



## Full wwPDB EM Validation Report ⓘ

Sep 22, 2025 – 11:13 AM EDT

PDB ID : 9NWP / pdb\_00009nwp  
EMDB ID : EMD-49889  
Title : Human delta 2 receptor activated by D-serine  
Authors : Wang, H.; Ahmed, F.; Kumar Mondal, A.; Twomey, E.C.  
Deposited on : 2025-03-24  
Resolution : 3.69 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](mailto: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>.

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

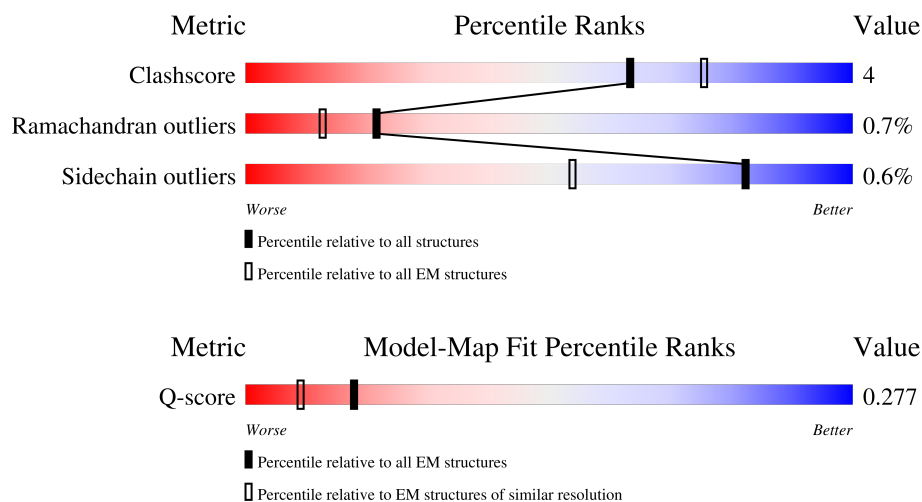
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 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 3.69 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11284 ( 3.19 - 4.18 )

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  $\geq 3$ , 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	836	<div> <div>8%</div> <div>91%</div> <div>8%</div> </div>
1	B	836	<div> <div>16%</div> <div>91%</div> <div>8%</div> </div>
1	C	836	<div> <div>54%</div> <div>89%</div> <div>10%</div> </div>
1	D	836	<div> <div>55%</div> <div>87%</div> <div>12%</div> </div>

## 2 Entry composition [i](#)

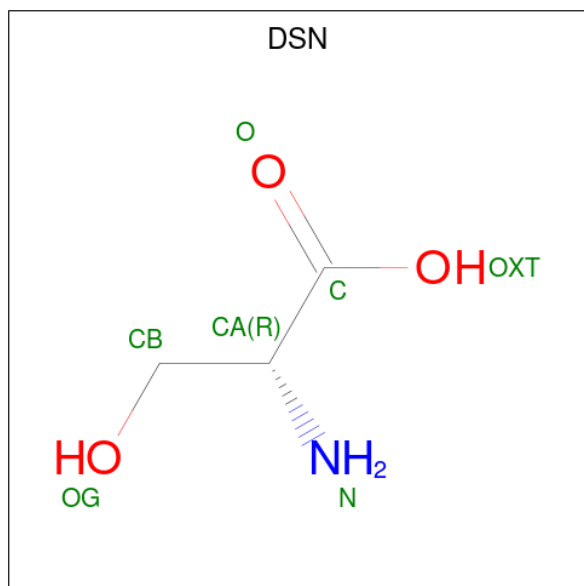
There are 2 unique types of molecules in this entry. The entry contains 26528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate receptor ionotropic, delta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	836	Total	C	N	O	S	0	0
			6625	4212	1132	1242	39		
1	B	836	Total	C	N	O	S	0	0
			6625	4212	1132	1242	39		
1	C	836	Total	C	N	O	S	0	0
			6625	4212	1132	1242	39		
1	D	836	Total	C	N	O	S	0	0
			6625	4212	1132	1242	39		

- Molecule 2 is D-SERINE (CCD ID: DSN) (formula:  $C_3H_7NO_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			7	3	1	3	
2	B	1	Total	C	N	O	0
			7	3	1	3	

*Continued on next page...*

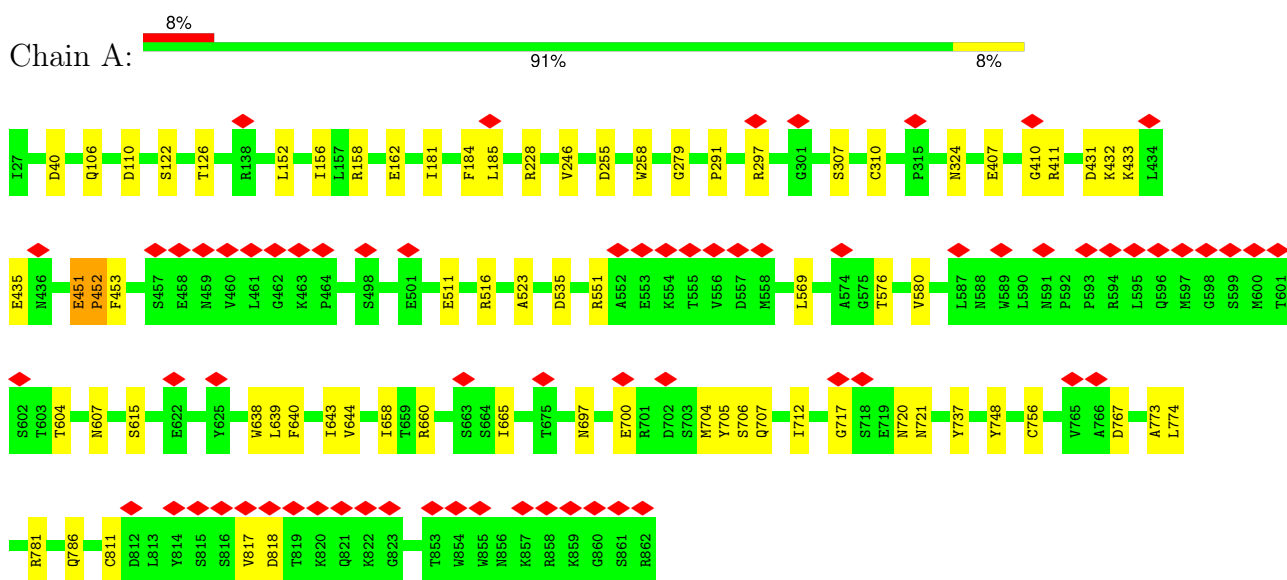
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			7	3	1	3	
2	D	1	Total	C	N	O	0
			7	3	1	3	

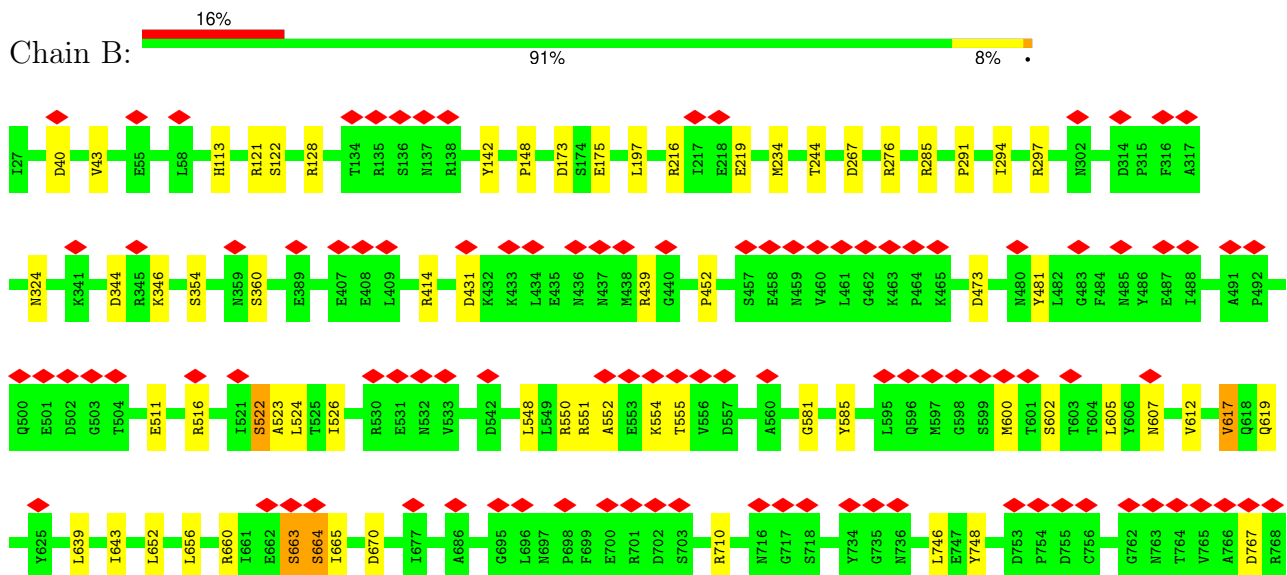
### 3 Residue-property plots

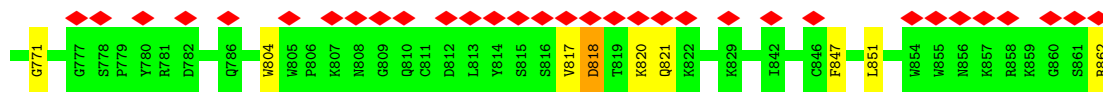
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor ionotropic, delta-2

