



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 07:16 am BST

PDB ID : 9I0H / pdb_00009i0h
EMDB ID : EMD-52558
Title : CryoEM structure of transit-GmNifEN
Authors : Paya Tormo, L.; Nguyen, T.Q.; Fyfe, C.; Basbous, H.; Dobrzynska, K.; Echavarri-Erasun, C.; Martin, L.; Caserta, G.; Legrand, P.; Thorn, A.; Amara, P.; Schoehn, G.; Cherrier, M.V.; Rubio, L.M.; Nicolet, Y.
Deposited on : 2025-01-15
Resolution : 2.62 Å(reported)
Based on initial model : .

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

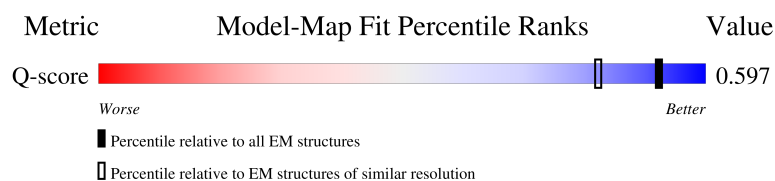
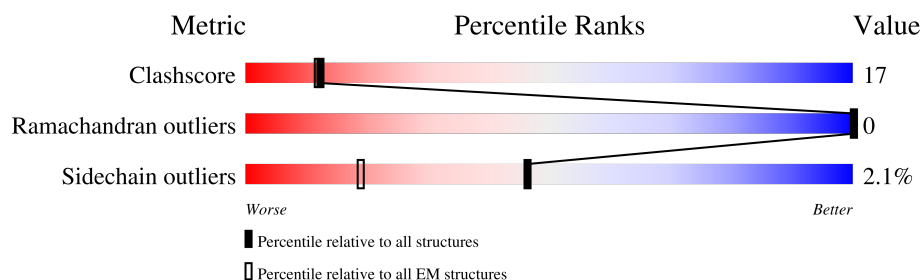
1 Overall quality at a glance

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	919	
1	B	919	

2 Entry composition [i](#)

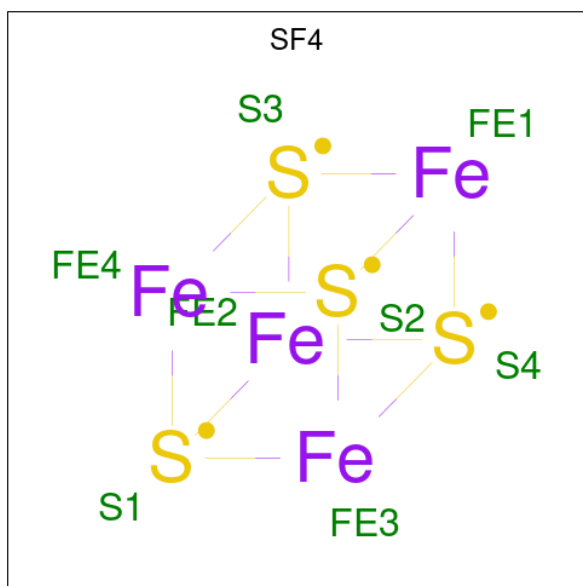
There are 4 unique types of molecules in this entry. The entry contains 12046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE.

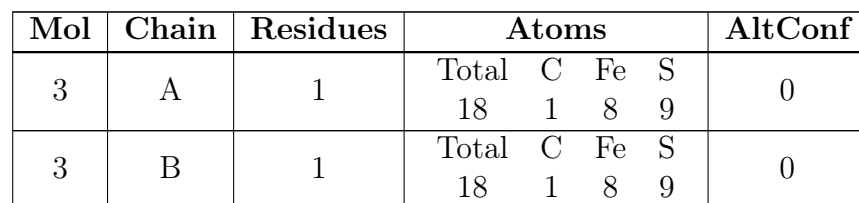
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			5994	3808	1044	1105	37		
1	B	783	Total	C	N	O	S	0	0
			5994	3808	1044	1105	37		

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	Fe	S	0
			8	4	4	
2	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 3 is FeFe cofactor (CCD ID: S5Q) (formula: CFe_8S_9).

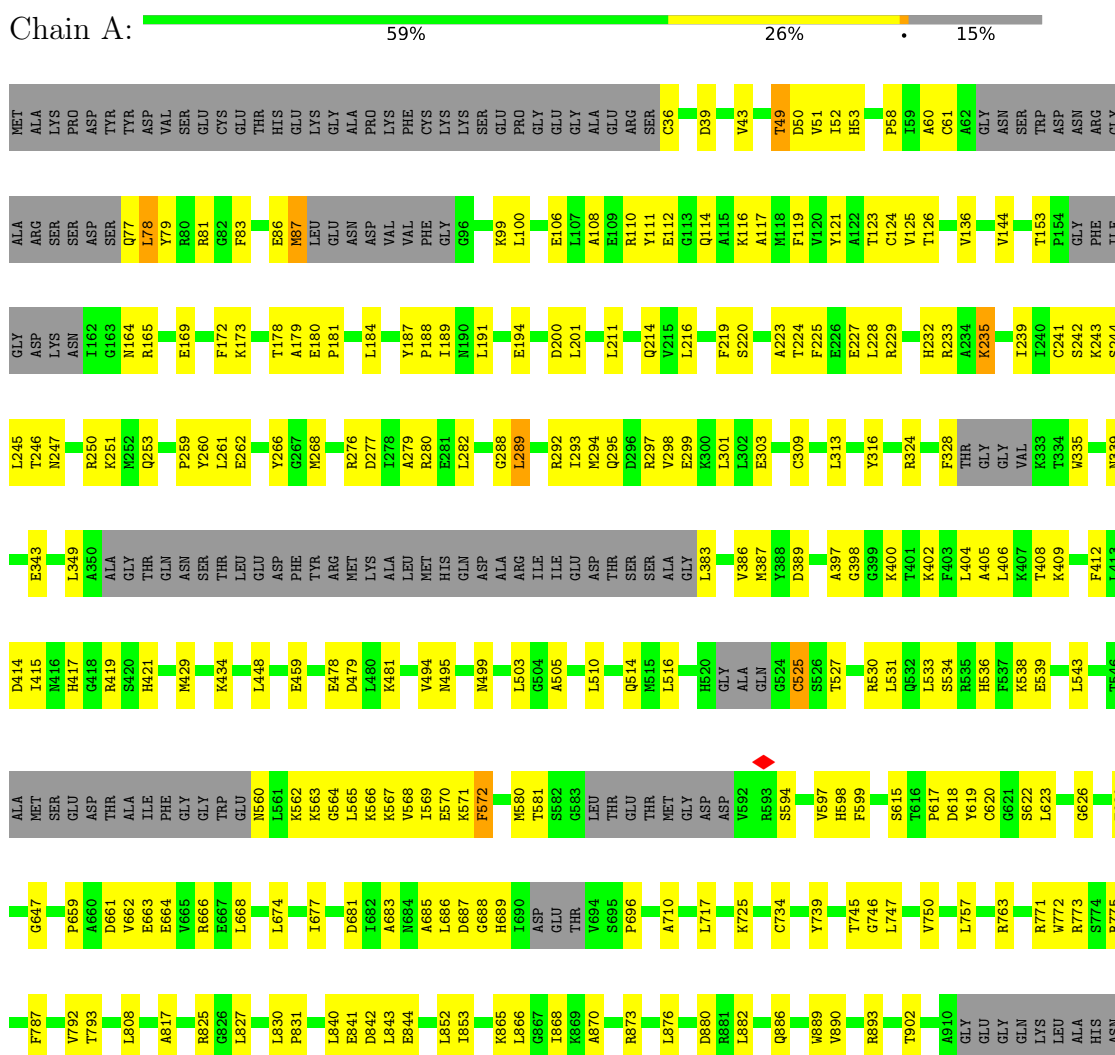


- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------|---------|
| 4 | A | 3 | Total O
3 3 | 0 |
| 4 | B | 3 | Total O
3 3 | 0 |

3 Residue-property plots

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

- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



V792	G647	MET	F412	N339	L245	GLY	ALA	MET
T793	P659	SER	L413	E343	T246	ASP	ARG	ALA
L808	A660	GLU	D414	E343	N247	LYS	SER	LYS
A817	D661	THR	I415	E343	R250	ASN	ASP	PRO
R825	V662	ALA	H416	L349	K251	I162	SER	TYR
L830	E663	ILE	G418	A350	M252	G163	TYR	TYR
P831	E664	PHE	R419	ALA	Q253	N164	ASP	ASP
D839	V665	GLY	S420	GLY	Q254	R165	VAL	VAL
L840	E666	GLY	H421	THR	R255	E169	R80	GLU
E841	E667	TRP	M429	GLN	Y256	V170	R81	SER
L843	L668	GLU	M560	ASN	P259	L171	CYS	GLY
E844	L674	LEU	K434	THR	Y260	F172	THR	THR
L852	T677	SER	E459	LEU	L261	K173	HIS	HIS
L853	D681	GLU	E478	GLU	E262	T178	GLU	GLU
L854	L682	ASP	L565	ASP	E266	A179	LYS	LYS
L855	A683	PHE	D479	TYR	G267	E180	GLY	GLY
L856	E684	ARG	L480	ARG	M268	ASN	ALA	ALA
L857	A685	MET	K481	ARG	R276	VAL	PRO	PRO
L858	L686	LYS	V494	LYS	D277	VAL	LYS	LYS
L859	E687	ILE	N495	ALA	I278	P188	PHE	PHE
L860	G688	GLY	M499	MET	A279	I189	GLY	GLY
L861	H689	ASP	L503	HIS	R280	G96	LYS	LYS
L862	A690	THR	G504	GLN	E281	L191	SER	SER
L863	G694	GLU	A505	ASP	L282	E194	GLU	GLU
L864	E695	LEU	L510	ARG	L289	D200	GLY	GLY
L865	P696	THR	Q514	ILE	R292	L201	ALA	ALA
L866	A710	GLU	L516	GLU	I293	R110	GLU	GLU
L867	L717	THR	H520	ASP	M294	E109	ARG	ARG
L868	M730	ASP	GLY	GLY	Q295	Y111	SER	SER
L869	C734	GLU	ALA	ALA	D296	E112	C36	C36
L870	Y739	THR	G524	L383	R297	Q114	D39	D39
L871	T745	GLY	S526	V386	V298	A115	V43	V43
L872	L747	ASP	T527	M387	E299	K116	T49	T49
L873	V750	ASP	R530	Y388	R300	M118	D50	D50
L874	R763	GLY	L531	D389	L301	F119	V51	V51
L875	A771	GLU	S534	A397	E303	V120	I52	I52
L876	R772	GLY	R535	G398	E309	Y121	H53	H53
L877	W773	GLY	H536	G399	L313	A122	P58	P58
L878	R774	GLY	F537	K400	Y316	T123	I59	I59
L879	S774	GLY	K402	T401	R229	C124	A60	A60
L880	R775	GLY	F403	K402	R233	V125	C61	C61
L881	F787	GLY	L404	F403	A234	T126	A62	A62
L882	T787	GLY	A405	L404	K235	V144	GLY	GLY
L883	T787	GLY	E539	A405	I239	ASP	ASN	ASN
L884	T787	GLY	L543	L406	GLY	TRP	TRP	TRP
L885	T787	GLY	T546	K407	VAL	ASP	ASP	ASP
L886	T787	GLY	ALA	T408	R333	GLY	ASN	ASN
L887	T787	GLY	ALA	K409	T334	PHE	ARG	ARG
L888	T787	GLY	ALA	ALA	W335	ILE	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	370821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.157	Depositor
Minimum map value	-0.129	Depositor
Average map value	-0.032	Depositor
Map value standard deviation	0.484	Depositor
Recommended contour level	0.75	Depositor
Map size (\AA)	276.87, 276.87, 276.87	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.839, 0.839, 0.839	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: S5Q, SF4

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	0.29	0/6100	0.51	4/8252 (0.0%)
1	B	0.29	0/6100	0.51	4/8252 (0.0%)
All	All	0.29	0/12200	0.51	8/16504 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	LEU	N-CA-C	-7.26	102.55	111.33
1	B	289	LEU	N-CA-C	-7.26	102.55	111.33
1	A	617	PRO	N-CA-C	6.69	122.33	113.57
1	B	617	PRO	N-CA-C	6.69	122.33	113.57
1	A	78	LEU	N-CA-C	-5.36	106.44	112.87
1	B	78	LEU	N-CA-C	-5.36	106.44	112.87
1	A	525	CYS	N-CA-C	-5.02	106.99	113.01
1	B	525	CYS	N-CA-C	-5.02	106.99	113.01

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	5994	0	6074	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5994	0	6074	214	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	12046	0	12148	411	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 17.

