HIS:NE2	2:B:600:TYR:OH	2.43	0.43
2:D:334:PHE:CE2	2:D:340:ASP:HB3	2.53	0.43
1:C:258:VAL:O	1:C:279:PRO:HA	2.19	0.43
1:C:306:GLU:OE2	1:C:309:ARG:NH1	2.42	0.43
2:D:30:PHE:CD1	2:D:63:PHE:HB2	2.54	0.43
2:D:257:THR:HG23	2:D:274:PRO:HG3	2.01	0.43
2:D:323:THR:HA	2:D:361:THR:O	2.18	0.43
2:B:68:TYR:CE1	2:B:73:VAL:HG21	2.54	0.43
2:D:99:CYS:SG	2:D:160:TRP:CZ3	3.12	0.43
2:D:541:HIS:NE2	2:D:600:TYR:OH	2.43	0.43
1:A:520:THR:HG1	1:A:534:PHE:HZ	1.61	0.43
2:B:350:ASN:OD1	2:B:472:ARG:N	2.51	0.43
2:B:503:GLY:O	2:B:526:SER:HA	2.18	0.43
1:A:258:VAL:O	1:A:279:PRO:HA	2.19	0.43
1:A:584:ILE:HG12	2:B:591:ARG:HD3	2.00	0.43
2:B:13:PRO:O	2:B:599:LYS:NZ	2.51	0.43
2:B:420:LEU:HD23	2:B:428:MET:CE	2.47	0.43
1:A:309:ARG:HA	1:A:316:LEU:HD21	2.01	0.42
2:B:334:PHE:CE2	2:B:340:ASP:HB3	2.53	0.42
2:B:433:PHE:HA	2:B:436:GLN:OE1	2.19	0.42
2:B:20:ASP:OD1	2:B:20:ASP:N	2.51	0.42
2:D:82:ALA:HB1	2:D:87:LEU:CB	2.49	0.42
2:D:185:GLY:HA3	2:D:248:ALA:HB2	2.01	0.42
2:D:503:GLY:O	2:D:526:SER:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:HA	1:C:316:LEU:HD21	2.02	0.42
1:C:638:ARG:NE	2:D:640:ALA:HB1	2.34	0.42
2:D:305:GLN:CG	2:D:320:LEU:HD13	2.49	0.42
2:D:549:GLY:HA2	2:D:585:GLN:HE21	1.82	0.42
1:A:68:TYR:CE1	1:A:73:VAL:HG21	2.54	0.42
1:A:505:PHE:CE1	1:A:515:THR:HG22	2.55	0.42
2:D:20:ASP:OD1	2:D:20:ASP:N	2.52	0.42
2:D:33:ALA:HB3	2:D:36:VAL:HG23	2.01	0.42
2:D:433:PHE:HA	2:D:436:GLN:OE1	2.20	0.42
1:A:416:MET:HE3	1:C:416:MET:HE3	2.00	0.42
2:B:82:ALA:HB1	2:B:87:LEU:HB2	2.01	0.42
2:B:531:LEU:HD12	2:B:555:ARG:HB3	2.02	0.42
1:C:505:PHE:CE1	1:C:515:THR:HG22	2.55	0.42
1:A:381:LYS:O	1:A:385:VAL:HG23	2.19	0.42
1:C:31:GLU:CD	1:C:50:LYS:HZ1	2.28	0.42
1:A:548:TYR:HE1	1:A:638:ARG:HB3	1.85	0.42
2:B:309:ARG:HA	2:B:316:LEU:HD21	2.02	0.42
1:C:553:LEU:HD11	1:C:567:LEU:N	2.35	0.42
2:B:256:THR:HG21	2:B:278:THR:CG2	2.50	0.42
1:C:520:THR:HG1	1:C:534:PHE:HZ	1.62	0.42
2:D:309:ARG:HA	2:D:316:LEU:HD21	2.02	0.42
2:D:505:PHE:CE1	2:D:515:THR:HG22	2.55	0.42
1:A:30:PHE:CD1	1:A:63:PHE:HB2	2.55	0.42
2:B:305:GLN:CG	2:B:320:LEU:HD13	2.50	0.42
2:B:505:PHE:CE1	2:B:515:THR:HG22	2.55	0.42
2:B:553:LEU:HD11	2:B:567:LEU:N	2.35	0.42
3:E:327:LYS:O	3:E:330:THR:HG22	2.20	0.42
1:C:313:TYR:O	1:C:437:ARG:NH2	2.46	0.42
1:A:553:LEU:HD11	1:A:567:LEU:N	2.35	0.41
2:B:28:VAL:HG13	2:B:175:VAL:HG22	2.01	0.41
2:D:256:THR:HG21	2:D:278:THR:CG2	2.50	0.41
1:C:30:PHE:CD1	1:C:63:PHE:HB2	2.55	0.41
1:C:126:LEU:HD11	1:C:149:ASN:HB3	2.01	0.41
1:C:381:LYS:O	1:C:385:VAL:HG23	2.20	0.41
2:D:531:LEU:HD12	2:D:555:ARG:HB3	2.02	0.41
1:A:257:THR:HG23	1:A:274:PRO:HG3	2.01	0.41
1:A:376:ASN:OD1	1:A:377:VAL:N	2.53	0.41
1:C:638:ARG:HE	2:D:640:ALA:HB1	1.85	0.41
2:D:33:ALA:CB	2:D:47:LEU:HD11	2.50	0.41
2:D:159:THR:HG22	2:D:194:ARG:NH1	2.36	0.41
1:A:637:PRO:O	1:A:638:ARG:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASN:OD1	1:C:472:ARG:N	2.53	0.41
2:D:28:VAL:HG13	2:D:175:VAL:HG22	2.01	0.41
2:D:553:LEU:HD11	2:D:567:LEU:N	2.35	0.41
1:A:383:GLN:HG3	1:A:488:LEU:HD12	2.02	0.41
2:B:159:THR:HG22	2:B:194:ARG:NH1	2.36	0.41
1:C:257:THR:HG23	1:C:274:PRO:HG3	2.01	0.41
2:D:258:VAL:O	2:D:279:PRO:HA	2.19	0.41
1:A:444:CYS:HB2	1:A:457:LEU:HD21	2.03	0.41
1:C:185:GLY:HA3	1:C:248:ALA:HB2	2.02	0.41
2:D:36:VAL:HB	2:D:66:GLY:HA3	2.01	0.41
2:B:152:VAL:HA	2:B:186:VAL:HG11	2.02	0.41
2:B:258:VAL:O	2:B:279:PRO:HA	2.20	0.41
1:A:313:TYR:O	1:A:437:ARG:NH2	2.47	0.41
2:D:350:ASN:OD1	2:D:472:ARG:N	2.53	0.41
1:A:103:PHE:CZ	1:A:113:LEU:HD22	2.56	0.41
1:A:185:GLY:HA3	1:A:248:ALA:HB2	2.02	0.41
2:B:33:ALA:CB	2:B:47:LEU:HD11	2.51	0.41
2:B:43:ILE:HG12	2:B:181:GLU:OE2	2.21	0.41
2:B:637:PRO:O	2:B:638:ARG:C	2.63	0.41
1:C:43:ILE:H	1:C:43:ILE:HD12	1.85	0.41
1:C:313:TYR:CD1	1:C:382:GLY:HA2	2.55	0.41
1:C:376:ASN:OD1	1:C:377:VAL:N	2.54	0.41
1:C:444:CYS:HB2	1:C:457:LEU:HD21	2.03	0.41
2:D:82:ALA:HB1	2:D:87:LEU:HB2	2.03	0.41
2:D:152:VAL:HA	2:D:186:VAL:HG11	2.03	0.41
2:D:534:PHE:HE1	2:D:596:LEU:HD11	1.85	0.41
1:A:43:ILE:H	1:A:43:ILE:HD12	1.85	0.41
2:D:43:ILE:HG12	2:D:181:GLU:OE2	2.21	0.41
1:C:125:ALA:O	1:C:126:LEU:C	2.64	0.40
2:B:33:ALA:HB3	2:B:36:VAL:HG23	2.02	0.40
1:C:103:PHE:CZ	1:C:113:LEU:HD22	2.57	0.40
1:A:313:TYR:CD1	1:A:382:GLY:HA2	2.56	0.40
2:B:432:ILE:O	2:B:436:GLN:OE1	2.40	0.40
1:C:175:VAL:HG12	1:C:198:VAL:HG13	2.03	0.40
1:C:305:GLN:CG	1:C:320:LEU:HD13	2.52	0.40
1:A:548:TYR:CD2	1:A:588:ARG:HB3	2.57	0.40
1:C:534:PHE:HE1	1:C:596:LEU:HD11	1.86	0.40
2:D:432:ILE:O	2:D:436:GLN:OE1	2.40	0.40
2:B:332:TYR:HH	2:B:454:ASP:CG	2.23	0.40
2:D:326:PHE:N	2:D:326:PHE:CD1	2.89	0.40
3:G:327:LYS:O	3:G:330:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/737 (83%)	592 (97%)	19 (3%)	0	100	100
1	C	611/737 (83%)	592 (97%)	19 (3%)	0	100	100
2	B	614/737 (83%)	598 (97%)	16 (3%)	0	100	100
2	D	614/737 (83%)	599 (98%)	15 (2%)	0	100	100
3	E	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
3	F	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
3	G	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
3	H	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
All	All	2574/4280 (60%)	2497 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/638 (83%)	529 (100%)	0	100	100
1	C	529/638 (83%)	529 (100%)	0	100	100
2	B	531/637 (83%)	531 (100%)	0	100	100
2	D	531/637 (83%)	531 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	29/294 (10%)	29 (100%)	0	100	100
3	F	29/294 (10%)	29 (100%)	0	100	100
3	G	29/294 (10%)	29 (100%)	0	100	100
3	H	29/294 (10%)	29 (100%)	0	100	100
All	All	2236/3726 (60%)	2236 (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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
2	B	268	HIS
2	B	447	ASN
1	C	268	HIS
2	D	268	HIS
2	D	447	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SEP	D	641	2	8,9,10	1.42	1 (12%)	7,12,14	1.48	1 (14%)
2	SEP	B	641	2	8,9,10	1.42	1 (12%)	7,12,14	1.47	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	D	641	2	-	0/6/8/10	-
2	SEP	B	641	2	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	641	SEP	P-O1P	3.16	1.60	1.50
2	D	641	SEP	P-O1P	3.14	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	641	SEP	OG-CB-CA	3.07	111.14	108.14
2	D	641	SEP	OG-CB-CA	3.03	111.09	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	641	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	641	SEP	1	0
2	B	641	SEP	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