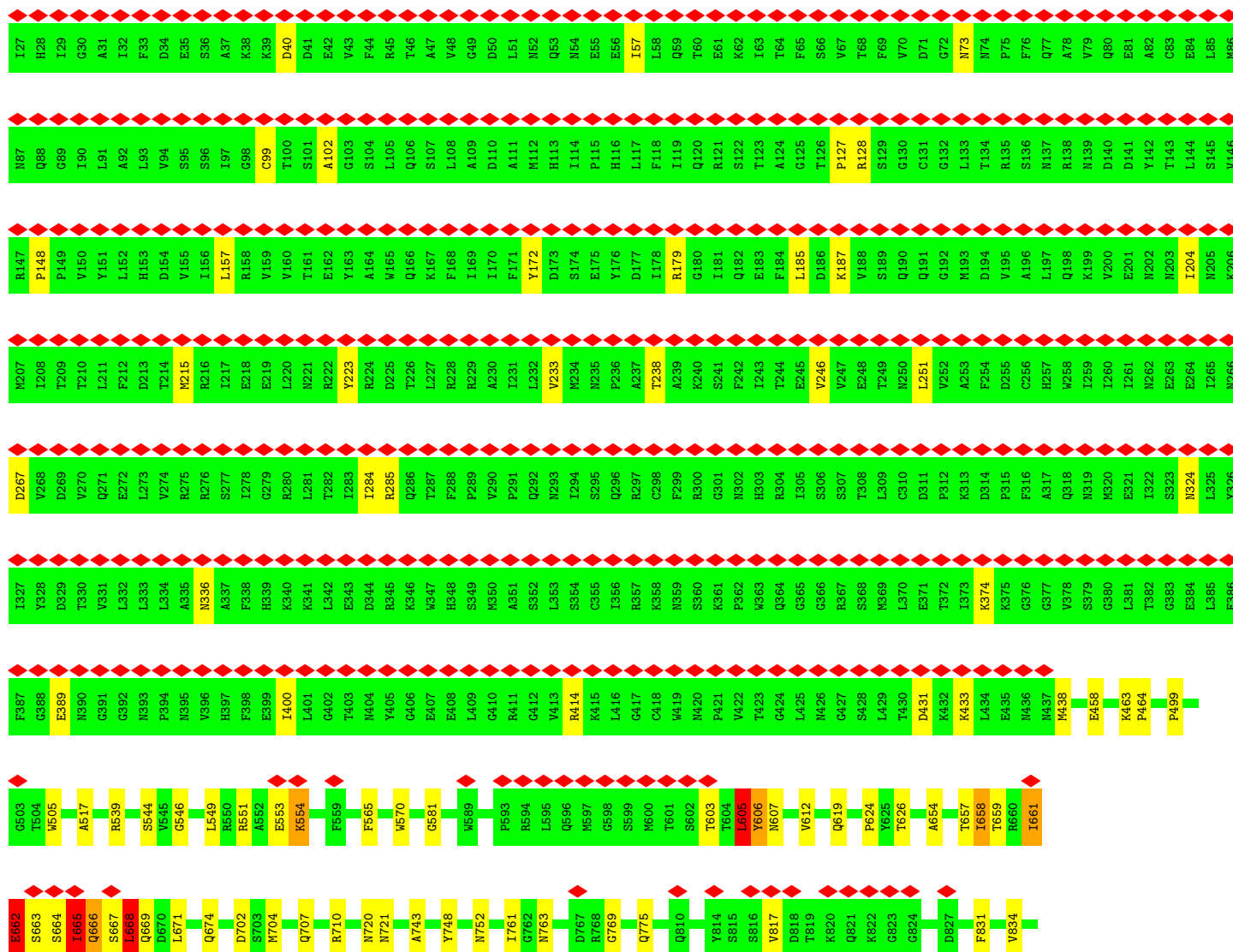
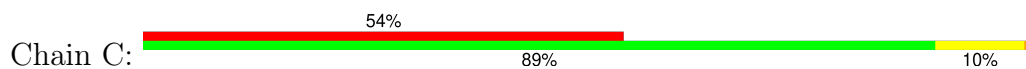


- Molecule 1: Glutamate receptor ionotropic, delta-2

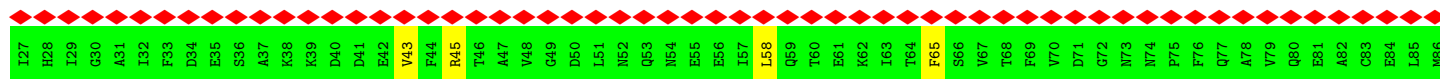
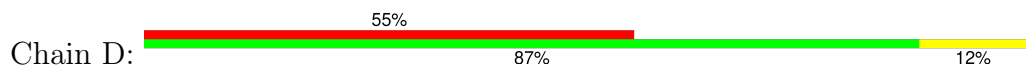




- Molecule 1: Glutamate receptor ionotropic, delta-2



- Molecule 1: Glutamate receptor ionotropic, delta-2



Q810	Q88	Q87	R147	M207	D267	I327	F387	M459	V606	Q810	Q88	Q87	R147	M207	D267	I327	F387	M459	V606
L813	G88	Q88	P148	I208	V268	Y328	G388	V460	M607	L813	G88	Q88	P148	I208	V268	Y328	G388	V460	M607
V817	G89	G89	P149	T209	D269	D329	E389	L461	V612	V817	G89	G89	P149	T209	D269	D329	E389	L461	V612
D816	I90	I90	V150	T210	V270	T330	N390	G462	V617	D816	I90	I90	V150	T210	V270	T330	N390	G462	V617
T819	L91	L91	Y151	L211	Q271	V331	G391	K463	V634	T819	L91	L91	Y151	L211	Q271	V331	G391	K463	V634
K820	A92	A92	L152	F212	E272	L332	G392	K465	V638	K820	A92	A92	L152	F212	E272	L332	G392	K465	V638
Q821	L93	L93	H153	D213	L273	L333	N393	P394	V639	Q821	L93	L93	H153	D213	L273	L333	N393	P394	V639
K822	V94	V94	D154	T214	V274	L334	N394	F484	V640	K822	V94	V94	D154	T214	V274	L334	N394	F484	V640
G823	S96	S96	I155	M215	R275	A335	N395	E487	V644	G823	S96	S96	I155	M215	R275	A335	N395	E487	V644
S845	I97	I97	L156	R216	R276	N336	V396	K495	V644	S845	I97	I97	L156	R216	R276	N336	V396	K495	V644
C846	G98	G98	L157	I217	S277	A337	H397	E501	V654	C846	G98	G98	L157	I217	S277	A337	H397	E501	V654
F847	C99	C99	R158	E218	I278	F338	F398	D502	V657	F847	C99	C99	R158	E218	I278	F338	F398	D502	V657
I848	T100	T100	V159	E219	G279	H339	E399	S503	V658	I848	T100	T100	V159	E219	G279	H339	E399	S503	V658
A849	S101	S101	T161	N221	L281	K341	L401	E507	V659	A849	S101	S101	T161	N221	L281	K341	L401	E507	V659
M850	A102	A102	E162	R222	T282	L342	G402	D509	V660	M850	A102	A102	E162	R222	T282	L342	G402	D509	V660
H854	G103	G103	Y163	Y223	I283	E343	I403	A517	V661	H854	G103	G103	Y163	Y223	I283	E343	I403	A517	V661
M855	S104	S104	A164	R224	I284	D344	M404	B516	V662	M855	S104	S104	A164	R224	I284	D344	M404	B516	V662
M856	L105	L105	W165	D225	R285	R345	Y405	I519	V663	M856	L105	L105	W165	D225	R285	R345	Y405	I519	V663
M857	Q106	Q106	Q166	T226	Q286	K346	G406	D529	V664	M857	Q106	Q106	Q166	T226	Q286	K346	G406	D529	V664
M858	S107	S107	K167	L227	T287	W347	E407	R530	V665	M858	S107	S107	K167	L227	T287	W347	E407	R530	V665
M859	L108	L108	F168	R228	F288	H348	E408	E531	V666	M859	L108	L108	F168	R228	F288	H348	E408	E531	V666
M860	A109	A109	I169	R229	P289	S349	L409	V534	V667	M860	A109	A109	I169	R229	P289	S349	L409	V534	V667
M861	D110	D110	I170	A230	V290	M350	G410	D535	V668	M861	D110	D110	I170	A230	V290	M350	G410	D535	V668
M862	A111	A111	F171	I231	P291	A351	R411	F536	V669	M862	A111	A111	F171	I231	P291	A351	R411	F536	V669
M112	M112	M112	Y172	I232	Q292	S352	G412	R539	V670	M112	M112	M112	Y172	I232	Q292	S352	G412	R539	V670
H113	H113	H113	D173	V233	N293	L353	V413	D542	V671	H113	H113	H113	D173	V233	N293	L353	V413	D542	V671
I114	I114	I114	S174	M234	I294	C354	R414	E553	V672	I114	I114	I114	S174	M234	I294	C354	R414	E553	V672
P115	P115	P115	E175	N235	S295	C355	M419	K554	V673	P115	P115	P115	E175	N235	S295	C355	M419	K554	V673
H116	H116	H116	Y176	P236	Q296	I356	N420	F565	V674	H116	H116	H116	Y176	P236	Q296	I356	N420	F565	V674
L117	L117	L117	D177	A237	R297	R357	G417	M570	V675	L117	L117	L117	D177	A237	R297	R357	G417	M570	V675
F118	F118	F118	I178	T238	C298	K358	C418	L562	V676	F118	F118	F118	I178	T238	C298	K358	C418	L562	V676
I119	I119	I119	R179	A239	F299	N359	M419	F565	V677	I119	I119	I119	R179	A239	F299	N359	M419	F565	V677
Q120	Q120	Q120	G180	R300	R300	S360	N420	L595	V678	Q120	Q120	Q120	G180	R300	R300	S360	N420	L595	V678
R121	R121	R121	I181	S241	G301	K361	P421	M570	V679	R121	R121	R121	I181	S241	G301	K361	P421	M570	V679
S122	S122	S122	Q182	N302	H303	P362	V422	G581	V680	S122	S122	S122	Q182	N302	H303	P362	V422	G581	V680
T123	T123	T123	E183	I243	H303	W363	G424	L586	V681	T123	T123	T123	E183	I243	H303	W363	G424	L586	V681
A124	A124	A124	F184	T244	R304	Q364	G424	P593	V682	A124	A124	A124	F184	T244	R304	Q364	G424	P593	V682
G125	G125	G125	L185	E245	I305	G365	L425	R594	V683	G125	G125	G125	L185	E245	I305	G365	L425	R594	V683
T126	T126	T126	D186	V246	S306	G366	M426	L595	V684	T126	T126	T126	D186	V246	S306	G366	M426	L595	V684
P127	P127	P127	K187	V247	S307	R367	G427	F596	V685	P127	P127	P127	K187	V247	S307	R367	G427	F596	V685
R128	R128	R128	V188	E248	S308	S368	S428	L597	V686	R128	R128	R128	V188	E248	S308	S368	S428	L597	V686
S129	S129	S129	S189	T249	L309	M369	L429	Q596	V687	S129	S129	S129	S189	T249	L309	M369	L429	Q596	V687
G130	G130	G130	Q190	N250	C310	L370	T430	M597	V688	G130	G130	G130	Q190	N250	C310	L370	T430	M597	V688
C131	C131	C131	Q191	L251	D311	E371	D431	G598	V689	C131	C131	C131	Q191	L251	D311	E371	D431	G598	V689
G132	G132	G132	G192	V252	P312	T372	K432	S599	V690	G132	G132	G132	G192	V252	P312	T372	K432	S599	V690
L133	L133	L133	M193	A253	K313	I373	K433	M600	V691	L133	L133	L133	M193	A253	K313	I373	K433	M600	V691
T134	T134	T134	D194	F254	D314	K374	L434	T601	V692	T134	T134	T134	D194	F254	D314	K374	L434	T601	V692
R135	R135	R135	V195	D255	F315	K375	M435	S602	V693	R135	R135	R135	V195	D255	F315	K375	M435	S602	V693
S136	S136	S136	A196	C256	F316	G376	M436	T603	V694	S136	S136	S136	A196	C256	F316	G376	M436	T603	V694
M137	M137	M137	L197	H257	A317	G377	M437	V604	V695	M137	M137	M137	L197	H257	A317	G377	M437	V604	V695
R138	R138	R138	Q198	W258	Q318	V378	M438	L605		R138	R138	R138	Q198	W258	Q318	V378	M438	L605	
M139	M139	M139	K199	I259	N319	S379	R439			M139	M139	M139	K199	I259	N319	S379	R439		
D140	D140	D140	V200	M320	G380	V440	G440			D140	D140	D140	V200	M320	G380	V440	G440		
D141	D141	D141	E201	I261	E321	L381	V441			D141	D141	D141	E201	I261	E321	L381	V441		
Y142	Y142	Y142	N202	N262	I322	T382	R442			Y142	Y142	Y142	N202	N262	I322	T382	R442		
T143	T143	T143	N203	E263	S323	G383	V443			T143	T143	T143	N203	E263	S323	G383	V443		
L144	L144	L144	I204	E264	N324	E384	V444			L144	L144	L144	I204	E264	N324	E384	V444		
S145	S145	S145	N205	I265	L325	L385	V445			S145	S145	S145	N205	I265	L325	L385	V445		
V146	V146	V146	K206	N266	Y326	E386				V146	V146	V146	K206	N266	Y326	E386			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69080	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.437	Depositor
Minimum map value	-0.299	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	407.40002, 407.40002, 407.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.14	0/6765	0.41	1/9171 (0.0%)
1	B	0.16	0/6765	0.39	0/9171
1	C	0.19	0/6765	0.41	1/9171 (0.0%)
1	D	0.17	0/6765	0.42	1/9171 (0.0%)
All	All	0.17	0/27060	0.41	3/36684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	605	LEU	N-CA-CB	6.25	119.42	110.16
1	D	431	ASP	N-CA-C	-5.47	107.86	114.75
1	A	451	GLU	C-N-CD	-5.23	103.54	125.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	817	VAL	Peptide
1	B	551	ARG	Sidechain
1	B	552	ALA	Peptide
1	B	664	SER	Peptide
1	C	551	ARG	Sidechain
1	C	817	VAL	Peptide
1	D	539	ARG	Sidechain