All (411) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:CG1	1:B:83:PHE:CD2	2.46	0.98
1:A:83:PHE:CD2	1:B:494:VAL:CG1	2.46	0.97
1:A:494:VAL:HG11	1:B:83:PHE:CD2	2.07	0.89
1:A:83:PHE:CD2	1:B:494:VAL:HG11	2.07	0.89
1:A:494:VAL:HG12	1:B:83:PHE:CD2	2.08	0.88
1:A:83:PHE:CD2	1:B:494:VAL:HG12	2.08	0.88
1:A:49:THR:HA	1:A:79:TYR:HB3	1.58	0.84
1:B:49:THR:HA	1:B:79:TYR:HB3	1.58	0.84
1:B:261:LEU:HD21	1:B:277:ASP:HB3	1.61	0.83
1:B:402:LYS:HG2	1:B:406:LEU:HD13	1.62	0.82
1:A:261:LEU:HD21	1:A:277:ASP:HB3	1.61	0.81
1:A:402:LYS:HG2	1:A:406:LEU:HD13	1.62	0.80
1:A:853:ILE:HD11	1:A:868:ILE:HD13	1.64	0.78
1:A:108:ALA:HB1	1:A:144:VAL:HG11	1.66	0.77
1:B:853:ILE:HD11	1:B:868:ILE:HD13	1.64	0.77
1:B:108:ALA:HB1	1:B:144:VAL:HG11	1.66	0.76
1:A:280:ARG:HG2	1:A:295:GLN:HE21	1.51	0.75
1:A:339:ASN:O	1:A:343:GLU:HG3	1.87	0.75
1:B:398:GLY:HA2	1:B:414:ASP:HA	1.67	0.75
1:B:328:PHE:HB2	1:B:397:ALA:HB2	1.68	0.75
1:A:398:GLY:HA2	1:A:414:ASP:HA	1.67	0.75
1:B:280:ARG:HG2	1:B:295:GLN:HE21	1.51	0.75
1:B:339:ASN:O	1:B:343:GLU:HG3	1.87	0.74
1:B:402:LYS:HG2	1:B:406:LEU:CD1	2.17	0.74
1:A:402:LYS:HG2	1:A:406:LEU:CD1	2.17	0.74
1:A:328:PHE:HB2	1:A:397:ALA:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:CG1	1:B:83:PHE:HD2	2.03	0.70
1:A:853:ILE:HD11	1:A:868:ILE:CD1	2.22	0.70
1:B:853:ILE:HD11	1:B:868:ILE:CD1	2.22	0.70
1:A:188:PRO:HG2	1:A:235:LYS:NZ	2.07	0.70
1:B:402:LYS:HG3	1:B:412:PHE:CE2	2.27	0.69
1:A:534:SER:O	1:A:538:LYS:N	2.25	0.69
1:B:188:PRO:HG2	1:B:235:LYS:NZ	2.07	0.69
1:A:510:LEU:HD23	1:A:686:LEU:HG	1.74	0.68
1:A:280:ARG:NH1	1:A:280:ARG:HB3	2.09	0.68
1:A:402:LYS:HG3	1:A:412:PHE:CE2	2.27	0.68
1:B:510:LEU:HD23	1:B:686:LEU:HG	1.74	0.68
1:B:534:SER:O	1:B:538:LYS:N	2.25	0.68
1:B:280:ARG:HB3	1:B:280:ARG:NH1	2.09	0.68
1:A:479:ASP:HB2	1:A:481:LYS:NZ	2.10	0.67
1:B:100:LEU:HD23	1:B:136:VAL:HG21	1.76	0.67
1:A:100:LEU:HD23	1:A:136:VAL:HG21	1.76	0.67
1:A:538:LYS:HZ2	1:A:882:LEU:HD21	1.60	0.66
1:B:479:ASP:HB2	1:B:481:LYS:NZ	2.10	0.66
1:A:83:PHE:HD2	1:B:494:VAL:CG1	2.03	0.65
1:B:539:GLU:OE1	1:B:689:HIS:HE1	1.79	0.65
1:B:188:PRO:HG2	1:B:235:LYS:HZ2	1.62	0.65
1:A:539:GLU:OE1	1:A:689:HIS:HE1	1.79	0.65
1:B:50:ASP:OD1	1:B:50:ASP:N	2.29	0.64
1:A:50:ASP:N	1:A:50:ASP:OD1	2.29	0.64
1:B:243:LYS:O	1:B:246:THR:N	2.31	0.64
1:A:494:VAL:HG11	1:B:83:PHE:CE2	2.33	0.63
1:B:292:ARG:NH1	1:B:295:GLN:OE1	2.31	0.63
1:A:194:GLU:HG2	1:A:201:LEU:HB2	1.81	0.63
1:A:402:LYS:CG	1:A:406:LEU:CD1	2.77	0.62
1:A:569:ILE:HD12	1:A:599:PHE:CZ	2.34	0.62
1:B:194:GLU:HG2	1:B:201:LEU:HB2	1.81	0.62
1:B:566:LYS:HE2	1:B:570:GLU:OE2	1.99	0.62
1:A:239:ILE:HD11	1:A:260:TYR:HB2	1.81	0.62
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.64	0.62
1:A:83:PHE:CE2	1:B:494:VAL:HG11	2.33	0.62
1:B:324:ARG:HG3	1:B:324:ARG:HH11	1.64	0.62
1:A:566:LYS:HE2	1:A:570:GLU:OE2	1.99	0.62
1:B:569:ILE:HD12	1:B:599:PHE:CZ	2.34	0.62
1:A:243:LYS:O	1:A:246:THR:N	2.31	0.62
1:B:239:ILE:HD11	1:B:260:TYR:HB2	1.81	0.62
1:A:663:GLU:HG2	1:A:683:ALA:HB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:HG2	1:B:683:ALA:HB1	1.82	0.61
1:A:86:GLU:HB2	1:A:99:LYS:HZ1	1.64	0.61
1:B:402:LYS:CG	1:B:406:LEU:CD1	2.77	0.61
1:B:844:GLU:HA	1:B:866:LEU:HD11	1.82	0.61
1:A:61:CYS:O	1:A:61:CYS:SG	2.59	0.61
1:A:188:PRO:HG2	1:A:235:LYS:HZ1	1.66	0.61
1:A:292:ARG:NH1	1:A:295:GLN:OE1	2.31	0.60
1:A:844:GLU:HA	1:A:866:LEU:HD11	1.82	0.60
1:B:61:CYS:SG	1:B:61:CYS:O	2.59	0.60
1:B:398:GLY:HA3	1:B:415:ILE:H	1.67	0.60
1:B:187:TYR:HD1	1:B:282:LEU:HD22	1.67	0.59
1:A:398:GLY:HA3	1:A:415:ILE:H	1.67	0.59
1:B:172:PHE:CD2	1:B:251:LYS:HE2	2.38	0.59
1:B:568:VAL:O	1:B:572:PHE:HD1	1.86	0.59
1:A:873:ARG:NH1	1:A:880:ASP:OD2	2.36	0.59
1:A:172:PHE:CD2	1:A:251:LYS:HE2	2.38	0.59
1:B:419:ARG:NH1	1:B:421:HIS:O	2.36	0.59
1:A:419:ARG:NH1	1:A:421:HIS:O	2.36	0.58
1:B:873:ARG:NH1	1:B:880:ASP:OD2	2.36	0.58
1:A:194:GLU:HG2	1:A:201:LEU:HD13	1.85	0.58
1:A:383:LEU:O	1:A:387:MET:HG3	2.04	0.58
1:B:280:ARG:HB3	1:B:280:ARG:HH11	1.68	0.58
1:A:568:VAL:O	1:A:572:PHE:HD1	1.86	0.58
1:A:279:ALA:HB2	1:A:298:VAL:HG11	1.86	0.58
1:B:194:GLU:HG2	1:B:201:LEU:HD13	1.85	0.58
1:B:383:LEU:O	1:B:387:MET:HG3	2.04	0.58
1:B:279:ALA:HB2	1:B:298:VAL:HG11	1.86	0.57
1:A:187:TYR:HD1	1:A:282:LEU:HD22	1.67	0.57
1:A:775:ARG:HG2	1:B:688:GLY:O	2.04	0.57
1:A:688:GLY:O	1:B:775:ARG:HG2	2.04	0.57
1:B:164:ASN:HB2	1:B:244:SER:HB2	1.86	0.57
1:A:402:LYS:CG	1:A:406:LEU:HD11	2.35	0.57
1:A:164:ASN:HB2	1:A:244:SER:HB2	1.86	0.57
1:A:280:ARG:HB3	1:A:280:ARG:HH11	1.68	0.56
1:B:402:LYS:CG	1:B:406:LEU:HD11	2.35	0.56
1:B:268:MET:HE2	1:B:429:MET:SD	2.46	0.56
1:B:294:MET:HE2	1:B:294:MET:HA	1.87	0.56
1:A:294:MET:HE2	1:A:294:MET:HA	1.87	0.56
1:A:717:LEU:HD23	1:A:739:TYR:HB2	1.88	0.56
1:A:505:ALA:HA	1:A:630:THR:HG21	1.87	0.56
1:A:268:MET:HE1	1:A:309:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:H	1:B:126:THR:HG22	1.71	0.56
1:B:106:GLU:OE2	1:B:110:ARG:NH2	2.39	0.56
1:A:123:THR:H	1:A:126:THR:HG22	1.71	0.55
1:A:268:MET:HE2	1:A:429:MET:SD	2.46	0.55
1:A:106:GLU:OE2	1:A:110:ARG:NH2	2.39	0.55
1:B:268:MET:HE1	1:B:309:CYS:SG	2.46	0.55
1:B:398:GLY:HA3	1:B:415:ILE:HD12	1.88	0.55
1:B:717:LEU:HD23	1:B:739:TYR:HB2	1.88	0.55
1:B:51:VAL:HG11	1:B:119:PHE:CD2	2.42	0.55
1:B:505:ALA:HA	1:B:630:THR:HG21	1.87	0.55
1:B:86:GLU:O	1:B:87:MET:C	2.50	0.55
1:B:530:ARG:HH12	1:B:543:LEU:HB3	1.71	0.55
1:A:51:VAL:HG11	1:A:119:PHE:CD2	2.42	0.54
1:A:398:GLY:HA3	1:A:415:ILE:HD12	1.88	0.54
1:B:299:GLU:O	1:B:303:GLU:HG2	2.07	0.54
1:B:53:HIS:HB3	1:B:121:TYR:HE2	1.73	0.54
1:B:792:VAL:HG22	1:B:852:LEU:HB3	1.90	0.54
1:A:53:HIS:HB3	1:A:121:TYR:HE2	1.73	0.54
1:A:572:PHE:HD2	1:A:696:PRO:HG2	1.73	0.54
1:A:86:GLU:O	1:A:87:MET:C	2.50	0.54
1:A:792:VAL:HG22	1:A:852:LEU:HB3	1.90	0.54
1:B:243:LYS:O	1:B:246:THR:HG23	2.08	0.54
1:A:299:GLU:O	1:A:303:GLU:HG2	2.07	0.54
1:B:626:GLY:O	1:B:630:THR:HG22	2.08	0.54
1:A:530:ARG:HH12	1:A:543:LEU:HB3	1.71	0.53
1:A:626:GLY:O	1:A:630:THR:HG22	2.08	0.53
1:A:81:ARG:HB3	1:A:83:PHE:CZ	2.43	0.53
1:A:763:ARG:HG3	1:A:763:ARG:HH11	1.73	0.53
1:B:58:PRO:HG3	1:B:125:VAL:HG21	1.90	0.53
1:A:685:ALA:O	1:A:689:HIS:CE1	2.62	0.53
1:B:572:PHE:N	1:B:572:PHE:CD1	2.77	0.53
1:A:243:LYS:O	1:A:246:THR:HG23	2.08	0.53
1:A:404:LEU:H	1:A:404:LEU:HD22	1.74	0.53
1:A:572:PHE:N	1:A:572:PHE:CD1	2.77	0.53
1:A:112:GLU:O	1:A:114:GLN:NE2	2.42	0.53
1:A:58:PRO:HG3	1:A:125:VAL:HG21	1.90	0.52
1:B:81:ARG:HB3	1:B:83:PHE:CZ	2.43	0.52
1:B:313:LEU:HD21	1:B:429:MET:HE2	1.92	0.52
1:B:479:ASP:HB2	1:B:481:LYS:HZ3	1.73	0.52
1:B:572:PHE:HD2	1:B:696:PRO:HG2	1.73	0.52
1:A:865:LYS:NZ	1:A:865:LYS:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:HD22	1:B:404:LEU:H	1.74	0.52
1:B:792:VAL:HG11	1:B:808:LEU:HD13	1.91	0.52
1:B:618:ASP:O	1:B:619:TYR:C	2.53	0.52
1:B:685:ALA:O	1:B:689:HIS:CE1	2.62	0.52
1:B:763:ARG:HG3	1:B:763:ARG:HH11	1.73	0.52
1:B:865:LYS:NZ	1:B:865:LYS:HB3	2.25	0.52
1:A:479:ASP:HB2	1:A:481:LYS:HZ3	1.73	0.51
1:A:539:GLU:OE1	1:A:689:HIS:CE1	2.62	0.51
1:A:840:LEU:HD22	1:A:843:LEU:HD22	1.92	0.51
1:B:172:PHE:HD2	1:B:251:LYS:HE2	1.75	0.51
1:B:840:LEU:HD22	1:B:843:LEU:HD22	1.92	0.51
1:A:618:ASP:HB3	1:A:620:CYS:HB3	1.93	0.51
1:A:313:LEU:HD21	1:A:429:MET:HE2	1.92	0.51
1:B:39:ASP:O	1:B:43:VAL:HG13	2.11	0.51
1:A:792:VAL:HG11	1:A:808:LEU:HD13	1.91	0.51
1:A:618:ASP:O	1:A:619:TYR:C	2.53	0.51
1:B:200:ASP:HB3	1:B:419:ARG:HH22	1.76	0.51
1:A:292:ARG:HD2	1:A:295:GLN:HB2	1.94	0.50
1:B:618:ASP:HB3	1:B:620:CYS:HB3	1.93	0.50
1:A:39:ASP:O	1:A:43:VAL:HG13	2.11	0.50
1:A:179:ALA:HB2	1:A:229:ARG:HH21	1.76	0.50
1:A:564:GLY:O	1:A:568:VAL:HG22	2.12	0.50
1:B:77:GLN:C	1:B:79:TYR:H	2.19	0.50
1:B:178:THR:HB	1:B:229:ARG:HD2	1.94	0.50
1:B:188:PRO:HA	1:B:214:GLN:O	2.12	0.50
1:A:188:PRO:HA	1:A:214:GLN:O	2.12	0.50
1:B:112:GLU:O	1:B:114:GLN:NE2	2.42	0.50
1:B:402:LYS:CG	1:B:406:LEU:HD13	2.37	0.50
1:B:539:GLU:OE1	1:B:689:HIS:CE1	2.62	0.50
1:B:564:GLY:O	1:B:568:VAL:HG22	2.12	0.50
1:A:77:GLN:C	1:A:79:TYR:H	2.19	0.50
1:A:200:ASP:HB3	1:A:419:ARG:HH22	1.76	0.50
1:A:172:PHE:HD2	1:A:251:LYS:HE2	1.75	0.49
1:A:243:LYS:O	1:A:245:LEU:N	2.45	0.49
1:B:179:ALA:HB2	1:B:229:ARG:HH21	1.76	0.49
1:B:292:ARG:HD2	1:B:295:GLN:HB2	1.94	0.49
1:A:86:GLU:CB	1:A:99:LYS:HZ1	2.26	0.49
1:A:169:GLU:O	1:A:173:LYS:HD3	2.12	0.49
1:A:664:GLU:O	1:A:668:LEU:HG	2.13	0.49
1:A:178:THR:HB	1:A:229:ARG:HD2	1.94	0.49
1:A:81:ARG:CB	1:A:83:PHE:CZ	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:LYS:HB2	1:B:572:PHE:CE1	2.48	0.49
1:B:666:ARG:NH1	1:B:681:ASP:OD2	2.36	0.49
1:A:81:ARG:O	1:A:83:PHE:CE1	2.66	0.49
1:A:562:LYS:HD3	1:A:598:HIS:HB3	1.95	0.49
1:B:243:LYS:O	1:B:245:LEU:N	2.45	0.49
1:B:414:ASP:OD1	1:B:414:ASP:N	2.43	0.49
1:A:543:LEU:HD11	1:A:580:MET:HE1	1.95	0.48
1:A:571:LYS:HB2	1:A:572:PHE:CD1	2.48	0.48
1:A:571:LYS:HB2	1:A:572:PHE:CE1	2.48	0.48
1:B:81:ARG:CB	1:B:83:PHE:CZ	2.96	0.48
1:B:402:LYS:HG3	1:B:406:LEU:HD11	1.95	0.48
1:B:664:GLU:O	1:B:668:LEU:HG	2.13	0.48
1:B:81:ARG:NH2	1:B:111:TYR:OH	2.46	0.48
1:B:677:ILE:HG21	1:B:710:ALA:HB2	1.96	0.48
1:B:543:LEU:HD11	1:B:580:MET:HE1	1.95	0.48
1:A:219:PHE:O	1:A:220:SER:OG	2.31	0.48
1:A:402:LYS:HG3	1:A:406:LEU:HD11	1.95	0.48
1:A:527:THR:O	1:A:531:LEU:HD22	2.13	0.48
1:B:169:GLU:O	1:B:173:LYS:HD3	2.12	0.48
1:B:239:ILE:HG22	1:B:241:CYS:O	2.14	0.48
1:A:293:ILE:CG1	1:A:297:ARG:HH21	2.27	0.48
1:A:659:PRO:HB3	1:A:683:ALA:HA	1.96	0.48
1:B:659:PRO:HB3	1:B:683:ALA:HA	1.96	0.48