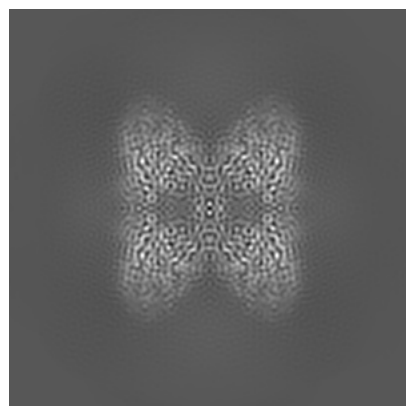
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14587. These allow visual inspection of the internal detail of the map and identification of artifacts.

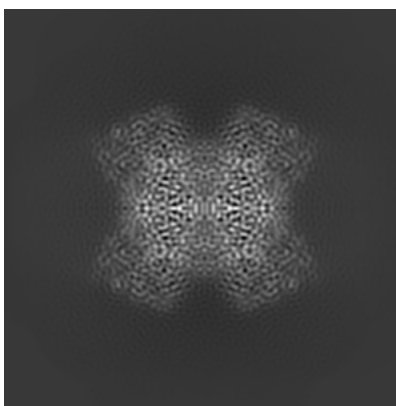
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

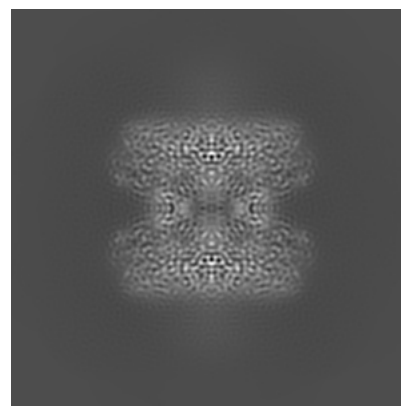
6.1.1 Primary map



X

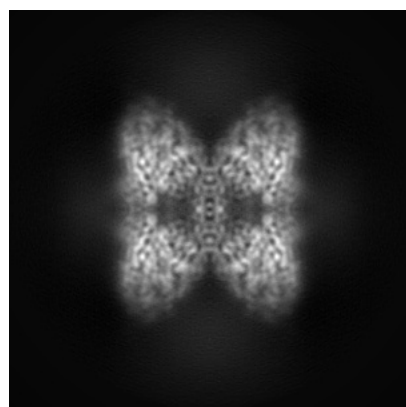


Y

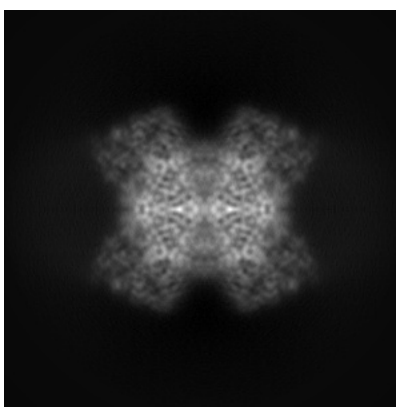


Z

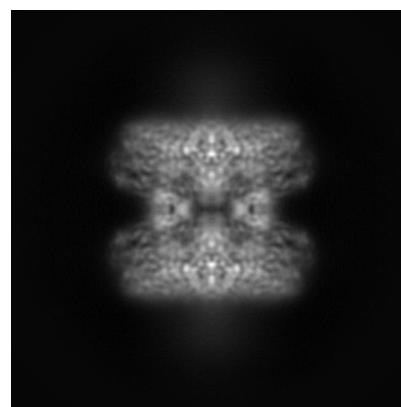
6.1.2 Raw map



X



Y

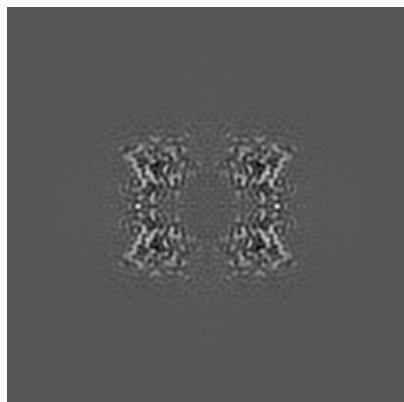


Z

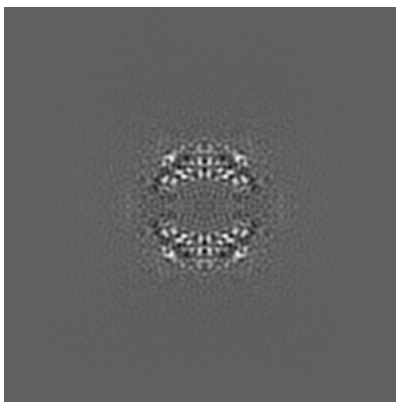
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

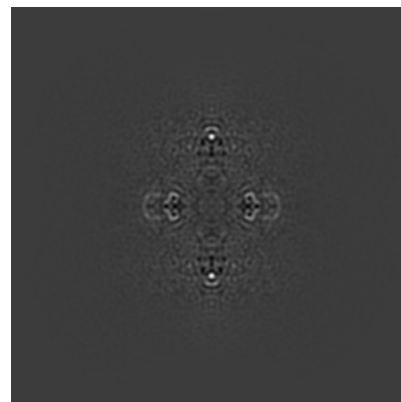
6.2.1 Primary map



X Index: 144

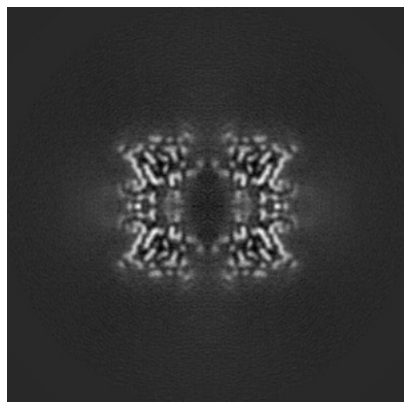


Y Index: 144

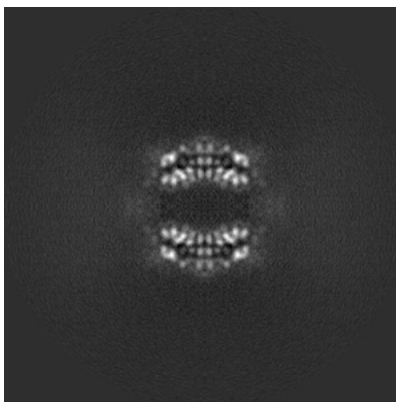


Z Index: 144

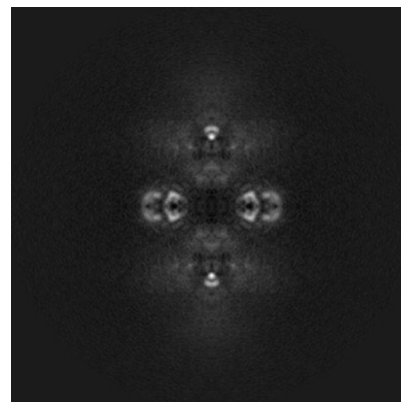
6.2.2 Raw map



X Index: 144



Y Index: 144

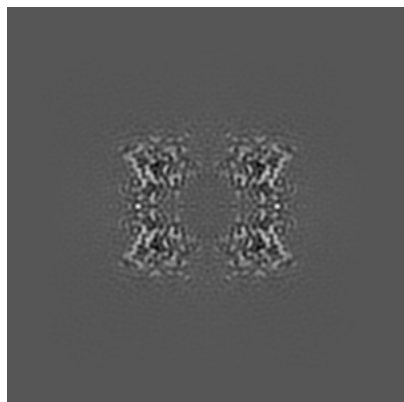


Z Index: 144

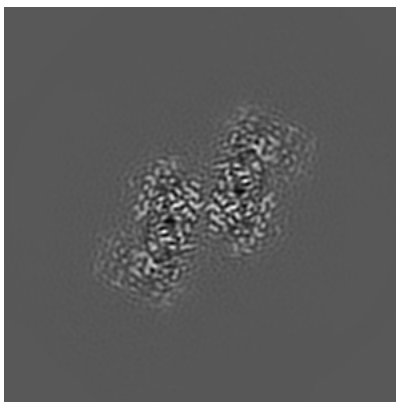
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