## 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	6625	0	6552	47	0
1	B	6625	0	6552	42	0
1	C	6625	0	6552	69	0
1	D	6625	0	6552	66	0
2	A	7	0	6	0	0
2	B	7	0	6	0	0
2	C	7	0	6	0	0
2	D	7	0	6	0	0
All	All	26528	0	26232	211	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 4.

All (211) 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:C:664:SER:CB	1:C:674:GLN:HG2	1.50	1.39
1:C:664:SER:HB3	1:C:674:GLN:CG	1.77	1.13
1:C:664:SER:CB	1:C:674:GLN:CG	2.34	1.05
1:C:665:ILE:HG12	1:C:761:ILE:HD13	1.55	0.87
1:C:664:SER:HB2	1:C:674:GLN:CG	2.08	0.83
1:C:664:SER:HB3	1:C:674:GLN:HG2	0.83	0.83
1:D:165:TRP:HZ2	1:D:257:HIS:HD2	1.28	0.81
1:D:657:THR:HG23	1:D:658:ILE:HG12	1.66	0.77
1:A:604:THR:OG1	1:A:607:ASN:ND2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:MET:HG2	1:A:705:TYR:H	1.57	0.69
1:C:664:SER:HB2	1:C:671:LEU:HA	1.75	0.68
1:B:817:VAL:HG23	1:B:818:ASP:H	1.59	0.68
1:A:451:GLU:O	1:A:453:PHE:N	2.26	0.67
1:D:581:GLY:HA2	1:D:612:VAL:HG21	1.76	0.66
1:B:40:ASP:OD2	1:B:121:ARG:NH2	2.30	0.65
1:B:581:GLY:HA2	1:B:612:VAL:HG21	1.77	0.65
1:D:267:ASP:OD1	1:D:285:ARG:NH1	2.23	0.62
1:C:223:TYR:OH	1:D:189:SER:O	2.17	0.62
1:C:605:LEU:C	1:C:607:ASN:N	2.55	0.62
1:A:535:ASP:OD2	1:A:781:ARG:NH1	2.32	0.61
1:C:664:SER:HB2	1:C:674:GLN:HG3	1.83	0.61
1:D:43:VAL:HG21	1:D:324:ASN:HB3	1.82	0.61
1:A:40:ASP:OD1	1:A:324:ASN:ND2	2.34	0.60
1:C:128:ARG:NH2	1:C:148:PRO:O	2.30	0.60
1:B:414:ARG:NH2	1:B:431:ASP:OD2	2.28	0.60
1:B:175:GLU:OE1	1:B:175:GLU:N	2.35	0.59
1:B:344:ASP:OD1	1:B:346:LYS:NZ	2.34	0.59
1:B:818:ASP:OD2	1:B:820:LYS:HG2	2.02	0.59
1:C:127:PRO:HG2	1:C:233:VAL:HG12	1.83	0.59
1:A:705:TYR:C	1:A:707:GLN:H	2.11	0.59
1:D:539:ARG:NH2	1:D:542:ASP:OD1	2.32	0.59
1:D:797:MET:O	1:D:801:LYS:NZ	2.28	0.59
1:C:664:SER:HB2	1:C:674:GLN:HG2	1.60	0.59
1:D:257:HIS:ND1	1:D:280:ARG:HB3	2.18	0.59
1:C:665:ILE:O	1:C:666:GLN:C	2.47	0.57
1:D:256:CYS:SG	1:D:258:TRP:NE1	2.77	0.57
1:D:640:PHE:O	1:D:644:VAL:HG23	2.03	0.57
1:B:522:SER:HB3	1:B:524:LEU:HD12	1.87	0.57
1:C:204:ILE:HD11	1:C:238:THR:HG23	1.87	0.57
1:A:432:LYS:HD3	1:A:435:GLU:HG3	1.87	0.57
1:D:750:ALA:HB1	1:D:813:LEU:HD22	1.87	0.56
1:B:660:ARG:NH1	1:D:654:ALA:O	2.39	0.56
1:C:215:MET:HE1	1:C:223:TYR:CD2	2.41	0.56
1:D:165:TRP:CZ2	1:D:257:HIS:HD2	2.16	0.56
1:A:639:LEU:O	1:A:643:ILE:HG12	2.06	0.56
1:B:511:GLU:OE2	1:B:516:ARG:NH1	2.34	0.56
1:C:246:VAL:HG13	1:C:251:LEU:HB2	1.87	0.56
1:C:581:GLY:HA2	1:C:612:VAL:HG21	1.87	0.56
1:D:817:VAL:HG22	1:D:818:ASP:H	1.71	0.56
1:C:665:ILE:CG1	1:C:761:ILE:HD13	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:ARG:NH1	1:D:593:PRO:O	2.39	0.55
1:B:600:MET:O	1:B:607:ASN:ND2	2.40	0.55
1:D:257:HIS:HE1	1:D:280:ARG:HH11	1.53	0.55
1:A:511:GLU:OE2	1:A:516:ARG:NH1	2.33	0.54
1:C:664:SER:O	1:C:665:ILE:C	2.50	0.54
1:A:615:SER:HB2	1:A:638:TRP:HE1	1.73	0.54
1:B:128:ARG:NH2	1:B:148:PRO:O	2.39	0.53
1:B:216:ARG:HB2	1:B:219:GLU:OE1	2.09	0.53
1:D:634:MET:HE3	1:D:638:TRP:HE1	1.74	0.53
1:D:439:ARG:NH2	1:D:487:GLU:OE2	2.41	0.53
1:A:291:PRO:HG2	1:A:297:ARG:HA	1.91	0.52
1:C:267:ASP:OD1	1:C:285:ARG:NH1	2.30	0.52
1:C:605:LEU:C	1:C:607:ASN:H	2.18	0.52
1:A:152:LEU:O	1:A:156:ILE:HG12	2.09	0.52
1:D:536:PHE:O	1:D:781:ARG:NE	2.42	0.52
1:D:665:ILE:HD11	1:D:674:GLN:HG2	1.92	0.52
1:C:624:PRO:O	1:C:626:THR:HG23	2.10	0.52
1:A:638:TRP:CD1	1:C:619:GLN:HG3	2.46	0.51
1:A:185:LEU:HD22	1:B:197:LEU:HB2	1.93	0.51
1:B:473:ASP:OD2	1:B:804:TRP:NE1	2.36	0.51
1:A:697:ASN:OD1	1:A:700:GLU:HG3	2.11	0.51
1:A:569:LEU:HD21	1:C:831:PHE:HE1	1.75	0.50
1:C:662:GLU:HG2	1:C:666:GLN:OE1	2.11	0.50
1:C:661:ILE:HD12	1:C:663:SER:H	1.76	0.50
1:B:660:ARG:HG3	1:B:821:GLN:O	2.11	0.50
1:C:707:GLN:HE22	1:C:710:ARG:HH21	1.59	0.50
1:A:717:GLY:O	1:A:721:ASN:ND2	2.37	0.49
1:B:113:HIS:ND1	1:B:142:TYR:OH	2.45	0.49
1:D:443:LEU:O	1:D:487:GLU:N	2.29	0.49
1:B:585:TYR:CE2	1:B:605:LEU:HD22	2.48	0.49
1:C:517:ALA:O	1:C:775:GLN:NE2	2.32	0.49
1:B:663:SER:OG	1:B:664:SER:N	2.45	0.49
1:A:640:PHE:O	1:A:644:VAL:HG23	2.13	0.48
1:D:120:GLN:OE1	1:D:128:ARG:NH1	2.37	0.48
1:D:246:VAL:HG13	1:D:251:LEU:HB2	1.95	0.48
1:B:665:ILE:HA	1:B:670:ASP:OD2	2.13	0.48
1:C:284:ILE:HG23	1:C:400:ILE:HG12	1.95	0.48
1:C:720:ASN:C	1:C:721:ASN:HD22	2.21	0.48
1:D:665:ILE:HG21	1:D:671:LEU:HB2	1.95	0.48
1:D:284:ILE:HG13	1:D:400:ILE:HG23	1.95	0.48
1:A:432:LYS:HE2	1:A:786:GLN:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:LYS:HG3	1:C:464:PRO:HD2	1.94	0.48
1:B:639:LEU:O	1:B:643:ILE:HG13	2.15	0.47
1:A:720:ASN:O	1:A:737:TYR:OH	2.27	0.47
1:A:122:SER:OG	1:A:126:THR:O	2.29	0.47
1:C:605:LEU:O	1:C:607:ASN:N	2.48	0.47
1:C:414:ARG:NH2	1:C:431:ASP:OD2	2.47	0.47
1:B:121:ARG:HG2	1:B:122:SER:N	2.29	0.47
1:A:246:VAL:HG11	1:A:258:TRP:CH2	2.50	0.47
1:C:661:ILE:H	1:C:661:ILE:HG13	1.34	0.47
1:B:526:ILE:HD11	1:B:771:GLY:HA3	1.97	0.46
1:A:106:GLN:NE2	1:A:110:ASP:OD2	2.39	0.46
1:A:453:PHE:CD2	1:A:523:ALA:HB2	2.51	0.46
1:D:529:ASP:OD1	1:D:529:ASP:N	2.48	0.46
1:D:152:LEU:HD11	1:D:263:GLU:HG3	1.98	0.46
1:A:307:SER:HA	1:A:310:CYS:SG	2.56	0.46
1:A:551:ARG:NH2	1:A:756:CYS:SG	2.80	0.46
1:D:441:VAL:HB	1:D:484:PHE:HA	1.97	0.46