1:A:414:ASP:OD1	1:A:414:ASP:N	2.43	0.48
1:B:527:THR:O	1:B:531:LEU:HD22	2.13	0.48
1:A:81:ARG:NH2	1:A:111:TYR:OH	2.46	0.47
1:B:200:ASP:OD1	1:B:201:LEU:N	2.47	0.47
1:B:571:LYS:HB2	1:B:572:PHE:CD1	2.48	0.47
1:A:250:ARG:NH1	1:A:250:ARG:HG3	2.29	0.47
1:B:81:ARG:O	1:B:83:PHE:CE1	2.66	0.47
1:B:293:ILE:CG1	1:B:297:ARG:HH21	2.27	0.47
1:A:200:ASP:OD1	1:A:201:LEU:N	2.47	0.47
1:B:562:LYS:HD3	1:B:598:HIS:HB3	1.95	0.47
1:A:666:ARG:NH1	1:A:681:ASP:OD2	2.36	0.47
1:A:239:ILE:HG22	1:A:241:CYS:O	2.14	0.47
1:B:536:HIS:HD2	1:B:876:LEU:HD23	1.80	0.47
1:B:386:VAL:HA	1:B:389:ASP:OD2	2.14	0.47
1:B:481:LYS:H	1:B:481:LYS:HD3	1.79	0.47
1:A:677:ILE:HG21	1:A:710:ALA:HB2	1.96	0.47
1:A:853:ILE:CD1	1:A:868:ILE:HD13	2.40	0.47
1:B:510:LEU:HD23	1:B:686:LEU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:HIS:H	1:B:232:HIS:CD2	2.33	0.47
1:A:536:HIS:HD2	1:A:876:LEU:HD23	1.80	0.46
1:B:224:THR:OG1	1:B:227:GLU:HB2	2.15	0.46
1:B:250:ARG:NH1	1:B:250:ARG:HG3	2.29	0.46
1:A:188:PRO:HG2	1:A:235:LYS:HZ2	1.79	0.46
1:A:316:TYR:CZ	1:A:434:LYS:HG2	2.51	0.46
1:A:386:VAL:HA	1:A:389:ASP:OD2	2.14	0.46
1:B:77:GLN:C	1:B:79:TYR:N	2.72	0.46
1:B:538:LYS:HZ2	1:B:882:LEU:HD21	1.78	0.46
1:A:402:LYS:CG	1:A:406:LEU:HD13	2.37	0.46
1:A:232:HIS:CD2	1:A:232:HIS:H	2.33	0.46
1:A:324:ARG:HD2	1:A:349:LEU:HD21	1.98	0.46
1:A:481:LYS:H	1:A:481:LYS:HD3	1.79	0.46
1:B:324:ARG:HD2	1:B:349:LEU:HD21	1.98	0.46
1:B:516:LEU:HD21	1:B:568:VAL:HB	1.97	0.46
1:A:189:ILE:HD12	1:A:191:LEU:HD21	1.98	0.46
1:A:516:LEU:HD21	1:A:568:VAL:HB	1.97	0.46
1:A:224:THR:OG1	1:A:227:GLU:HB2	2.15	0.46
1:B:560:ASN:HA	1:B:563:LYS:HD2	1.98	0.46
1:B:853:ILE:CD1	1:B:868:ILE:HD13	2.40	0.46
1:A:478:GLU:O	1:A:825:ARG:NH1	2.50	0.46
1:A:481:LYS:HD3	1:A:481:LYS:N	2.31	0.46
1:B:241:CYS:SG	1:B:242:SER:N	2.89	0.46
1:A:745:THR:HG22	1:A:889:TRP:O	2.16	0.45
1:B:661:ASP:HB3	1:B:890:VAL:HG21	1.99	0.45
1:B:165:ARG:HD3	1:B:247:ASN:ND2	2.32	0.45
1:B:180:GLU:OE2	1:B:233:ARG:HD2	2.17	0.45
1:B:189:ILE:HD12	1:B:191:LEU:HD21	1.98	0.45
1:A:108:ALA:CB	1:A:144:VAL:HG11	2.42	0.45
1:B:316:TYR:CZ	1:B:434:LYS:HG2	2.51	0.45
1:B:481:LYS:HD3	1:B:481:LYS:N	2.31	0.45
1:A:292:ARG:HD2	1:A:295:GLN:CB	2.47	0.45
1:B:747:LEU:HD11	1:B:773:ARG:HG3	1.99	0.45
1:A:180:GLU:OE2	1:A:233:ARG:HD2	2.17	0.45
1:B:536:HIS:CD2	1:B:876:LEU:HD23	2.52	0.45
1:A:246:THR:O	1:A:250:ARG:HG3	2.17	0.45
1:A:661:ASP:HB3	1:A:890:VAL:HG21	1.99	0.45
1:A:560:ASN:HA	1:A:563:LYS:HD2	1.98	0.45
1:B:60:ALA:O	1:B:61:CYS:HB3	2.16	0.45
1:B:188:PRO:HG2	1:B:235:LYS:HZ1	1.82	0.45
1:B:246:THR:O	1:B:250:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLU:O	1:B:825:ARG:NH1	2.50	0.45
1:A:747:LEU:HD11	1:A:773:ARG:HG3	1.99	0.44
1:A:165:ARG:HD3	1:A:247:ASN:ND2	2.32	0.44
1:B:294:MET:O	1:B:298:VAL:HG13	2.18	0.44
1:A:83:PHE:HD2	1:B:494:VAL:HG11	1.67	0.44
1:A:687:ASP:OD1	1:A:886:GLN:NE2	2.51	0.44
1:B:292:ARG:HD2	1:B:295:GLN:CB	2.47	0.44
1:A:241:CYS:SG	1:A:242:SER:N	2.89	0.44
1:A:594:SER:HA	1:A:597:VAL:HG12	2.00	0.44
1:B:687:ASP:OD1	1:B:886:GLN:NE2	2.51	0.44
1:A:60:ALA:O	1:A:61:CYS:HB3	2.16	0.44
1:A:536:HIS:CD2	1:A:876:LEU:HD23	2.52	0.44
1:A:841:GLU:HG3	1:A:842:ASP:N	2.32	0.44
1:B:745:THR:HG22	1:B:889:TRP:O	2.16	0.44
1:A:77:GLN:C	1:A:79:TYR:N	2.72	0.44
1:A:250:ARG:HG3	1:A:250:ARG:HH11	1.82	0.44
1:A:530:ARG:NH1	1:A:543:LEU:HB3	2.33	0.44
1:B:536:HIS:HD1	1:B:536:HIS:C	2.25	0.44
1:A:223:ALA:HB1	1:A:228:LEU:HD11	2.00	0.44
1:A:184:LEU:CD1	1:A:188:PRO:HG3	2.49	0.43
1:A:294:MET:O	1:A:298:VAL:HG13	2.18	0.43
1:A:852:LEU:HD12	1:A:870:ALA:HB1	2.00	0.43
1:A:292:ARG:O	1:A:292:ARG:HG3	2.19	0.43
1:A:495:ASN:HB3	1:A:840:LEU:HB2	1.99	0.43
1:A:787:PHE:CZ	1:A:902:THR:HB	2.53	0.43
1:B:223:ALA:HB1	1:B:228:LEU:HD11	2.00	0.43
1:B:830:LEU:HA	1:B:831:PRO:HD3	1.88	0.43
1:B:841:GLU:HG3	1:B:842:ASP:N	2.32	0.43
1:A:83:PHE:CD1	1:A:83:PHE:N	2.87	0.43
1:A:266:TYR:OH	1:A:419:ARG:NH2	2.51	0.43
1:A:510:LEU:HD23	1:A:686:LEU:CG	2.44	0.43
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.80	0.43
1:B:108:ALA:CB	1:B:144:VAL:HG11	2.42	0.43
1:B:184:LEU:CD1	1:B:188:PRO:HG3	2.49	0.43
1:B:250:ARG:HG3	1:B:250:ARG:HH11	1.82	0.43
1:B:495:ASN:HB3	1:B:840:LEU:HB2	1.99	0.43
1:B:51:VAL:HG11	1:B:119:PHE:HD2	1.80	0.43
1:A:51:VAL:HG11	1:A:119:PHE:HD2	1.80	0.43
1:A:662:VAL:HB	1:A:683:ALA:HB2	2.01	0.43
1:B:295:GLN:O	1:B:299:GLU:HG2	2.18	0.43
1:B:530:ARG:NH1	1:B:543:LEU:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:HG13	1:A:117:ALA:C	2.44	0.43
1:A:114:GLN:N	1:A:114:GLN:CD	2.76	0.43
1:A:295:GLN:O	1:A:299:GLU:HG2	2.18	0.43
1:A:494:VAL:HG23	1:A:841:GLU:HB3	2.01	0.43
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.91	0.43
1:B:494:VAL:HG23	1:B:841:GLU:HB3	2.01	0.43
1:B:503:LEU:HD23	1:B:623:LEU:HD12	2.01	0.43
1:B:292:ARG:O	1:B:292:ARG:HG3	2.19	0.43
1:B:594:SER:HA	1:B:597:VAL:HG12	2.00	0.43
1:B:763:ARG:HG3	1:B:763:ARG:NH1	2.33	0.43
1:A:763:ARG:HG3	1:A:763:ARG:NH1	2.33	0.43
1:A:772:TRP:CZ3	1:A:893:ARG:HG3	2.54	0.43
1:B:51:VAL:HG13	1:B:117:ALA:C	2.44	0.43
1:B:204:MET:HE3	1:B:204:MET:HB3	1.84	0.43
1:B:243:LYS:HE2	1:B:262:GLU:OE1	2.19	0.43
1:B:852:LEU:HD12	1:B:870:ALA:HB1	2.00	0.43
1:A:225:PHE:CE2	1:A:229:ARG:HD3	2.54	0.42
1:A:243:LYS:HE2	1:A:262:GLU:OE1	2.19	0.42
1:A:400:LYS:C	1:A:402:LYS:H	2.27	0.42
1:B:114:GLN:N	1:B:114:GLN:CD	2.76	0.42
1:B:191:LEU:HD12	1:B:201:LEU:HD11	2.01	0.42
1:B:276:ARG:NH1	1:B:299:GLU:OE2	2.52	0.42
1:B:772:TRP:CZ3	1:B:893:ARG:HG3	2.54	0.42
1:A:409:LYS:HD3	1:A:409:LYS:HA	1.64	0.42
1:B:459:GLU:OE1	1:B:459:GLU:N	2.52	0.42
1:A:503:LEU:HD23	1:A:623:LEU:HD12	2.01	0.42
1:A:725:LYS:HB2	1:A:725:LYS:HE3	1.82	0.42
1:A:746:GLY:O	1:A:750:VAL:HG23	2.19	0.42
1:B:180:GLU:OE1	1:B:181:PRO:HD2	2.20	0.42
1:B:266:TYR:OH	1:B:419:ARG:NH2	2.51	0.42
1:B:787:PHE:CZ	1:B:902:THR:HB	2.53	0.42
1:A:412:PHE:CZ	1:A:414:ASP:HB3	2.54	0.42
1:A:180:GLU:OE1	1:A:181:PRO:HD2	2.20	0.42
1:A:618:ASP:O	1:A:619:TYR:CG	2.73	0.42
1:B:565:LEU:O	1:B:569:ILE:HG13	2.20	0.42
1:B:83:PHE:CD1	1:B:83:PHE:N	2.87	0.42
1:B:225:PHE:CE2	1:B:229:ARG:HD3	2.54	0.42
1:B:565:LEU:HD12	1:B:565:LEU:HA	1.89	0.42
1:A:194:GLU:CG	1:A:201:LEU:HD13	2.49	0.42
1:B:536:HIS:O	1:B:536:HIS:ND1	2.45	0.42
1:B:746:GLY:O	1:B:750:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD12	1:A:201:LEU:HD11	2.01	0.42
1:A:216:LEU:O	1:A:227:GLU:HG2	2.20	0.42
1:A:459:GLU:N	1:A:459:GLU:OE1	2.52	0.42
1:B:402:LYS:HG3	1:B:406:LEU:CD1	2.50	0.42
1:B:412:PHE:CZ	1:B:414:ASP:HB3	2.54	0.42
1:B:581:THR:O	1:B:615:SER:HA	2.20	0.42
1:A:211:LEU:HG	1:A:301:LEU:HD13	2.02	0.42
1:A:235:LYS:HZ3	1:A:235:LYS:HG3	1.11	0.42
1:B:216:LEU:O	1:B:227:GLU:HG2	2.20	0.42
1:B:793:THR:HG23	1:B:817:ALA:HB3	2.02	0.42
1:A:565:LEU:O	1:A:569:ILE:HG13	2.20	0.42
1:A:830:LEU:HA	1:A:831:PRO:HD3	1.88	0.42
1:B:335:TRP:NE1	1:B:339:ASN:HD21	2.18	0.42
1:B:662:VAL:HB	1:B:683:ALA:HB2	2.01	0.42
1:B:873:ARG:H	1:B:873:ARG:HG2	1.69	0.42
1:A:276:ARG:NH1	1:A:299:GLU:OE2	2.52	0.41
1:B:143:LYS:HB2	1:B:143:LYS:HE2	1.84	0.41
1:A:253:GLN:NE2	1:A:259:PRO:HA	2.36	0.41
1:A:288:GLY:O	1:A:289:LEU:C	2.62	0.41
1:B:402:LYS:O	1:B:405:ALA:N	2.53	0.41
1:B:408:THR:HG22	1:B:408:THR:O	2.20	0.41
1:B:409:LYS:HA	1:B:409:LYS:HD3	1.64	0.41
1:B:647:GLY:HA2	1:B:674:LEU:HD23	2.02	0.41
1:A:402:LYS:O	1:A:405:ALA:N	2.53	0.41
1:A:581:THR:O	1:A:615:SER:HA	2.20	0.41
1:A:335:TRP:NE1	1:A:339:ASN:HD21	2.18	0.41
1:A:408:THR:O	1:A:408:THR:HG22	2.20	0.41
1:A:499:ASN:O	1:A:622:SER:HA	2.20	0.41
1:A:564:GLY:HA2	1:A:567:LYS:HD3	2.02	0.41
1:B:618:ASP:O	1:B:619:TYR:CG	2.73	0.41
1:A:793:THR:HG23	1:A:817:ALA:HB3	2.02	0.41
1:B:400:LYS:C	1:B:402:LYS:H	2.27	0.41
1:B:499:ASN:O	1:B:622:SER:HA	2.20	0.41
1:B:211:LEU:HG	1:B:301:LEU:HD13	2.02	0.41
1:B:253:GLN:NE2	1:B:259:PRO:HA	2.36	0.41
1:B:50:ASP:OD1	1:B:224:THR:HA	2.20	0.41
1:B:81:ARG:HB2	1:B:83:PHE:CE1	2.56	0.41
1:B:618:ASP:C	1:B:620:CYS:N	2.77	0.41
1:A:647:GLY:HA2	1:A:674:LEU:HD23	2.02	0.41
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.87	0.41
1:A:771:ARG:O	1:A:775:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:MET:HE2	1:B:730:MET:HB3	1.97	0.41
1:B:839:ASP:OD1	1:B:839:ASP:N	2.40	0.41
1:B:52:ILE:HD11	1:B:111:TYR:HB2	2.04	0.40
1:B:328:PHE:HD1	1:B:328:PHE:HA	1.76	0.40
1:A:530:ARG:NH1	1:A:530:ARG:HB2	2.36	0.40
1:B:194:GLU:CG	1:B:201:LEU:HD13	2.49	0.40
1:A:50:ASP:OD1	1:A:224:THR:HA	2.20	0.40
1:A:827:LEU:HD23	1:A:827:LEU:HA	1.94	0.40
1:B:771:ARG:O	1:B:775:ARG:HG3	2.21	0.40
1:A:52:ILE:HD11	1:A:111:TYR:HB2	2.04	0.40
1:A:235:LYS:HE2	1:A:282:LEU:HD21	2.04	0.40
1:B:211:LEU:HD21	1:B:298:VAL:HG12	2.04	0.40
1:B:255:ASN:C	1:B:256:TYR:HD1	2.29	0.40
1:B:564:GLY:HA2	1:B:567:LYS:HD3	2.02	0.40
1:A:757:LEU:HD23	1:A:757:LEU:HA	1.91	0.40
1:B:256:TYR:HD1	1:B:256:TYR:N	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	763/919 (83%)	737 (97%)	26 (3%)	0	100	100
1	B	763/919 (83%)	737 (97%)	26 (3%)	0	100	100
All	All	1526/1838 (83%)	1474 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	626/732 (86%)	613 (98%)	13 (2%)	47	72
1	B	626/732 (86%)	613 (98%)	13 (2%)	47	72
All	All	1252/1464 (86%)	1226 (98%)	26 (2%)	46	72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	CYS
1	A	49	THR
1	A	78	LEU
1	A	87	MET
1	A	116	LYS
1	A	124	CYS
1	A	153	THR
1	A	235	LYS
1	A	417	HIS
1	A	514	GLN
1	A	525	CYS
1	A	572	PHE
1	A	734	CYS
1	B	36	CYS
1	B	49	THR
1	B	78	LEU
1	B	87	MET
1	B	116	LYS
1	B	124	CYS
1	B	153	THR
1	B	235	LYS
1	B	417	HIS
1	B	514	GLN
1	B	525	CYS
1	B	572	PHE
1	B	734	CYS