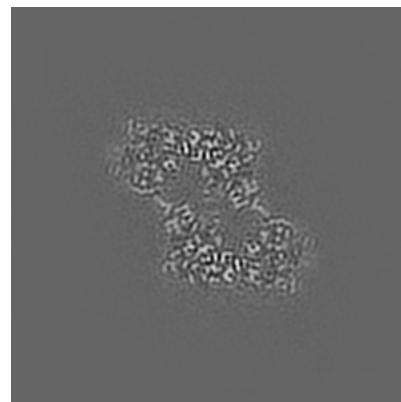
6.3.1 Primary map



X Index: 144

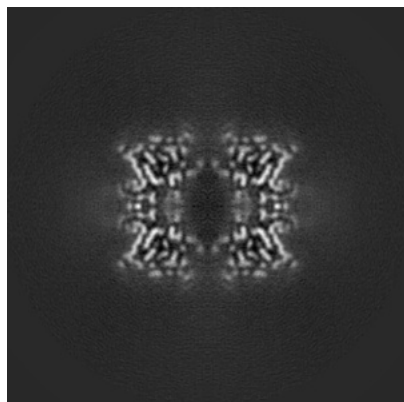


Y Index: 184

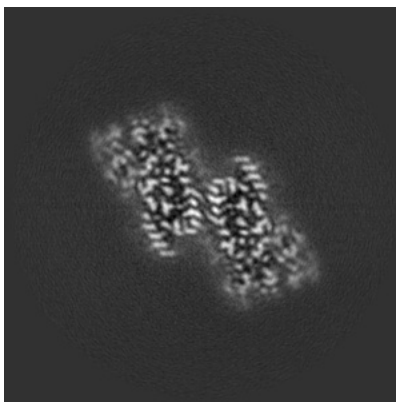


Z Index: 115

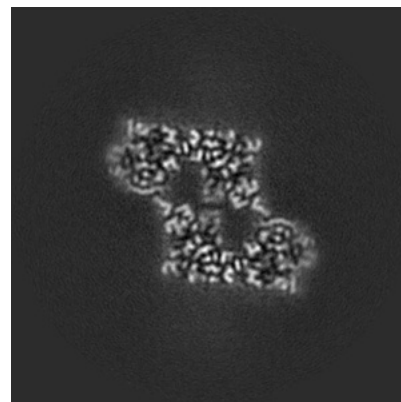
6.3.2 Raw map



X Index: 144



Y Index: 100

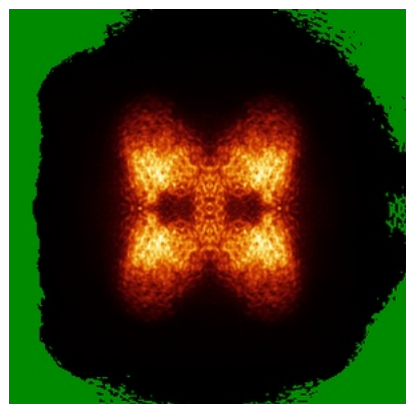


Z Index: 115

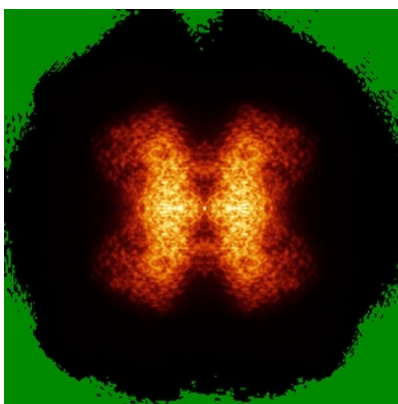
The images above show the largest variance slices of the map in three orthogonal directions.

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

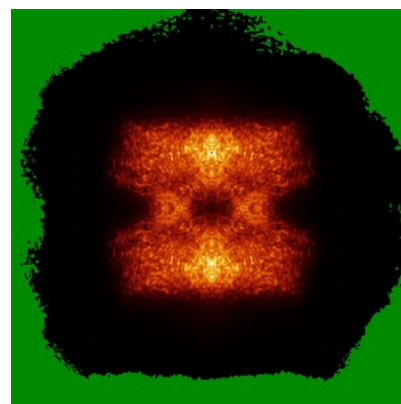
6.4.1 Primary map



X

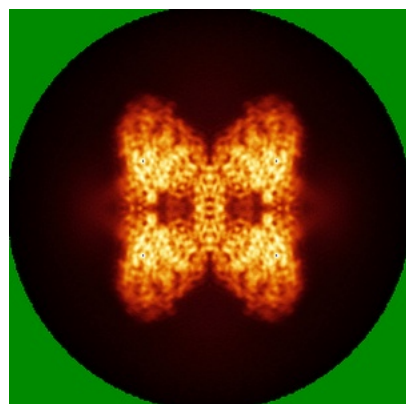


Y

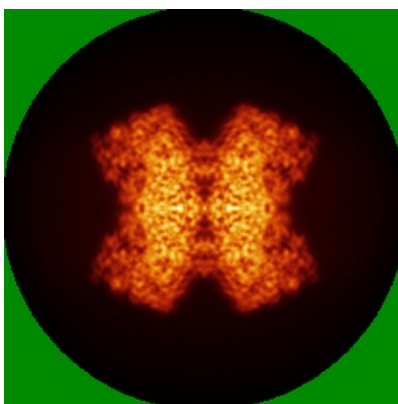


Z

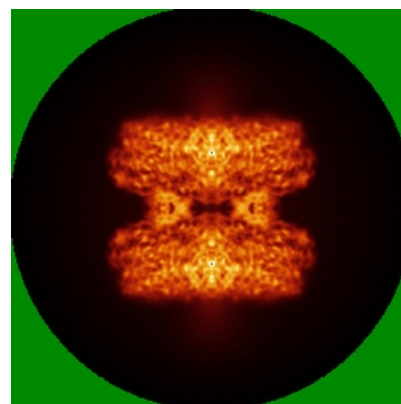
6.4.2 Raw map



X



Y

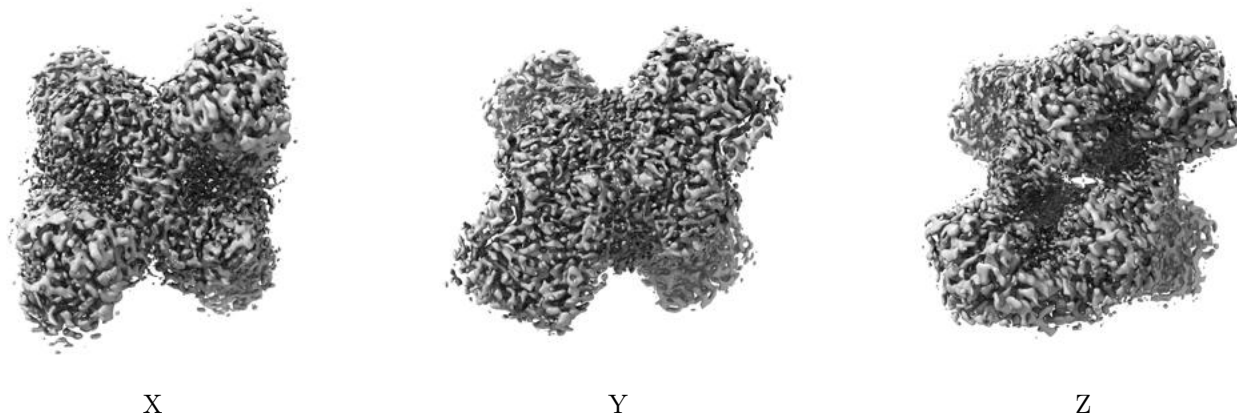


Z

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.