1:D:639:LEU:O	1:D:643:ILE:HG13	2.16	0.46
1:A:704:MET:HG2	1:A:705:TYR:N	2.29	0.46
1:C:539:ARG:HD2	1:C:769:GLY:HA3	1.98	0.46
1:D:165:TRP:HZ2	1:D:257:HIS:CD2	2.18	0.46
1:A:181:ILE:O	1:A:184:PHE:HD1	1.98	0.46
1:C:654:ALA:O	1:C:657:THR:HG23	2.15	0.46
1:A:228:ARG:NE	1:A:255:ASP:OD2	2.47	0.45
1:A:452:PRO:HD3	1:A:748:TYR:CD2	2.52	0.45
1:D:531:GLU:HA	1:D:534:VAL:O	2.14	0.45
1:C:157:LEU:HD22	1:C:187:LYS:HD3	1.97	0.45
1:A:705:TYR:O	1:A:707:GLN:N	2.41	0.45
1:D:274:VAL:HG13	1:D:403:THR:HG22	1.98	0.45
1:D:262:ASN:HB3	1:D:265:ILE:HG13	1.98	0.45
1:D:416:LEU:HB3	1:D:429:LEU:HD22	1.99	0.45
1:B:173:ASP:HB3	1:B:234:MET:HB2	1.99	0.45
1:D:661:ILE:HD12	1:D:661:ILE:HA	1.80	0.45
1:C:458:GLU:OE1	1:C:463:LYS:NZ	2.49	0.45
1:C:99:CYS:HA	1:C:102:ALA:HB3	1.99	0.44
1:C:544:SER:OG	1:C:763:ASN:O	2.30	0.44
1:D:225:ASP:OD1	1:D:228:ARG:NH1	2.48	0.44
1:C:748:TYR:O	1:C:752:ASN:ND2	2.37	0.44
1:D:809:GLY:O	1:D:810:GLN:C	2.60	0.44
1:D:117:LEU:HD22	1:D:330:THR:HG23	1.98	0.44
1:C:664:SER:OG	1:C:665:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:ALA:O	1:D:775:GLN:NE2	2.41	0.44
1:C:57:ILE:HD13	1:C:336:ASN:HD21	1.82	0.44
1:C:374:LYS:HE2	1:C:389:GLU:HA	2.00	0.44
1:C:669:GLN:HA	1:C:704:MET:SD	2.57	0.44
1:A:158:ARG:O	1:A:162:GLU:HG2	2.17	0.44
1:A:658:ILE:HG21	1:C:659:THR:HG21	1.98	0.44
1:C:172:TYR:OH	1:D:186:ASP:OD1	2.28	0.44
1:D:495:LYS:HD3	1:D:684:ASP:OD2	2.18	0.44
1:C:657:THR:O	1:C:658:ILE:C	2.61	0.43
1:D:443:LEU:HD13	1:D:519:ILE:HD12	1.99	0.43
1:B:40:ASP:OD1	1:B:324:ASN:ND2	2.51	0.43
1:C:702:ASP:OD2	1:C:704:MET:HB3	2.18	0.43
1:B:452:PRO:HB3	1:B:748:TYR:CE2	2.52	0.43
1:C:73:ASN:HB2	1:D:136:SER:HB2	2.00	0.43
1:C:846:CYS:O	1:C:850:MET:HG2	2.18	0.43
1:B:121:ARG:HG2	1:B:122:SER:H	1.83	0.43
1:C:662:GLU:CG	1:C:666:GLN:OE1	2.67	0.43
1:D:565:PHE:HB2	1:D:570:TRP:NE1	2.33	0.43
1:C:707:GLN:NE2	1:C:710:ARG:HH21	2.16	0.43
1:D:535:ASP:OD2	1:D:777:GLY:N	2.43	0.43
1:D:603:THR:HB	1:D:607:ASN:HB2	2.00	0.43
1:C:215:MET:HE1	1:C:223:TYR:CE2	2.54	0.43
1:C:40:ASP:OD1	1:C:324:ASN:ND2	2.44	0.43
1:D:45:ARG:HG2	1:D:65:PHE:CZ	2.54	0.43
1:D:797:MET:O	1:D:797:MET:HG3	2.18	0.43
1:C:185:LEU:HD13	1:D:197:LEU:HD22	2.01	0.42
1:C:57:ILE:HD13	1:C:336:ASN:ND2	2.35	0.42
1:D:142:TYR:CD2	1:D:370:LEU:HD22	2.54	0.42
1:C:605:LEU:O	1:C:606:TYR:C	2.62	0.42
1:B:43:VAL:HG21	1:B:324:ASN:HB3	2.01	0.42
1:C:179:ARG:HA	1:D:178:ILE:HD11	2.00	0.42
1:D:617:VAL:O	1:D:617:VAL:HG12	2.19	0.42
1:A:432:LYS:HE3	1:A:432:LYS:HB3	1.83	0.42
1:D:435:GLU:HB2	1:D:441:VAL:HG12	2.02	0.42
1:A:811:CYS:HA	1:B:710:ARG:NH2	2.35	0.42
1:B:548:LEU:HB2	1:B:746:LEU:HD13	2.01	0.42
1:B:652:LEU:O	1:B:656:LEU:HG	2.19	0.42
1:D:717:GLY:O	1:D:721:ASN:ND2	2.43	0.42
1:A:451:GLU:C	1:A:453:PHE:H	2.21	0.42
1:B:291:PRO:HB2	1:B:297:ARG:HG2	2.02	0.42
1:C:546:GLY:HA3	1:C:743:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LYS:NZ	1:A:435:GLU:OE2	2.38	0.41
1:A:640:PHE:CE1	1:C:834:VAL:HG12	2.54	0.41
1:B:522:SER:OG	1:B:523:ALA:N	2.53	0.41
1:D:662:GLU:HB2	1:D:663:SER:H	1.62	0.41
1:B:244:THR:OG1	1:B:276:ARG:NH1	2.44	0.41
1:B:267:ASP:OD1	1:B:285:ARG:NH1	2.45	0.41
1:B:617:VAL:O	1:B:619:GLN:HG3	2.20	0.41
1:C:549:LEU:HD22	1:C:665:ILE:HB	2.02	0.41
1:C:565:PHE:HB2	1:C:570:TRP:NE1	2.35	0.41
1:A:432:LYS:HD2	1:A:433:LYS:O	2.21	0.41
1:A:712:ILE:O	1:A:717:GLY:HA2	2.19	0.41
1:A:279:GLY:C	1:A:411:ARG:HH22	2.28	0.41
1:A:576:THR:O	1:A:580:VAL:HG23	2.20	0.41
1:A:660:ARG:H	1:A:660:ARG:HG2	1.64	0.41
1:D:120:GLN:O	1:D:147:ARG:NH1	2.50	0.41
1:D:121:ARG:NH1	1:D:323:SER:OG	2.54	0.41
1:D:819:THR:O	1:D:822:LYS:NZ	2.53	0.41
1:D:201:GLU:O	1:D:204:ILE:HG13	2.21	0.41
1:D:204:ILE:HG23	1:D:208:ILE:HD12	2.02	0.41
1:D:445:VAL:N	1:D:487:GLU:O	2.51	0.41
1:B:294:ILE:HD12	1:B:294:ILE:H	1.86	0.41
1:B:439:ARG:NH1	1:B:481:TYR:O	2.53	0.41
1:D:327:ILE:O	1:D:331:VAL:HG23	2.21	0.41
1:A:705:TYR:C	1:A:707:GLN:N	2.75	0.40
1:C:554:LYS:HG2	1:C:658:ILE:HG23	2.03	0.40
1:C:662:GLU:HG3	1:C:665:ILE:HD13	2.04	0.40
1:B:818:ASP:CG	1:B:820:LYS:HG2	2.46	0.40
1:C:499:PRO:HD3	1:C:505:TRP:CH2	2.56	0.40
1:A:407:GLU:C	1:A:410:GLY:H	2.28	0.40
1:B:847:PHE:CE2	1:B:851:LEU:HD11	2.56	0.40
1:D:741:TRP:HA	1:D:741:TRP:CE3	2.56	0.40
1:C:603:THR:HG23	1:C:607:ASN:HB2	2.02	0.40
1:C:668:LEU:HD23	1:C:668:LEU:HA	1.74	0.40
1:A:431:ASP:C	1:A:433:LYS:H	2.30	0.40
1:A:773:ALA:C	1:A:774:LEU:HD12	2.46	0.40
1:B:354:SER:O	1:B:360:SER:OG	2.39	0.40
1:D:112:MET:HE3	1:D:353:LEU:HD13	2.02	0.40
1:D:242:PHE:CE1	1:D:246:VAL:HG21	2.56	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	834/836 (100%)	767 (92%)	62 (7%)	5 (1%)	22	54
1	B	834/836 (100%)	786 (94%)	42 (5%)	6 (1%)	19	51
1	C	834/836 (100%)	776 (93%)	49 (6%)	9 (1%)	12	43
1	D	834/836 (100%)	776 (93%)	53 (6%)	5 (1%)	22	54
All	All	3336/3344 (100%)	3105 (93%)	206 (6%)	25 (1%)	21	51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	452	PRO
1	C	665	ILE
1	B	663	SER
1	C	433	LYS
1	C	658	ILE
1	C	662	GLU
1	C	666	GLN
1	D	58	LEU
1	A	706	SER
1	A	818	ASP
1	C	667	SER
1	C	668	LEU
1	A	665	ILE
1	A	767	ASP
1	B	602	SER
1	B	767	ASP
1	D	662	GLU
1	D	665	ILE
1	B	522	SER
1	B	818	ASP
1	C	438	MET
1	C	606	TYR