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

Mol	Chain	Res	Type
1	A	339	ASN
1	A	385	GLN
1	A	491	ASN
1	A	495	ASN
1	A	497	GLN
1	A	858	ASN
1	A	885	HIS
1	B	339	ASN
1	B	385	GLN
1	B	491	ASN
1	B	495	ASN
1	B	858	ASN
1	B	885	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
3	S5Q	A	1002	1	18,30,30	2.55	10 (55%)	-		
2	SF4	A	1001	1	0,12,12	-	-	-		
2	SF4	B	1001	1	0,12,12	-	-	-		
3	S5Q	B	1002	1	18,30,30	2.55	10 (55%)	-		

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	SF4	A	1001	1	-	-	0/6/5/5
2	SF4	B	1001	1	-	-	0/6/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	S5Q	S3A-FE4	-4.27	2.14	2.24
3	B	1002	S5Q	S3A-FE4	-4.27	2.14	2.24
3	A	1002	S5Q	S4A-FE4	-4.23	2.22	2.32
3	B	1002	S5Q	S4A-FE4	-4.23	2.22	2.32
3	A	1002	S5Q	S3B-FE6	-3.94	2.22	2.32
3	B	1002	S5Q	S3B-FE6	-3.94	2.22	2.32
3	A	1002	S5Q	S1B-FE6	-3.49	2.23	2.32
3	B	1002	S5Q	S1B-FE6	-3.49	2.23	2.32
3	A	1002	S5Q	S2A-FE3	-3.18	2.24	2.32
3	B	1002	S5Q	S2A-FE3	-3.18	2.24	2.32
3	A	1002	S5Q	S1B-FE5	-2.84	2.25	2.32
3	B	1002	S5Q	S1B-FE5	-2.84	2.25	2.32
3	A	1002	S5Q	S2B-FE6	-2.81	2.18	2.24
3	B	1002	S5Q	S2B-FE6	-2.81	2.18	2.24
3	A	1002	S5Q	S1A-FE2	-2.57	2.26	2.32
3	B	1002	S5Q	S1A-FE2	-2.57	2.26	2.32
3	A	1002	S5Q	S4A-FE3	-2.50	2.26	2.32
3	B	1002	S5Q	S4A-FE3	-2.50	2.26	2.32
3	A	1002	S5Q	S1A-FE4	-2.47	2.26	2.32
3	B	1002	S5Q	S1A-FE4	-2.47	2.26	2.32

There are no bond angle outliers.