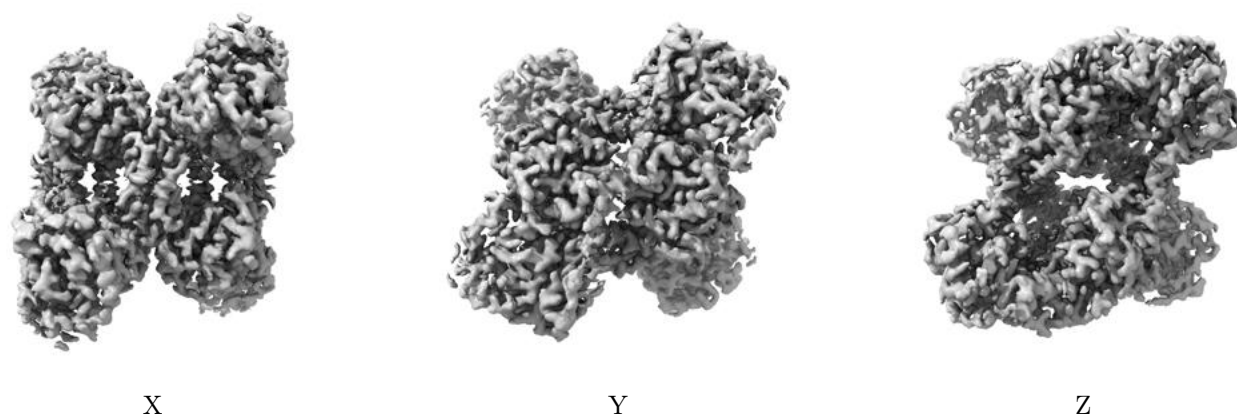
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

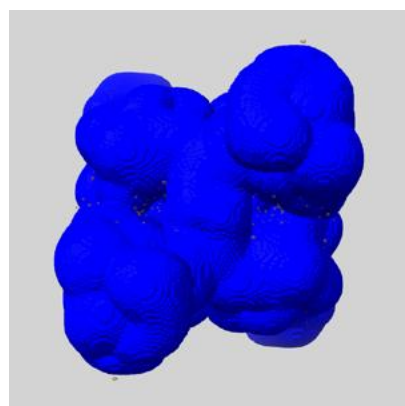
6.6 Mask visualisation [i](#)

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

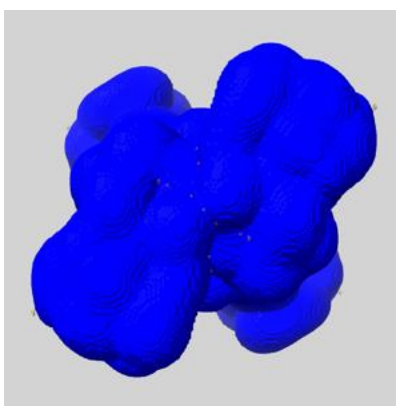
A mask typically either:

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

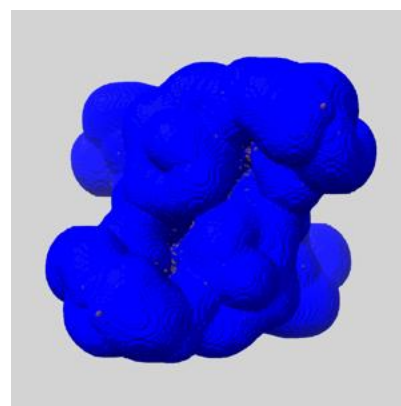
6.6.1 emd_14587_msk_1.map [i](#)