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Mol	Chain	Res	Type
1	D	432	LYS
1	D	658	ILE
1	B	617	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/726 (100%)	726 (100%)	0	100	100
1	B	726/726 (100%)	723 (100%)	3 (0%)	89	93
1	C	726/726 (100%)	719 (99%)	7 (1%)	73	82
1	D	726/726 (100%)	720 (99%)	6 (1%)	79	85
All	All	2904/2904 (100%)	2888 (99%)	16 (1%)	82	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	550	ARG
1	B	554	LYS
1	B	555	THR
1	C	553	GLU
1	C	554	LYS
1	C	605	LEU
1	C	661	ILE
1	C	662	GLU
1	C	665	ILE
1	C	668	LEU
1	D	661	ILE
1	D	662	GLU
1	D	663	SER
1	D	665	ILE
1	D	666	GLN
1	D	810	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	A	607	ASN
1	B	397	HIS
1	B	666	GLN
1	B	716	ASN
1	C	73	ASN
1	C	336	ASN
1	C	494	HIS
1	C	669	GLN
1	C	736	ASN
1	D	106	GLN
1	D	339	HIS
1	D	459	ASN
1	D	669	GLN
1	D	690	HIS
1	D	763	ASN
1	D	776	HIS
1	D	808	ASN

### 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	$\# Z  > 2$
2	DSN	C	901	-	4,6,6	1.22	1 (25%)	2,7,7	1.84	1 (50%)
2	DSN	D	901	-	4,6,6	1.17	1 (25%)	2,7,7	1.98	1 (50%)
2	DSN	B	901	-	4,6,6	1.17	1 (25%)	2,7,7	1.93	1 (50%)
2	DSN	A	901	-	4,6,6	1.17	1 (25%)	2,7,7	1.94	1 (50%)

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	DSN	C	901	-	-	0/6/6/6	-
2	DSN	D	901	-	-	0/6/6/6	-
2	DSN	B	901	-	-	0/6/6/6	-
2	DSN	A	901	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	DSN	OXT-C	-2.35	1.23	1.30
2	A	901	DSN	OXT-C	-2.24	1.23	1.30
2	D	901	DSN	OXT-C	-2.24	1.23	1.30
2	B	901	DSN	OXT-C	-2.23	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	DSN	OXT-C-O	-2.79	117.76	124.08
2	A	901	DSN	OXT-C-O	-2.72	117.90	124.08
2	B	901	DSN	OXT-C-O	-2.69	117.97	124.08
2	C	901	DSN	OXT-C-O	-2.59	118.20	124.08

There are no chirality outliers.

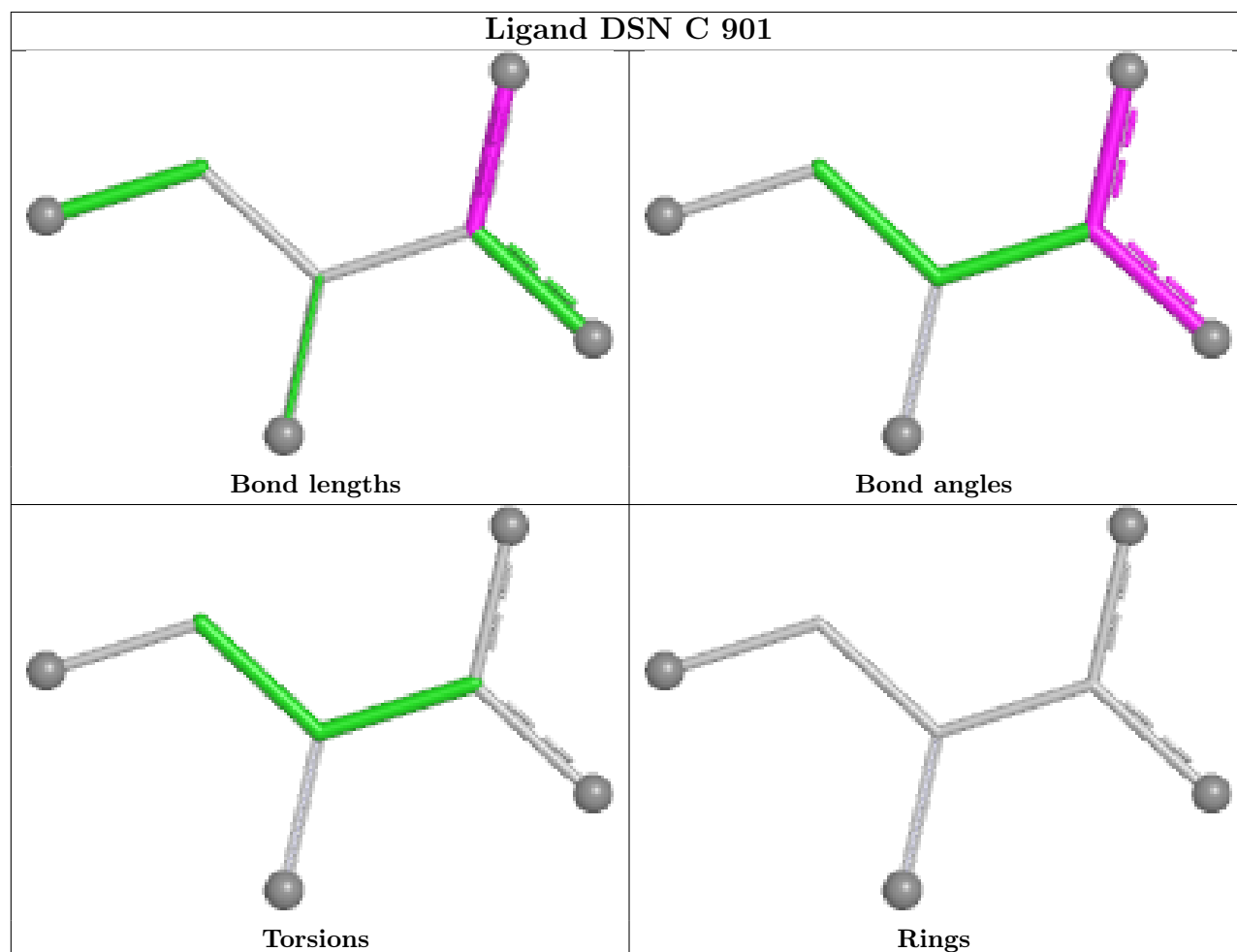
There are no torsion outliers.