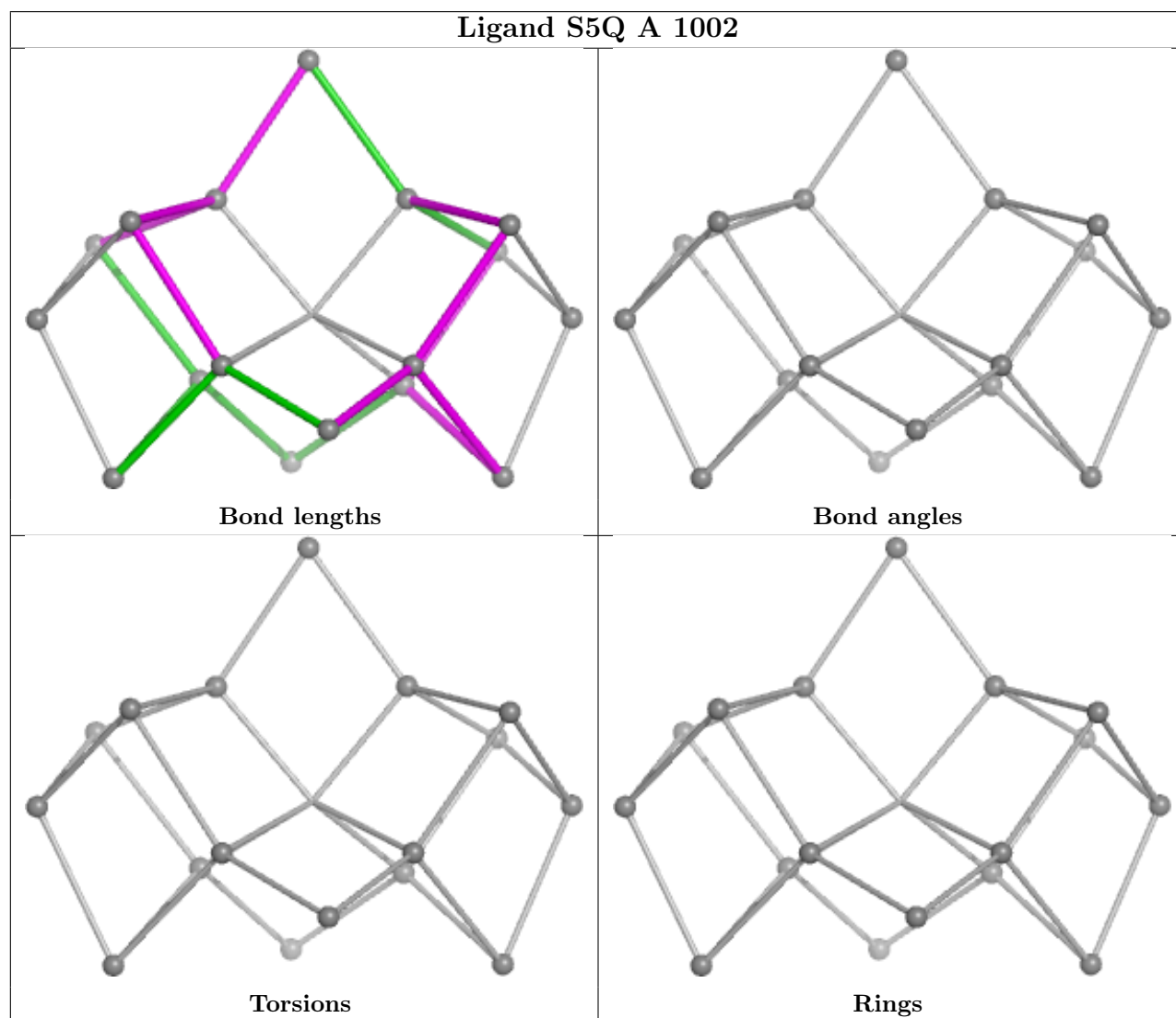
There are no chirality outliers.

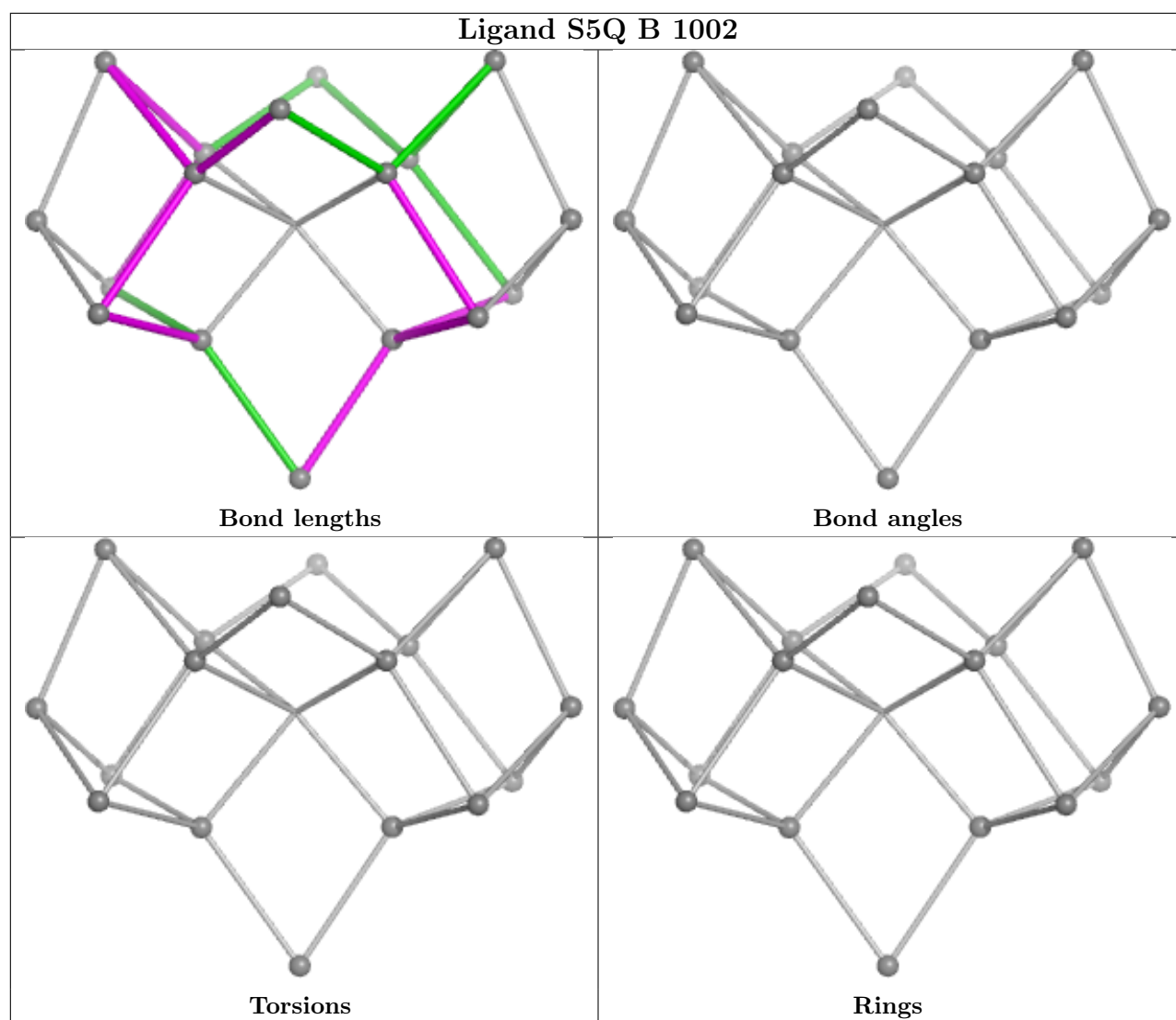
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

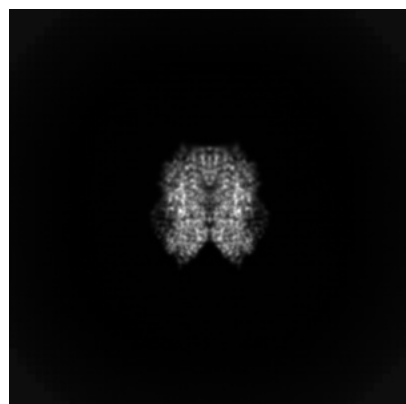
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52558. These allow visual inspection of the internal detail of the map and identification of artifacts.

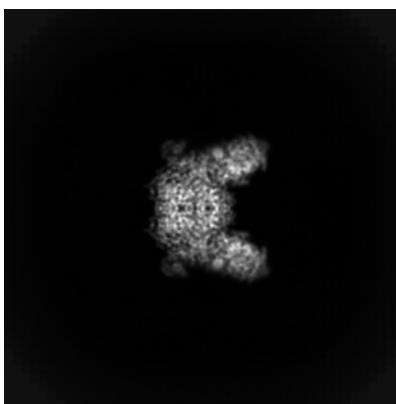
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

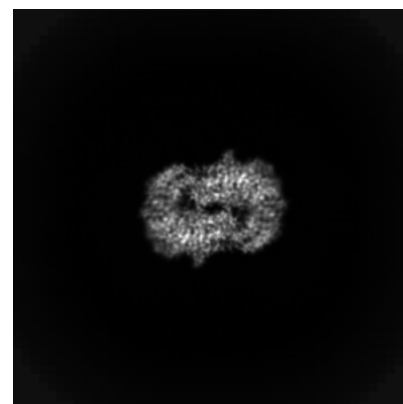
6.1.1 Primary map



X

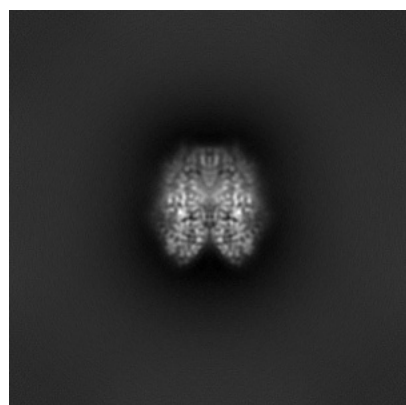


Y

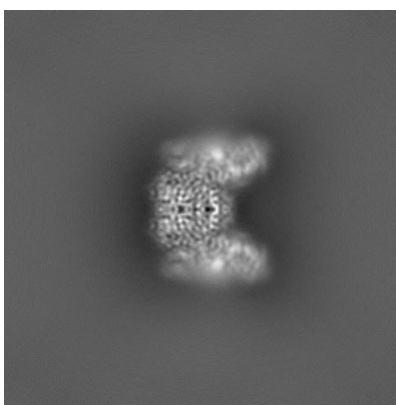


Z

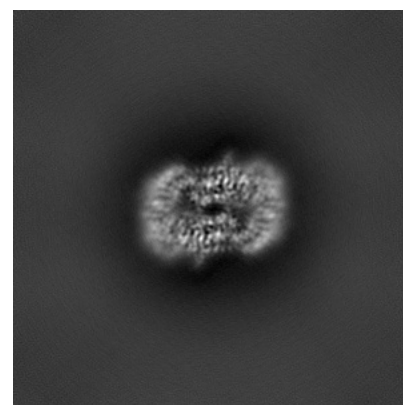
6.1.2 Raw map



X



Y

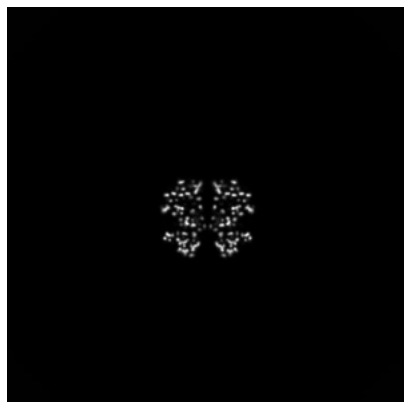


Z

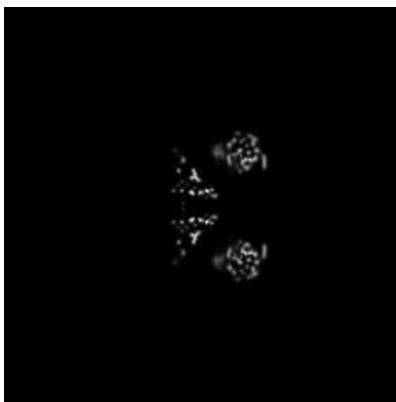
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