X



Y

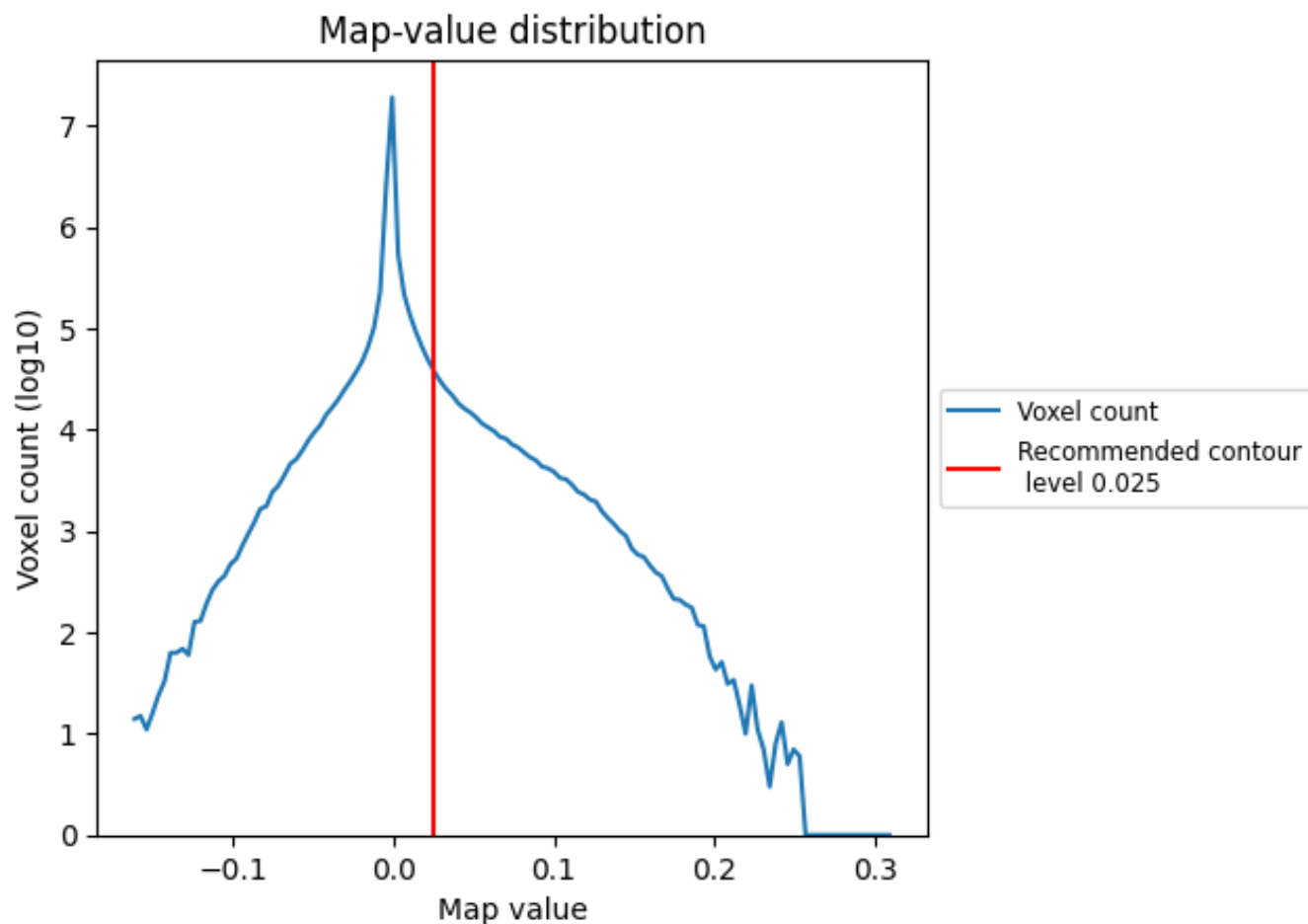


Z

7 Map analysis [i](#)

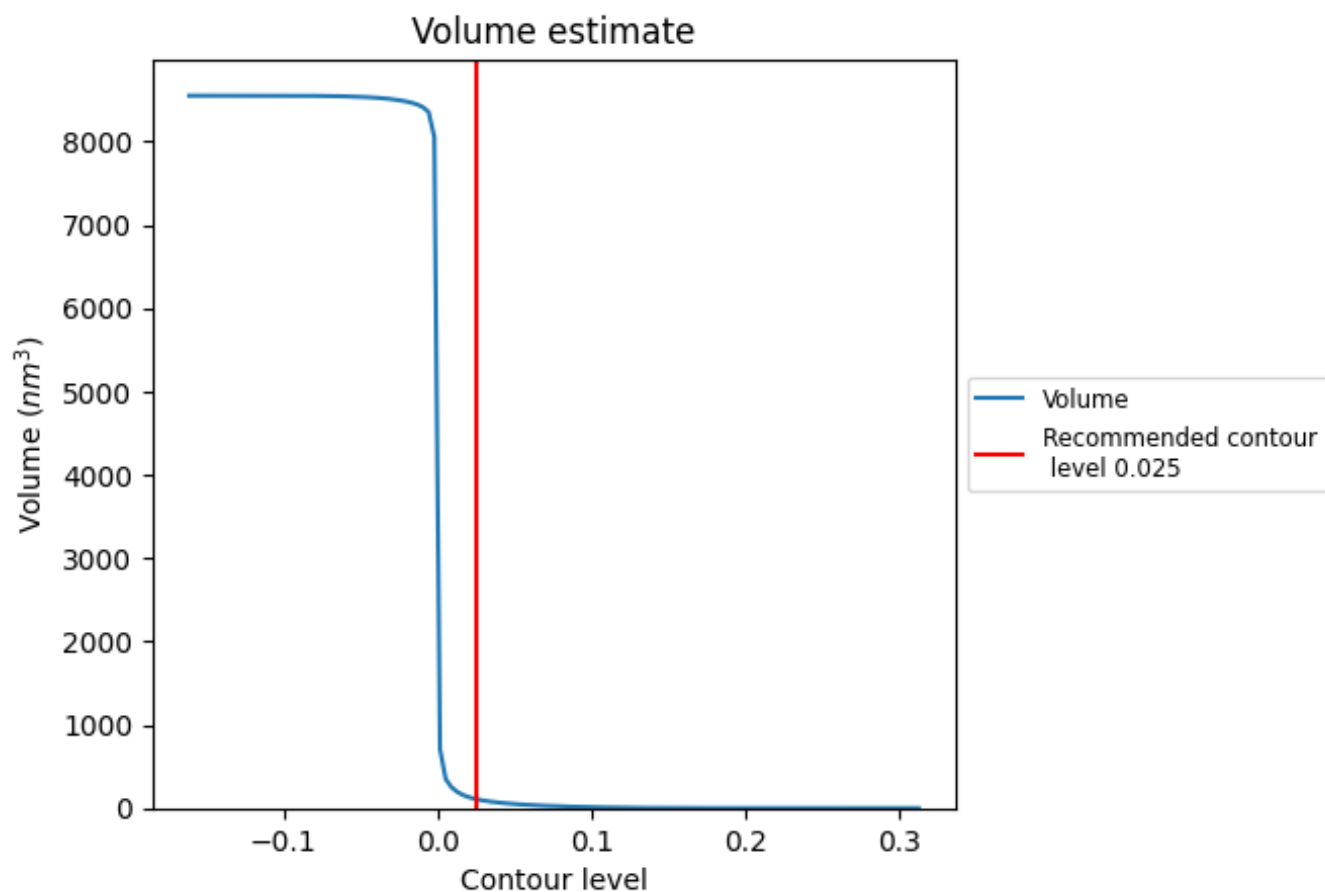
This section contains the results of statistical analysis of the map.