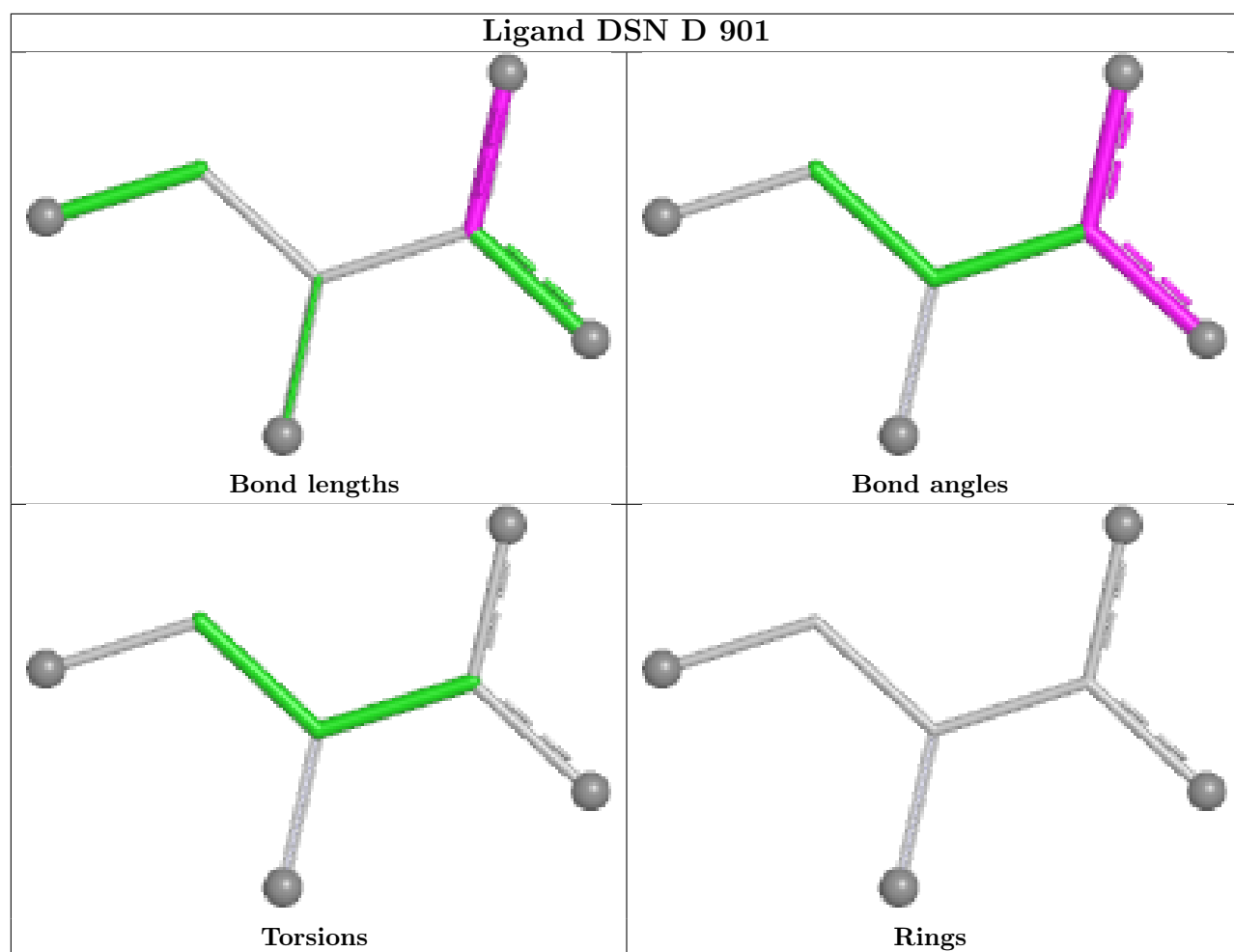
There are no ring outliers.

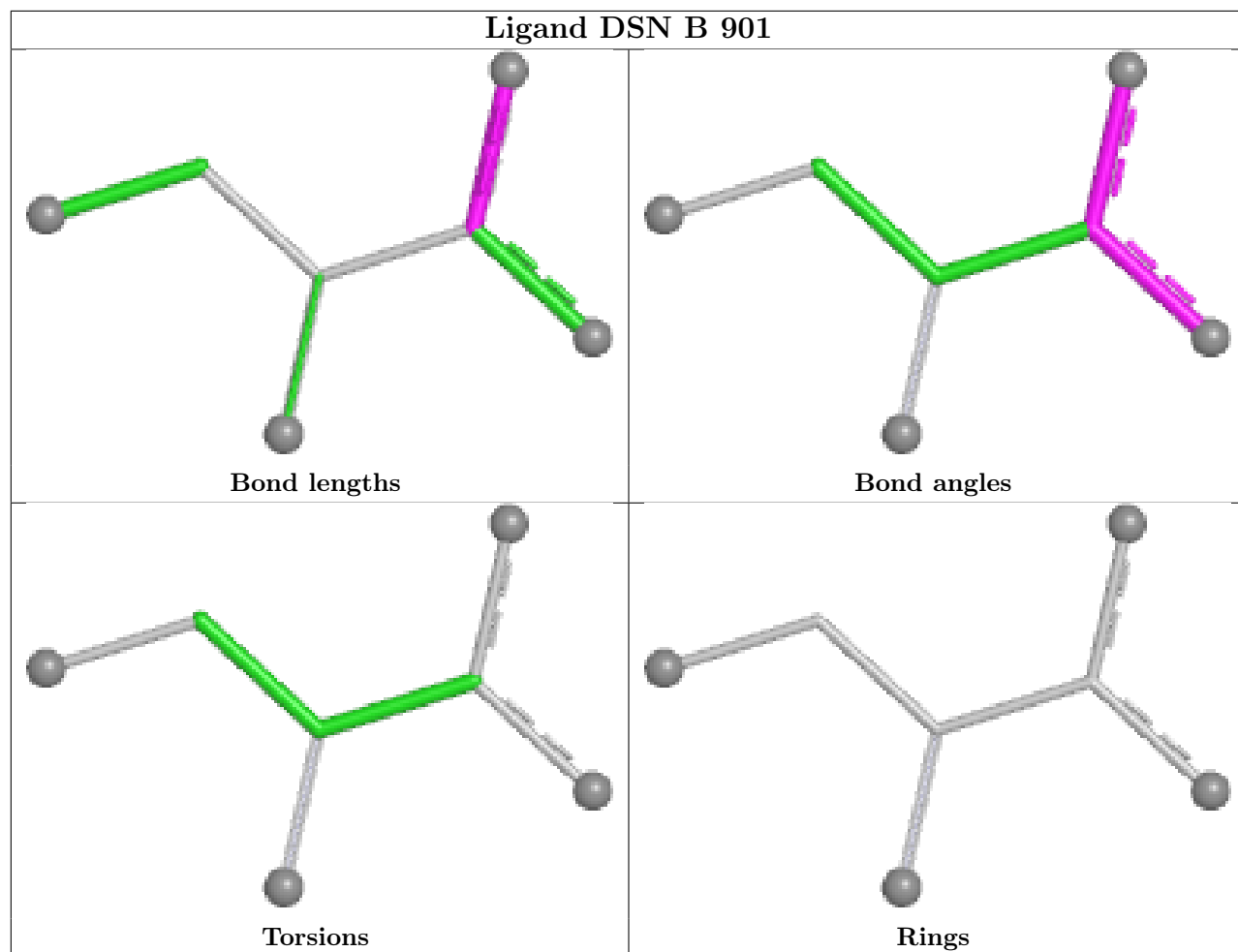
No monomer is involved in short contacts.

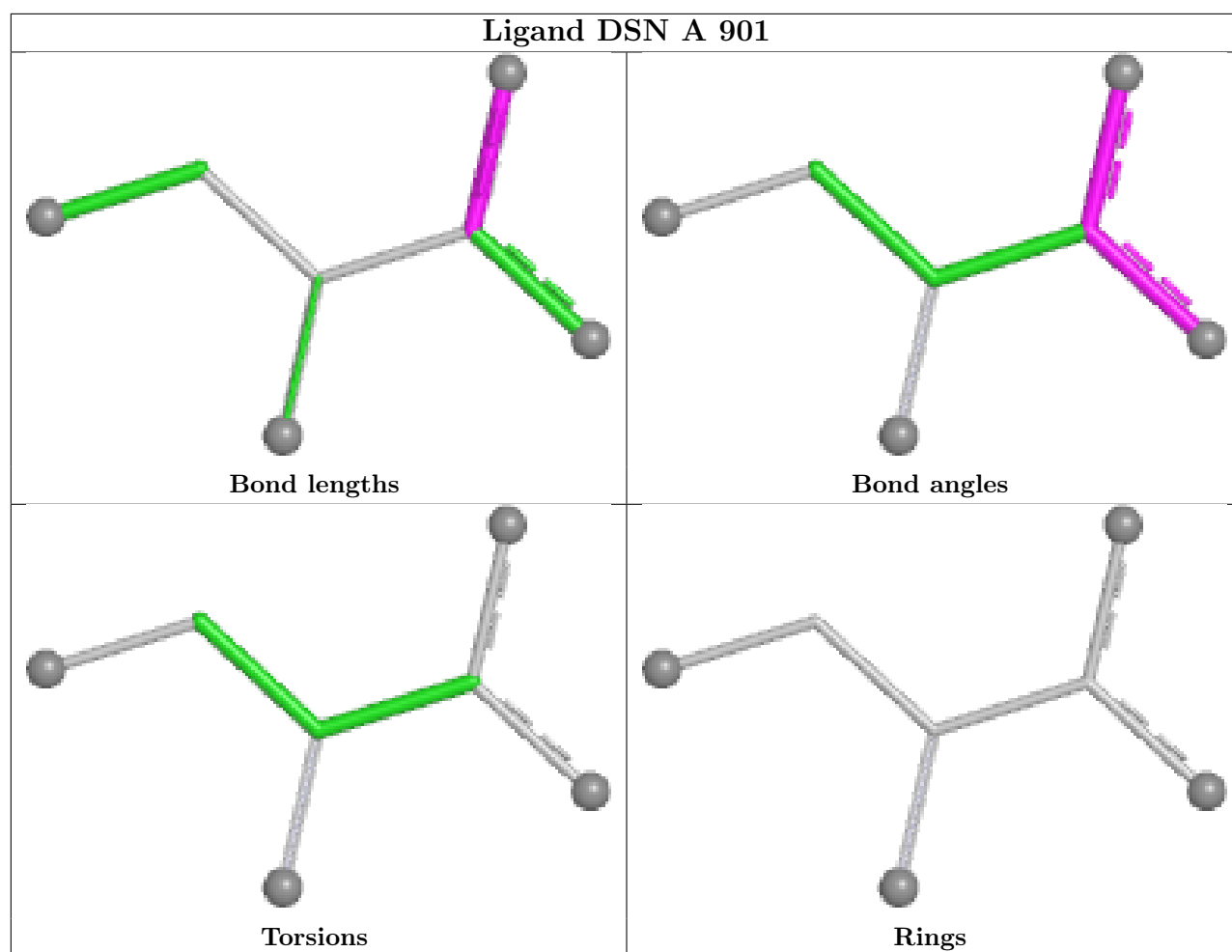
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

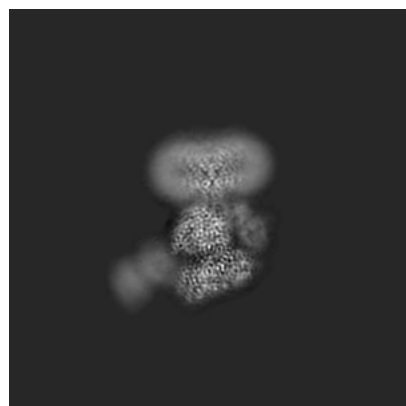
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49889. These allow visual inspection of the internal detail of the map and identification of artifacts.