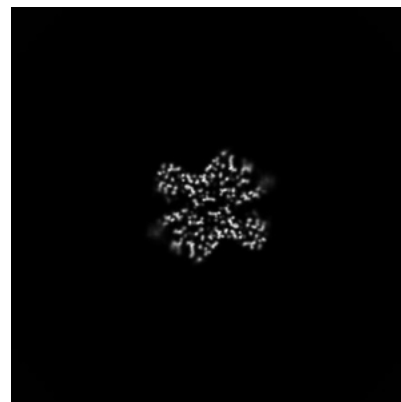
6.2.1 Primary map



X Index: 165

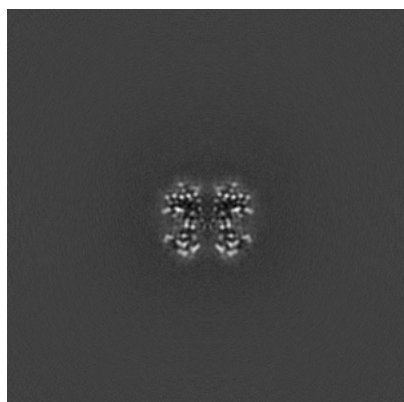


Y Index: 165

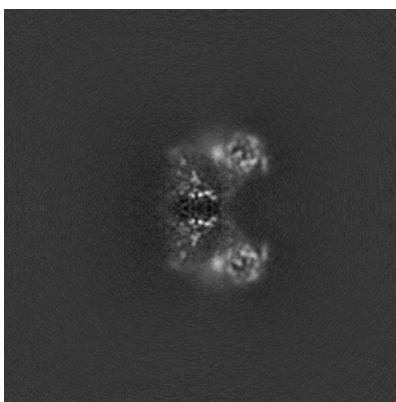


Z Index: 165

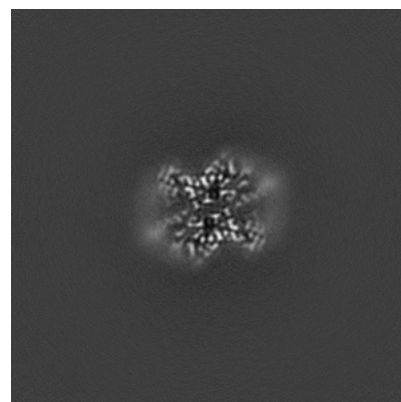
6.2.2 Raw map



X Index: 165



Y Index: 165

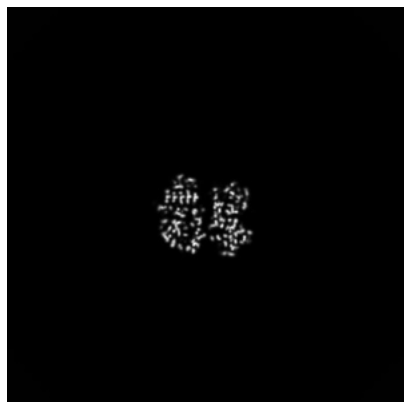


Z Index: 165

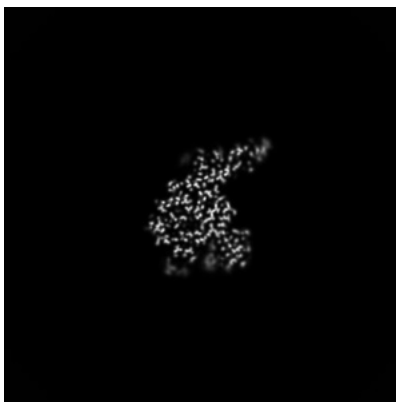
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

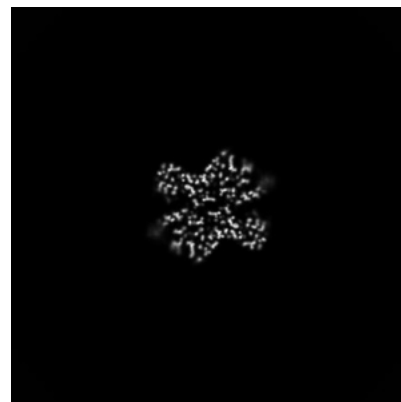
6.3.1 Primary map



X Index: 161

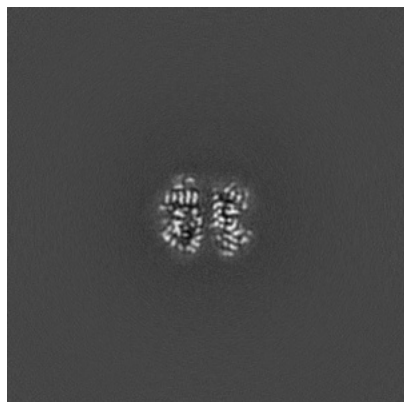


Y Index: 143

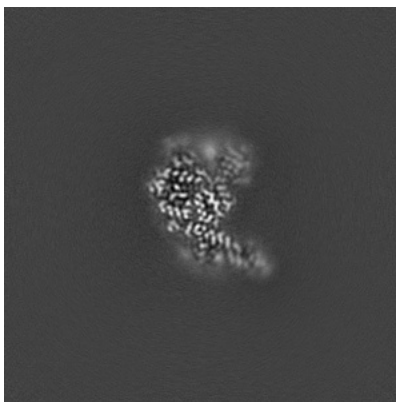


Z Index: 165

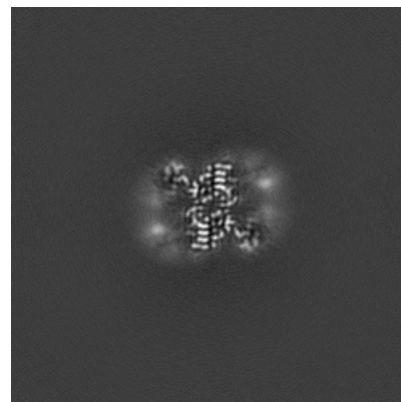
6.3.2 Raw map



X Index: 161



Y Index: 187

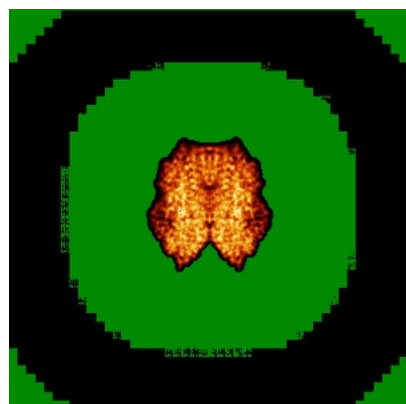


Z Index: 171

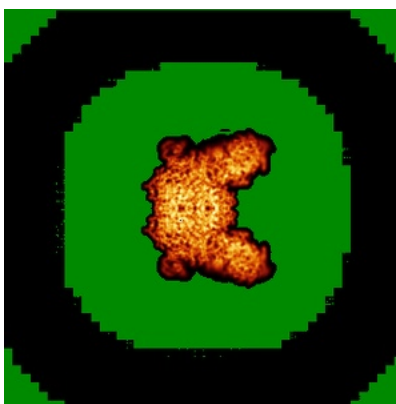
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

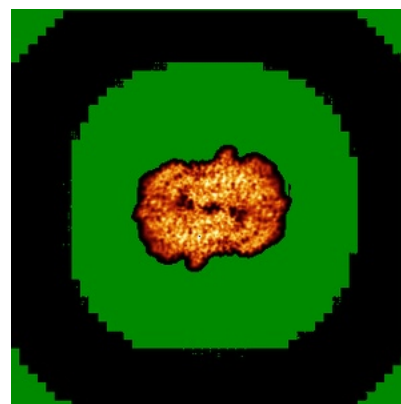
6.4.1 Primary map



X

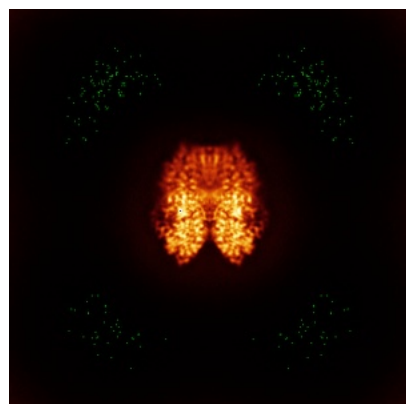


Y

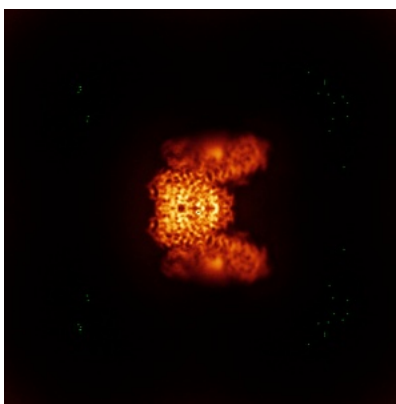


Z

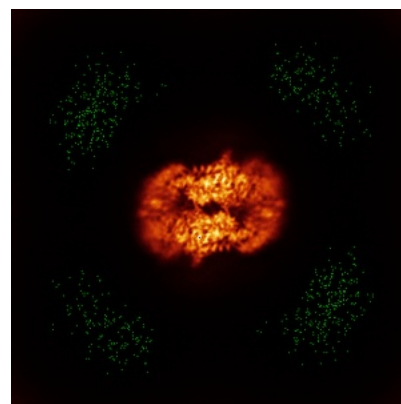
6.4.2 Raw map



X



Y

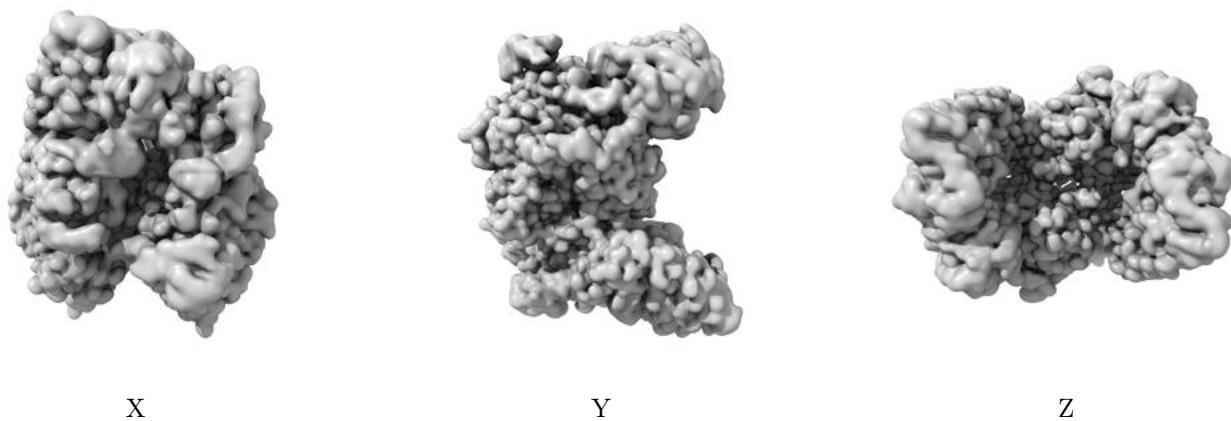


Z

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.

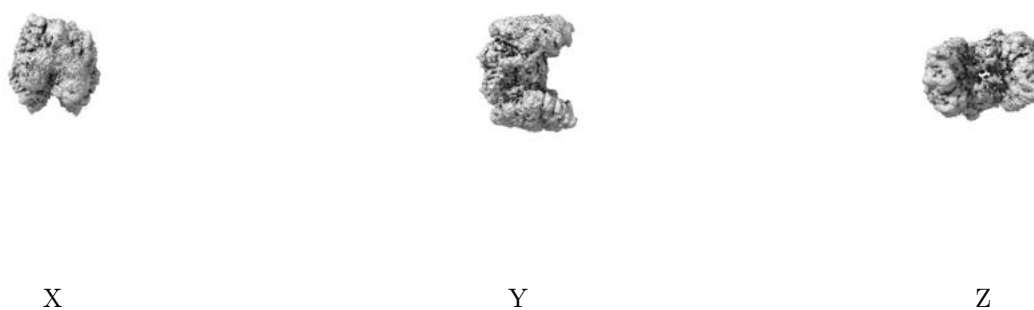
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. 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.