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.

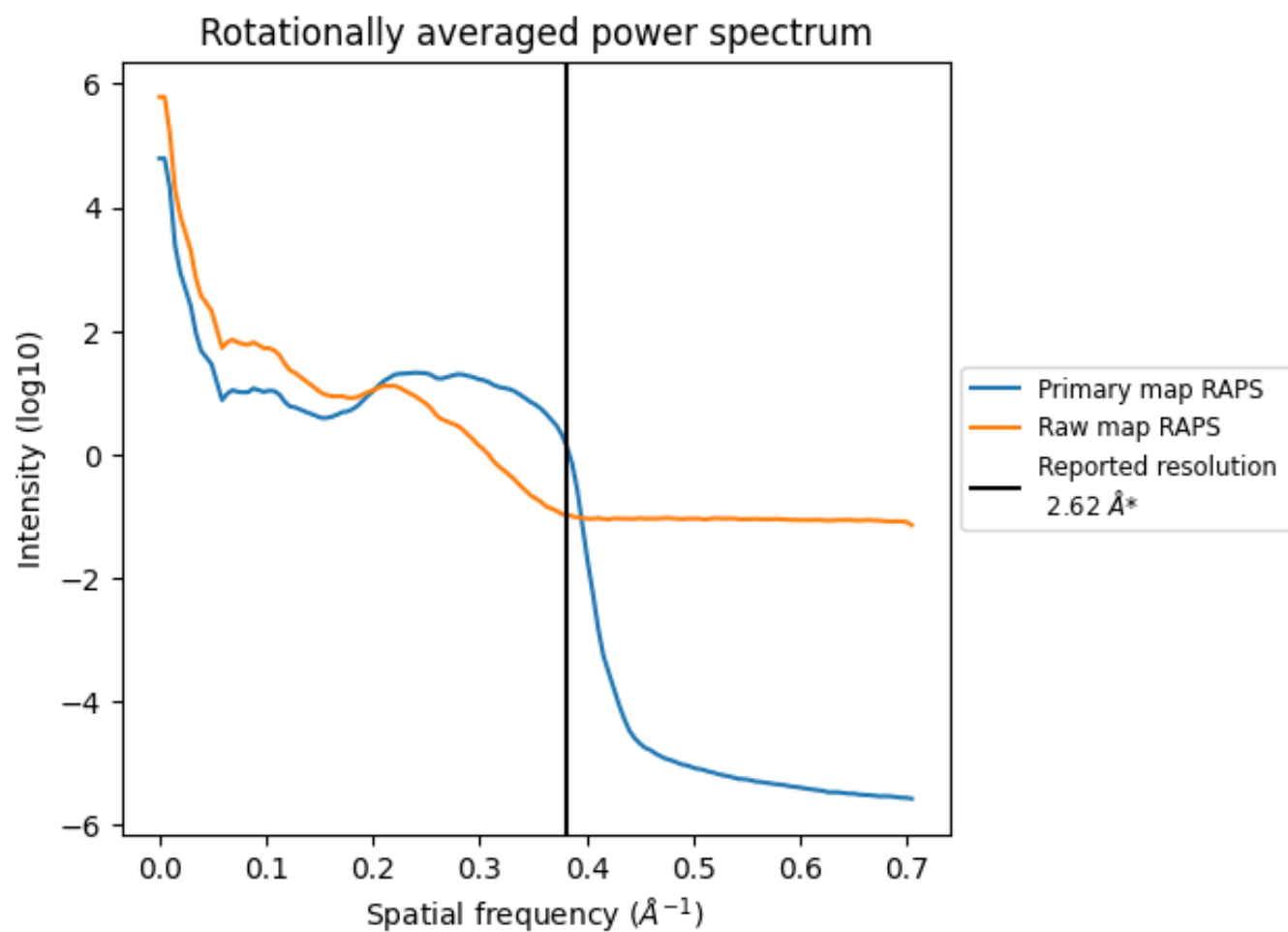
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 99 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 ⓘ