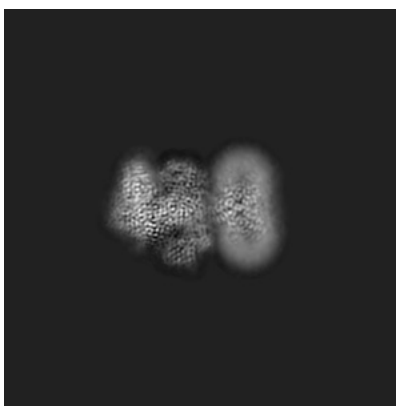
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

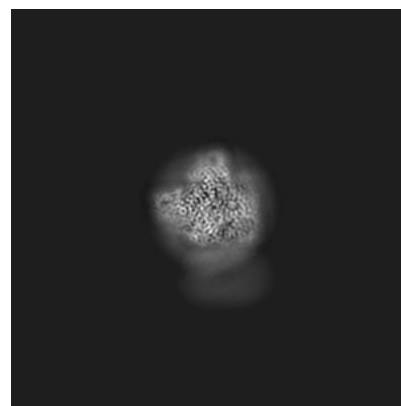
#### 6.1.1 Primary map



X

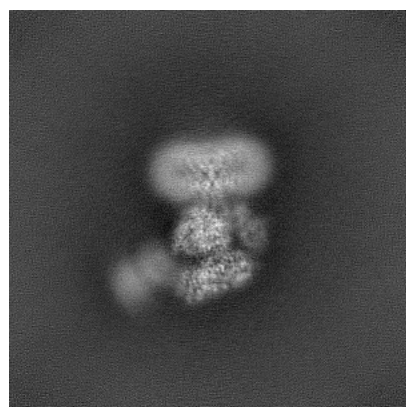


Y

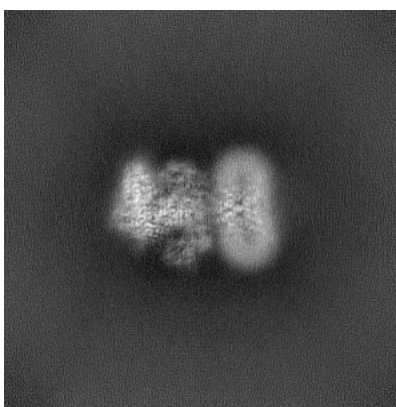


Z

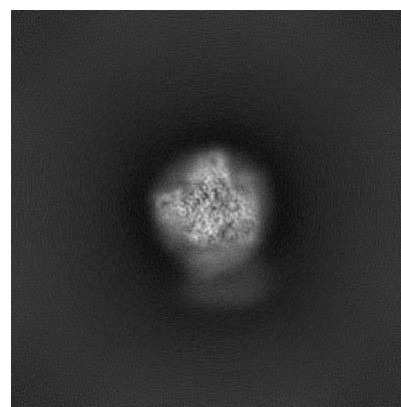
#### 6.1.2 Raw map



X



Y



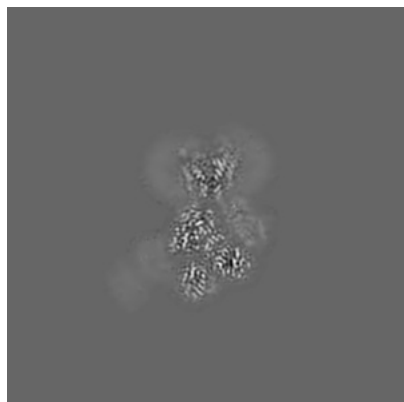
Z

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

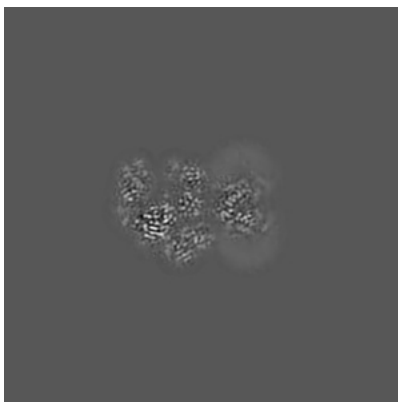


## 6.2 Central slices [i](#)

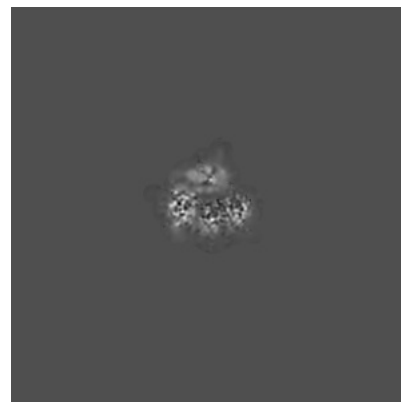
### 6.2.1 Primary map



X Index: 210

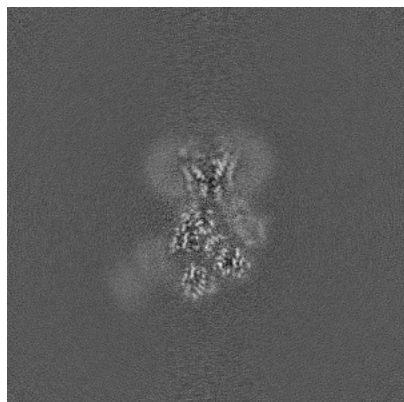


Y Index: 210

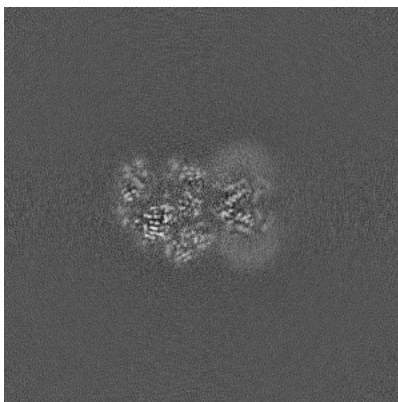


Z Index: 210

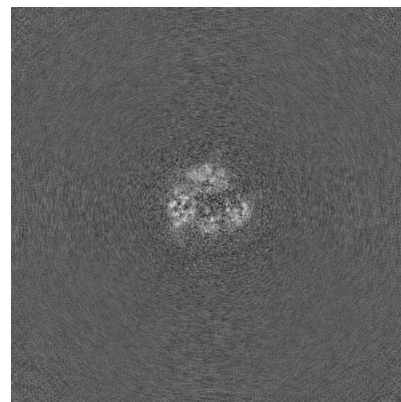
### 6.2.2 Raw map



X Index: 210



Y Index: 210

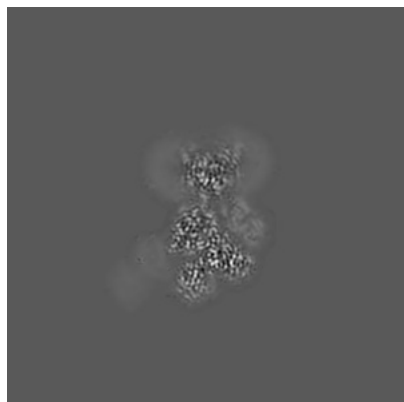


Z Index: 210

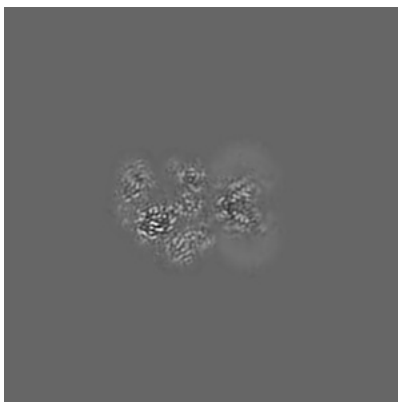
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