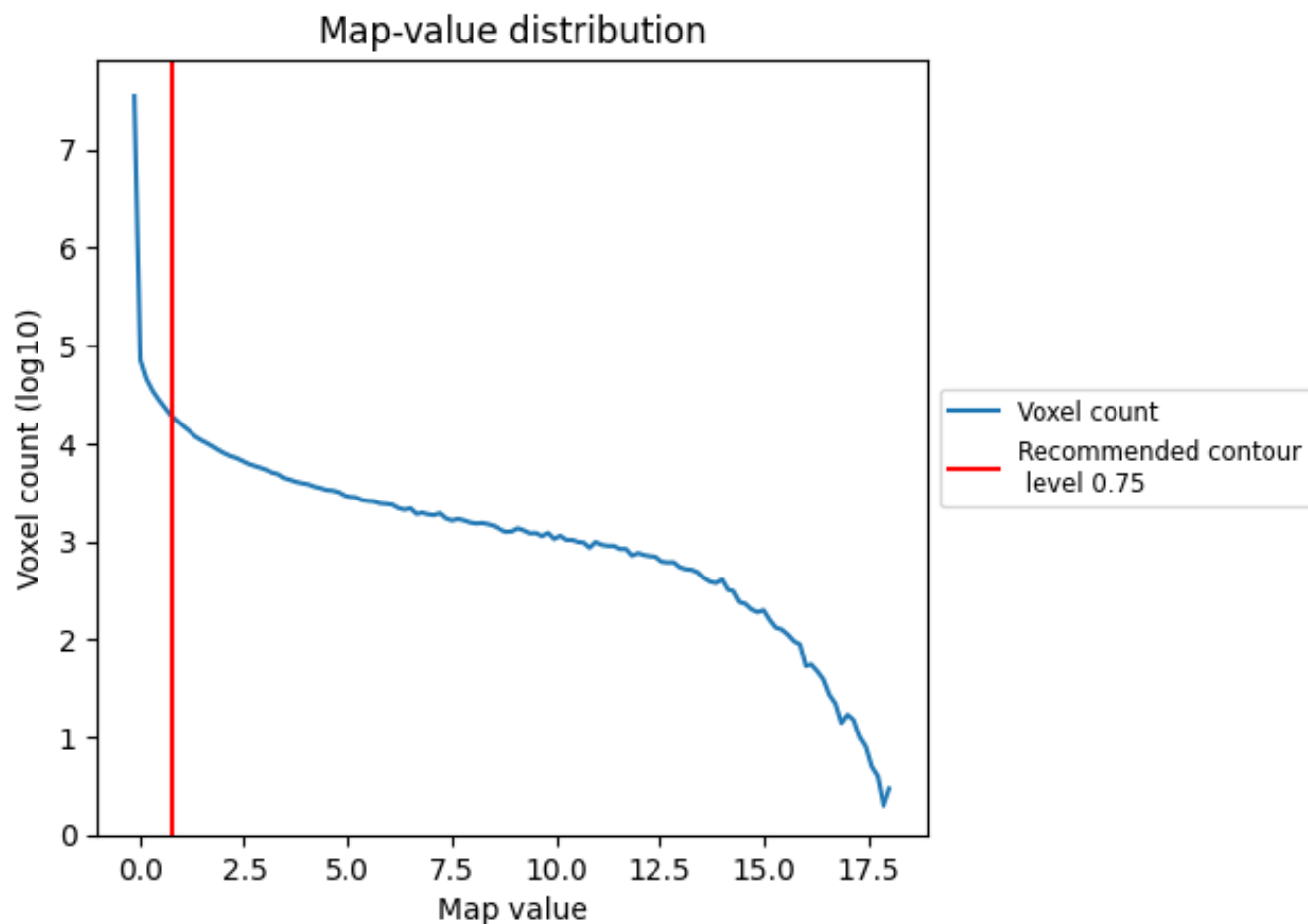
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

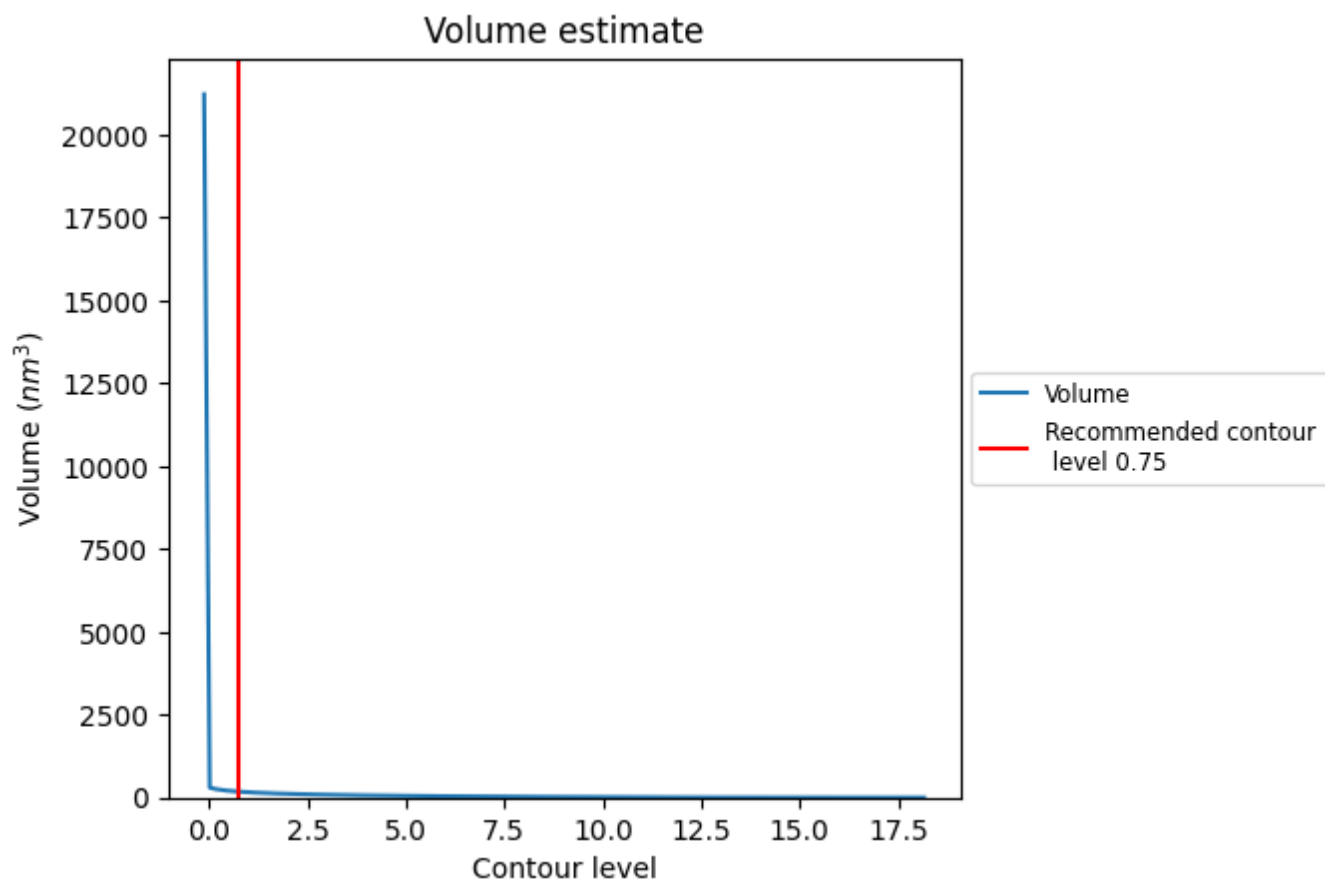
This section contains the results of statistical analysis of the map.

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.

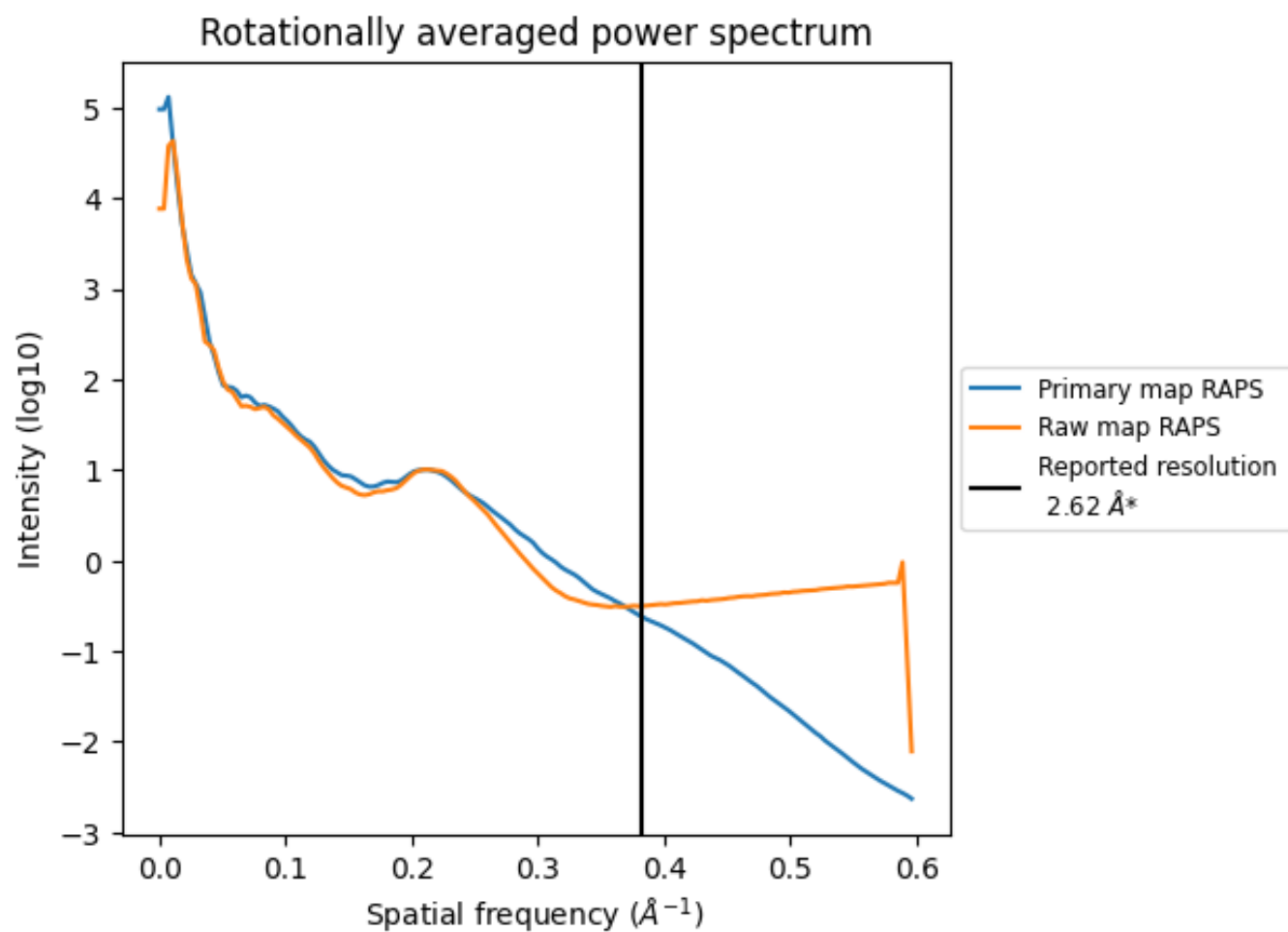
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm³; this corresponds to an approximate mass of 162 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 ⓘ