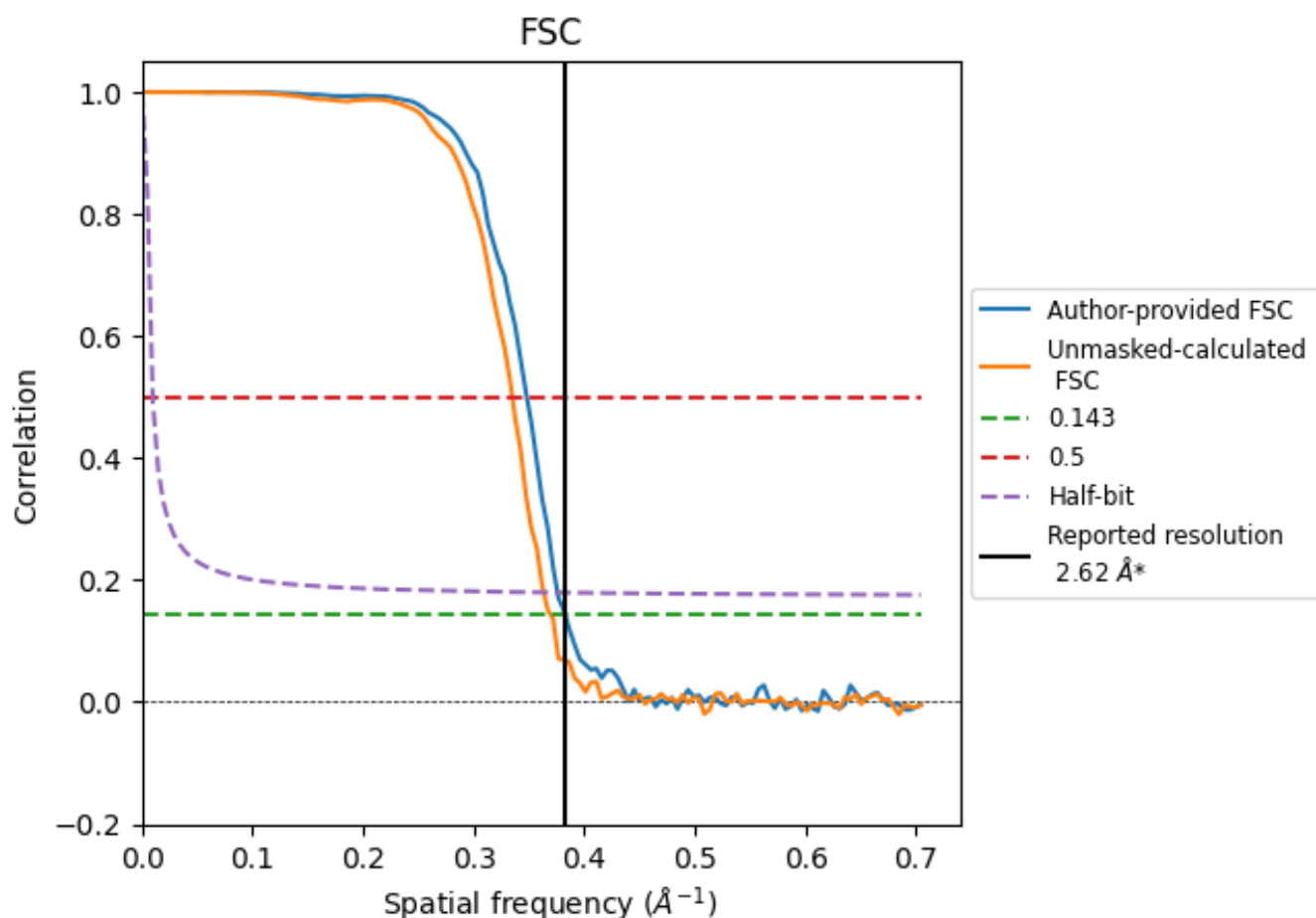


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

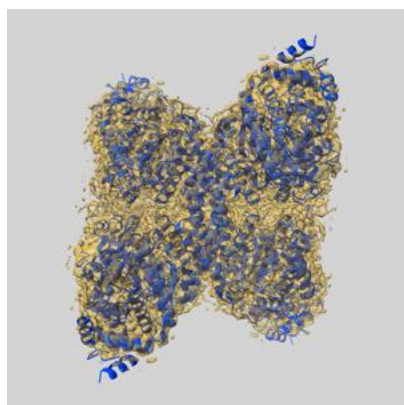
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.61	2.87	2.66
Unmasked-calculated*	2.71	2.99	2.75

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

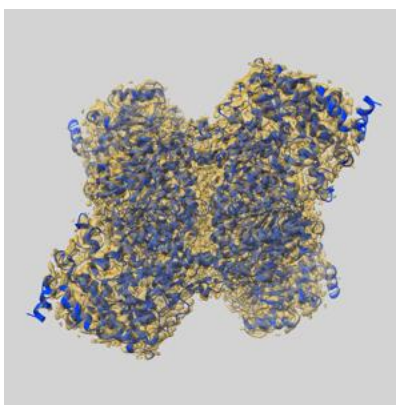
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14587 and PDB model 7ZBN. Per-residue inclusion information can be found in section 3 on page 6.

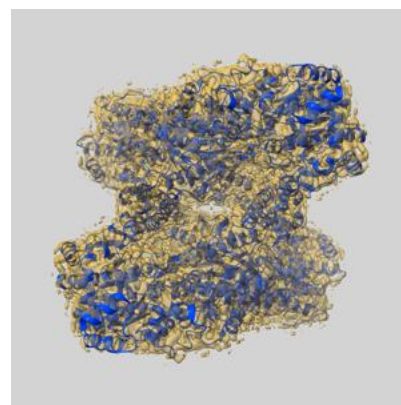
9.1 Map-model overlay [i](#)



X



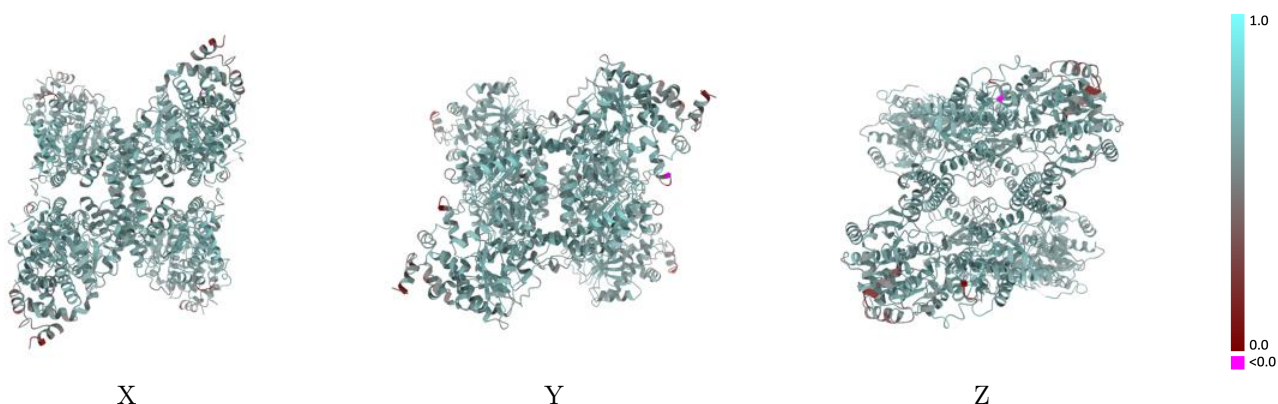
Y



Z

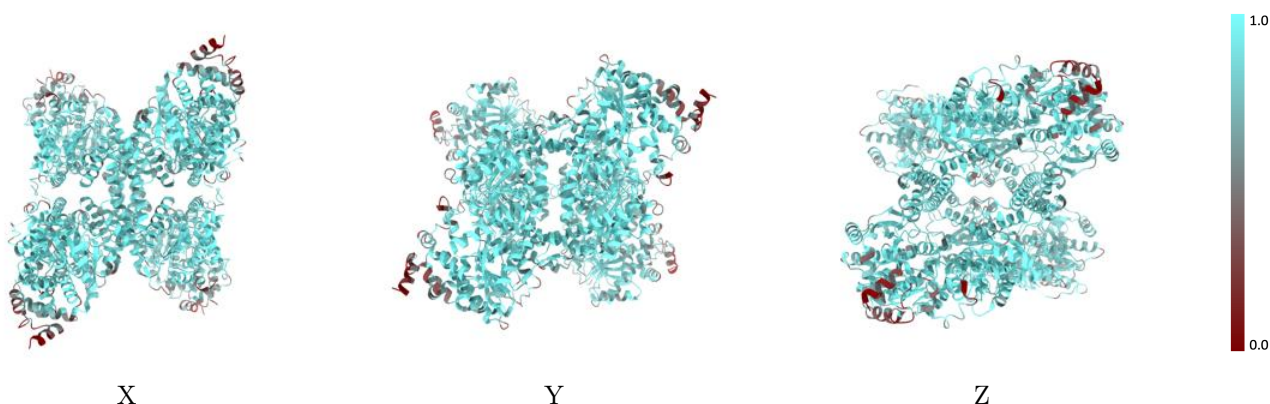
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



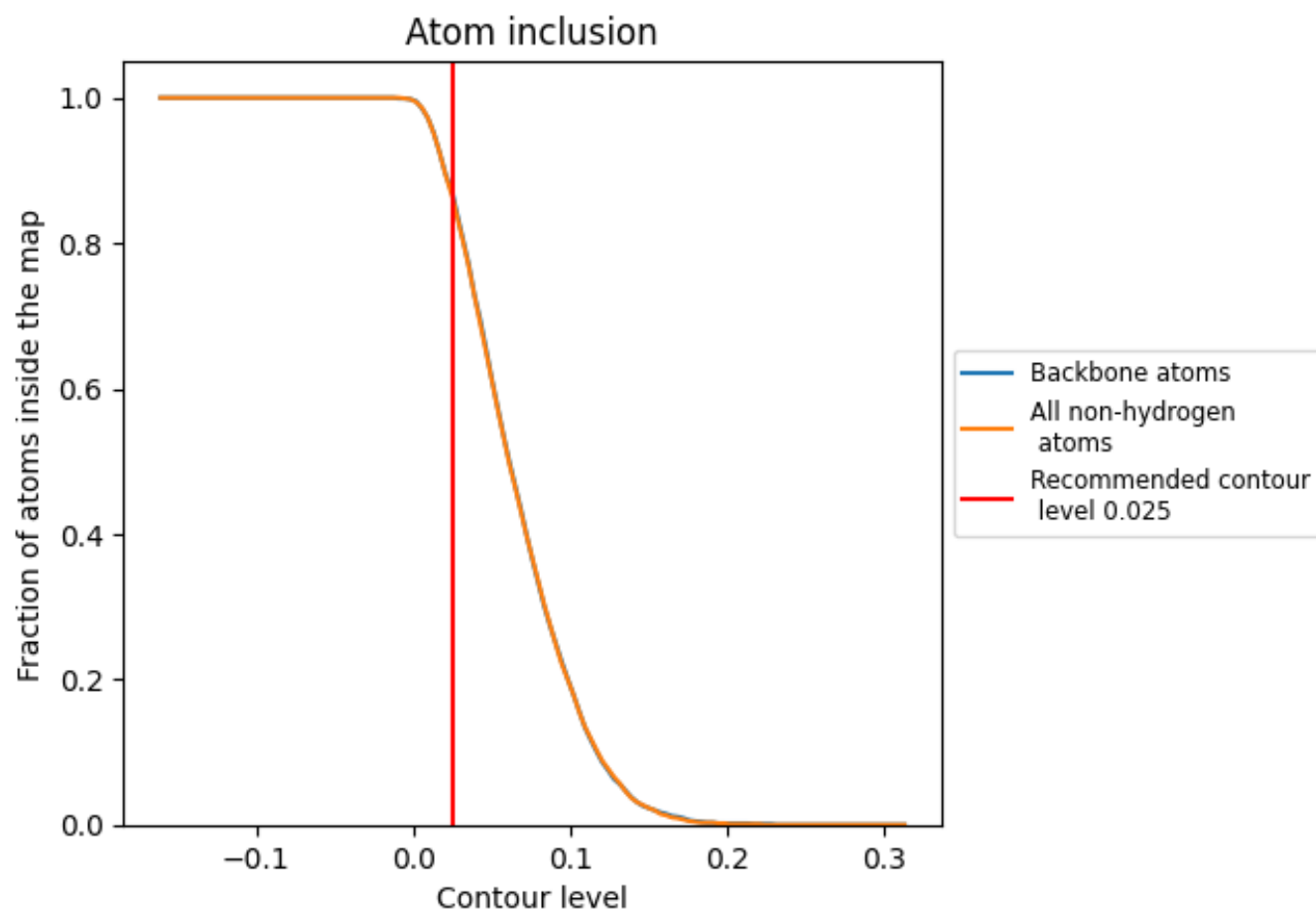
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.6200
A	0.8910	0.6290
B	0.8890	0.6280
C	0.8920	0.6300
D	0.8910	0.6290
E	0.3720	0.4620
F	0.3680	0.4690
G	0.3720	0.4700
H	0.3640	0.4720

1.0

0.0

<0.0