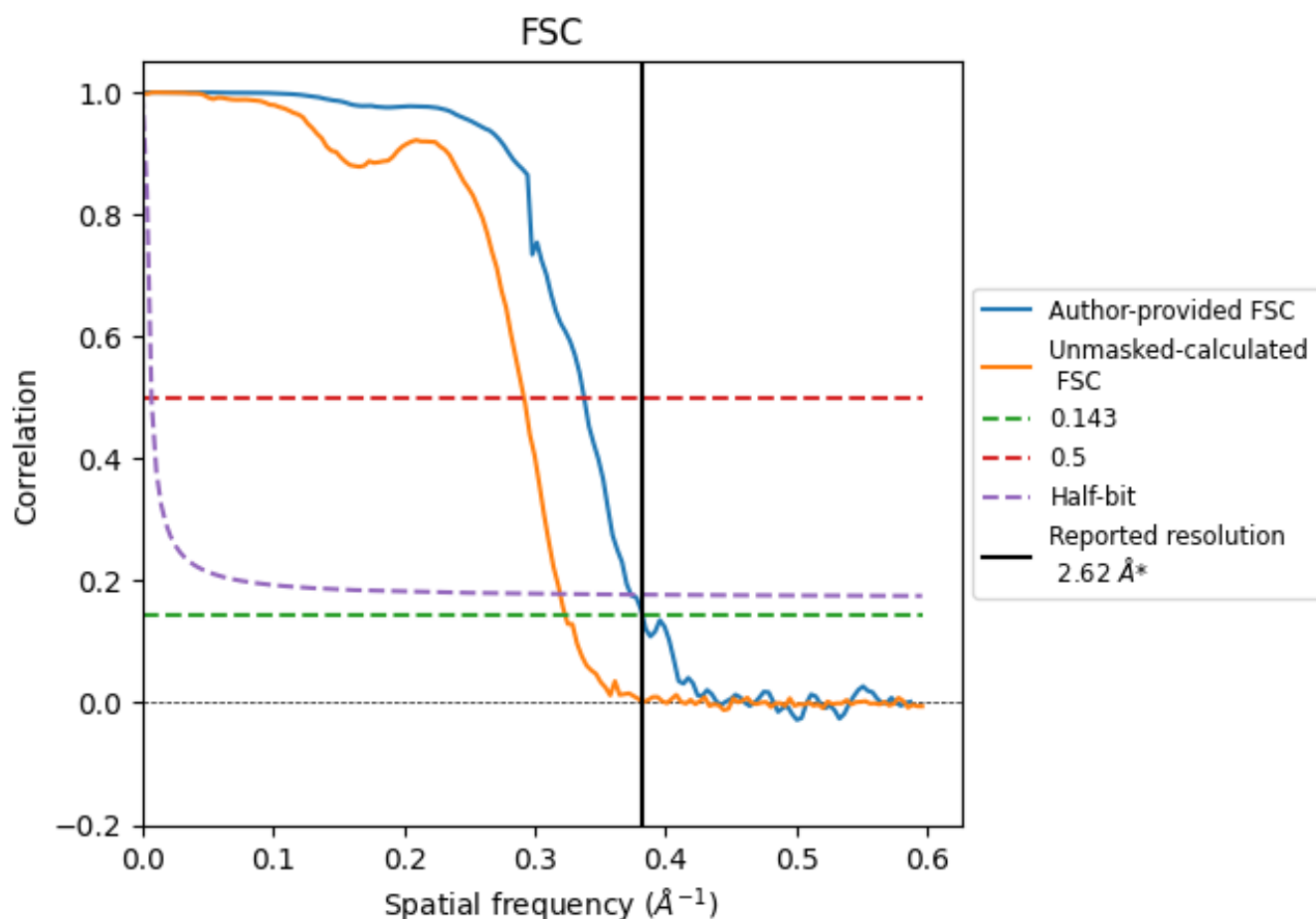


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

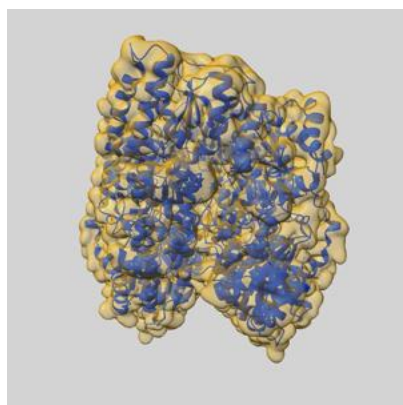
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.96	2.68
Unmasked-calculated*	3.09	3.43	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.62 by more than 10 %

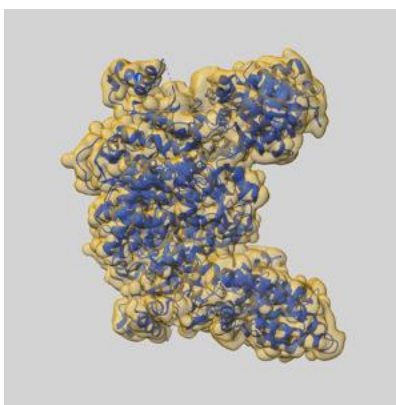
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52558 and PDB model 9I0H. Per-residue inclusion information can be found in section 3 on page 5.

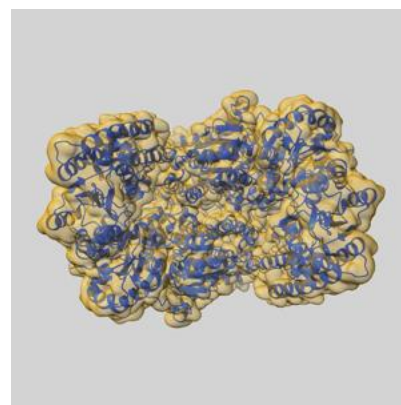
9.1 Map-model overlay [i](#)



X



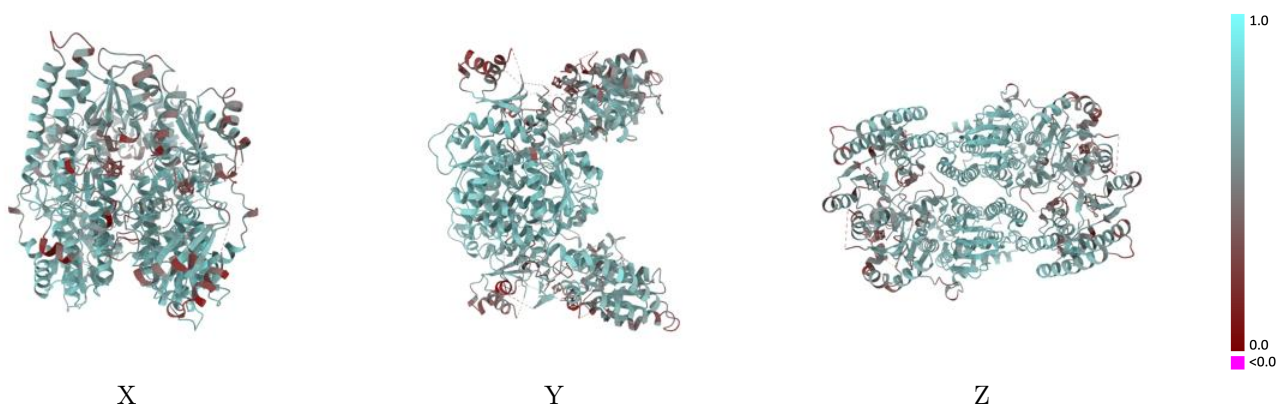
Y



Z

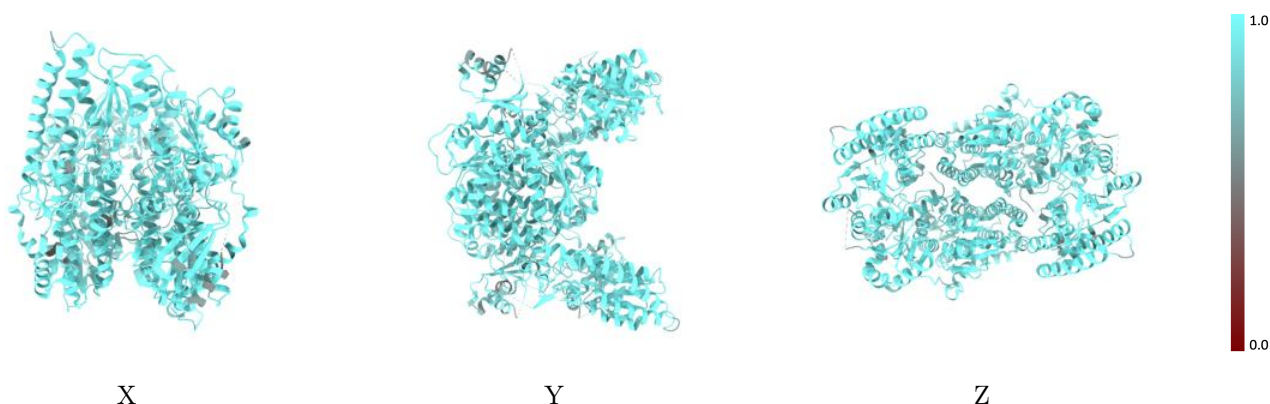
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



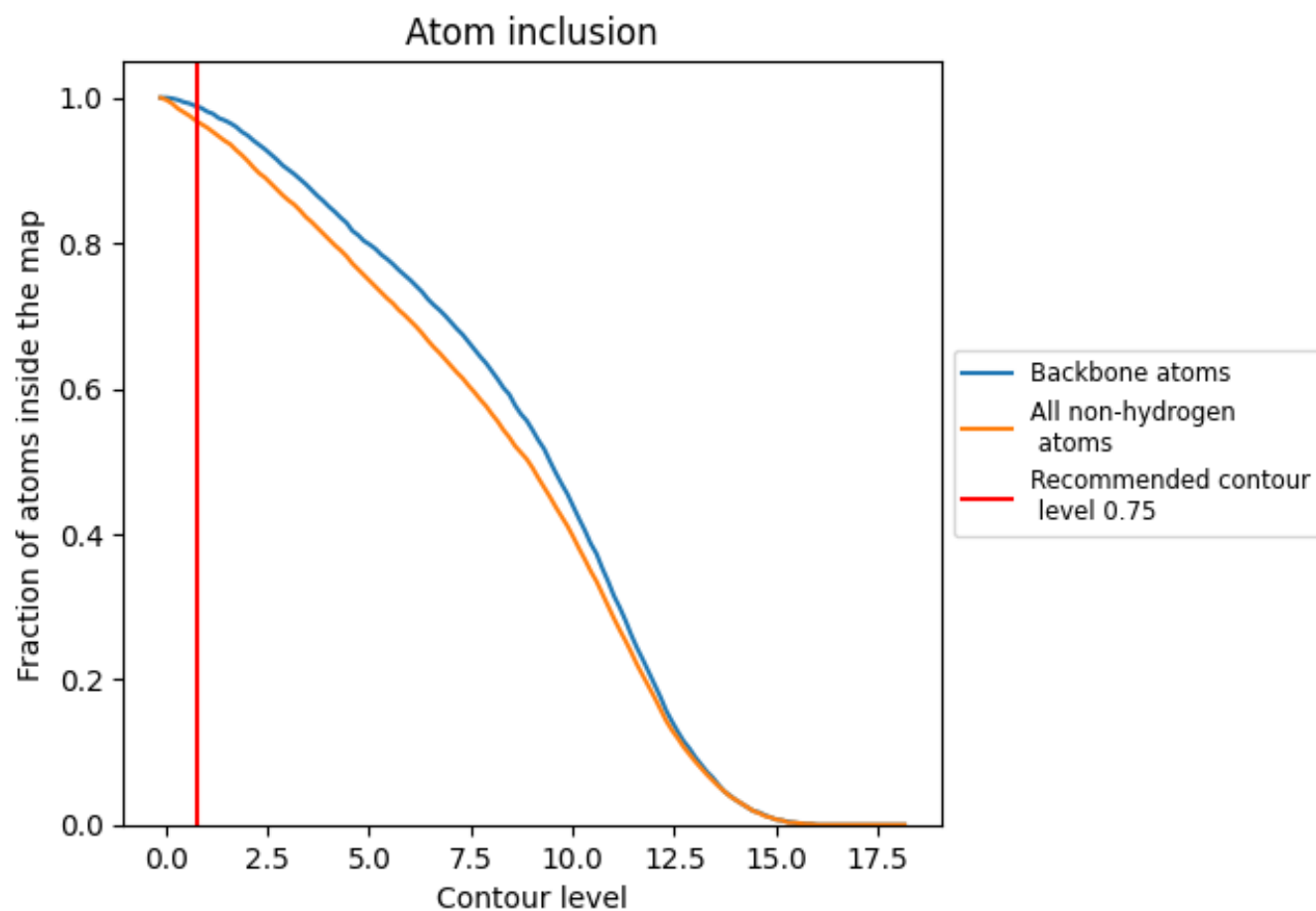
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9680	<div></div> 0.5970
A	<div></div> 0.9690	<div></div> 0.5980
B	<div></div> 0.9710	<div></div> 0.5970