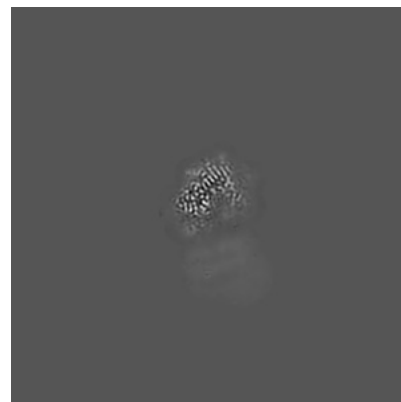
### 6.3.1 Primary map



X Index: 206

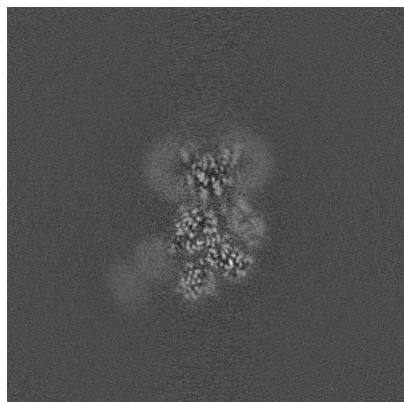


Y Index: 212

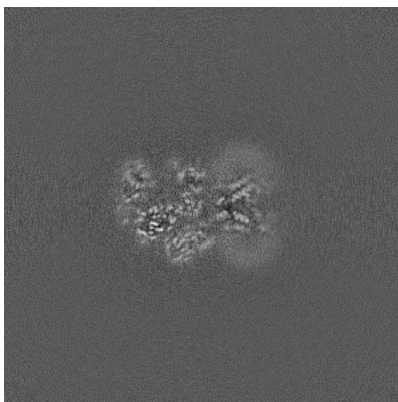


Z Index: 153

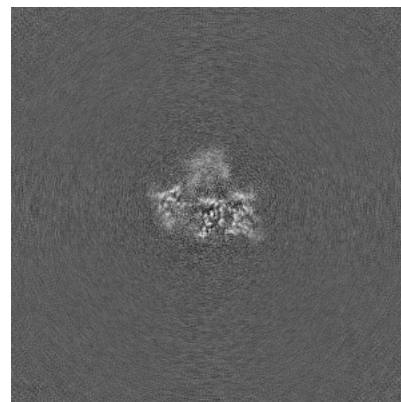
### 6.3.2 Raw map



X Index: 207



Y Index: 212

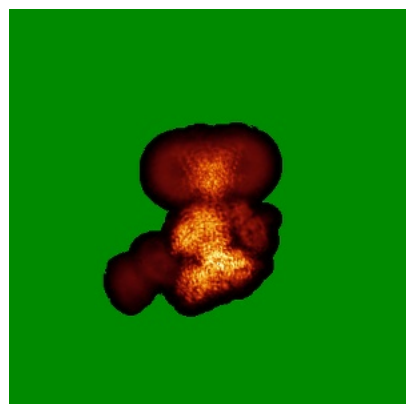


Z Index: 193

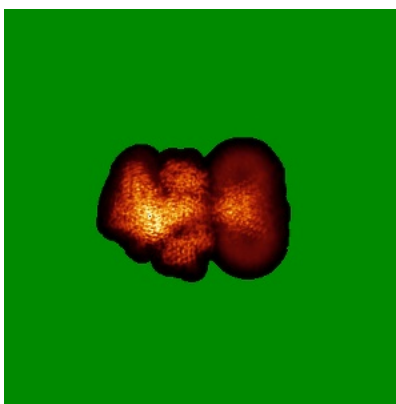
The images above show the largest variance slices of the map in three orthogonal directions.

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

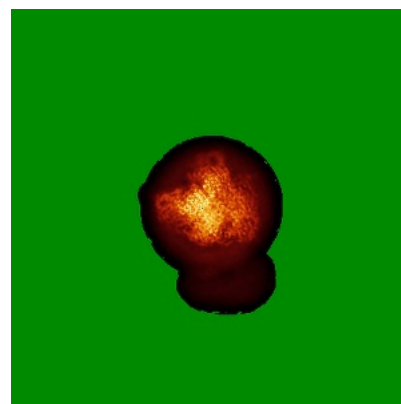
### 6.4.1 Primary map



X

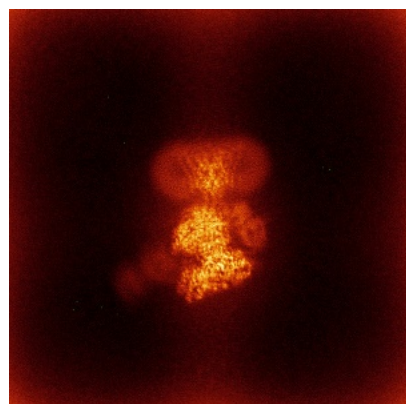


Y

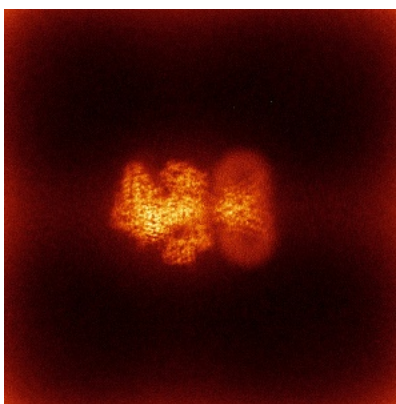


Z

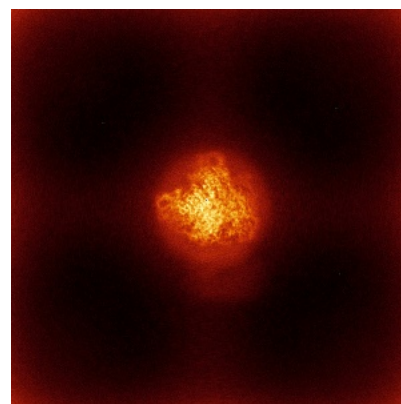
### 6.4.2 Raw map



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.

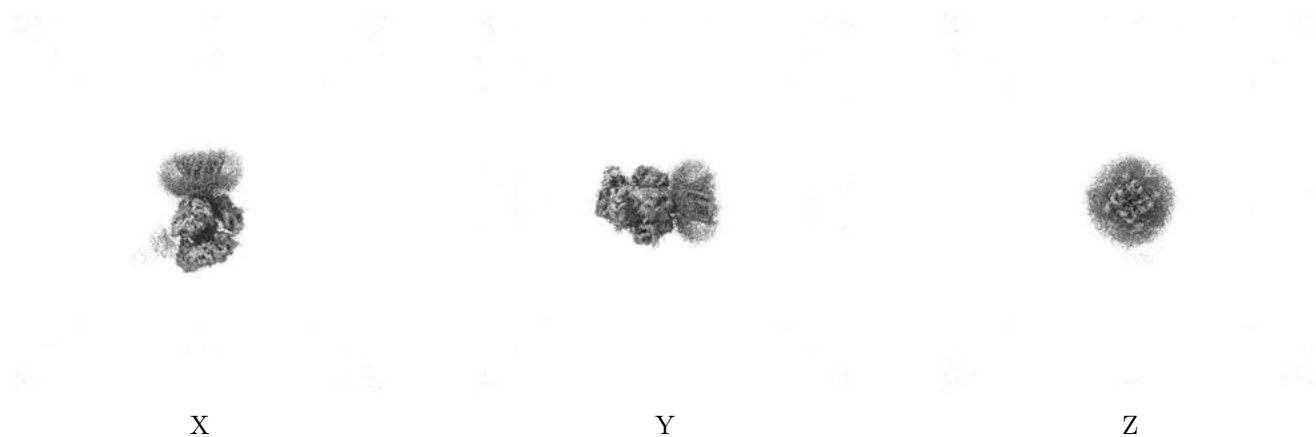
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

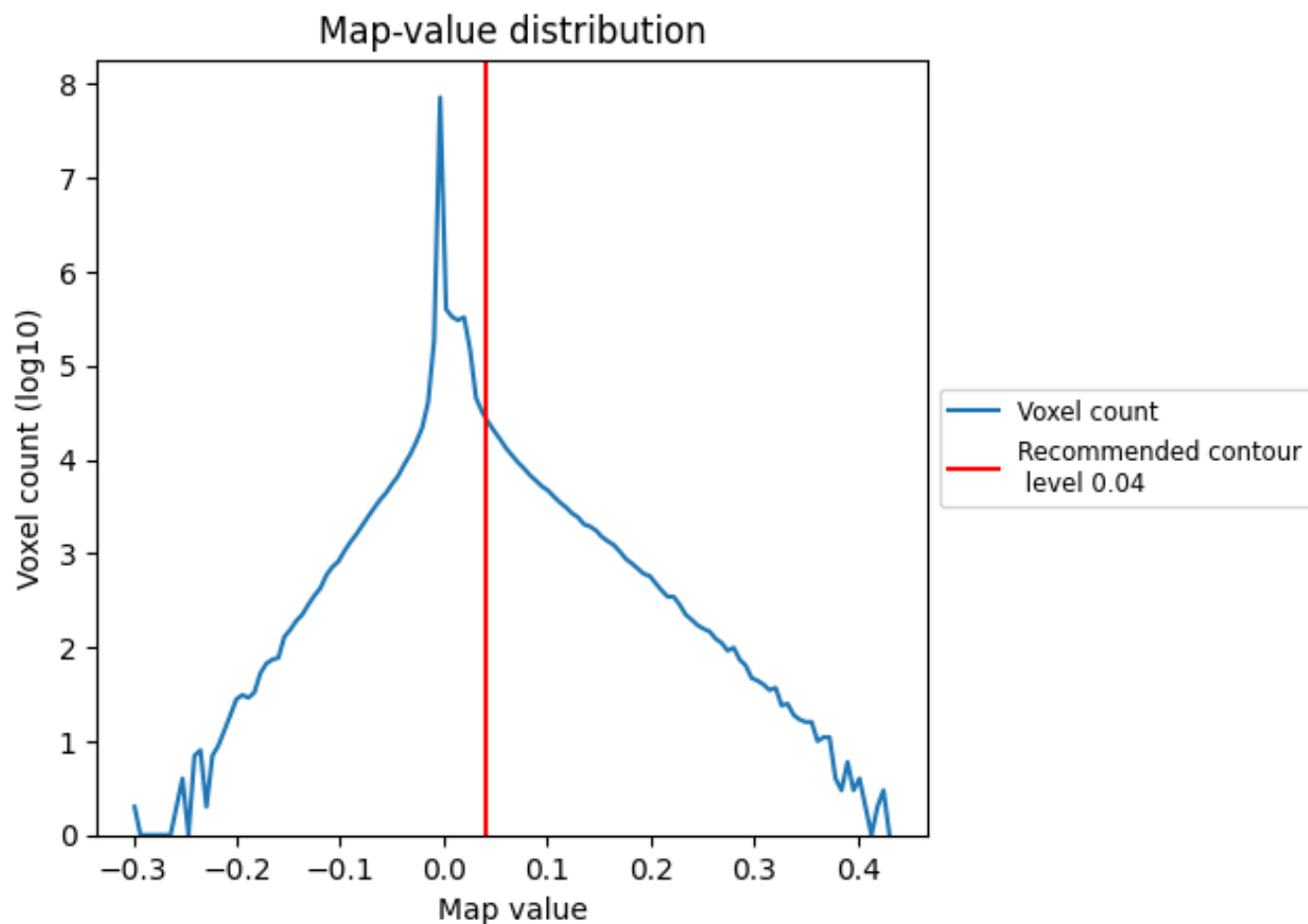
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

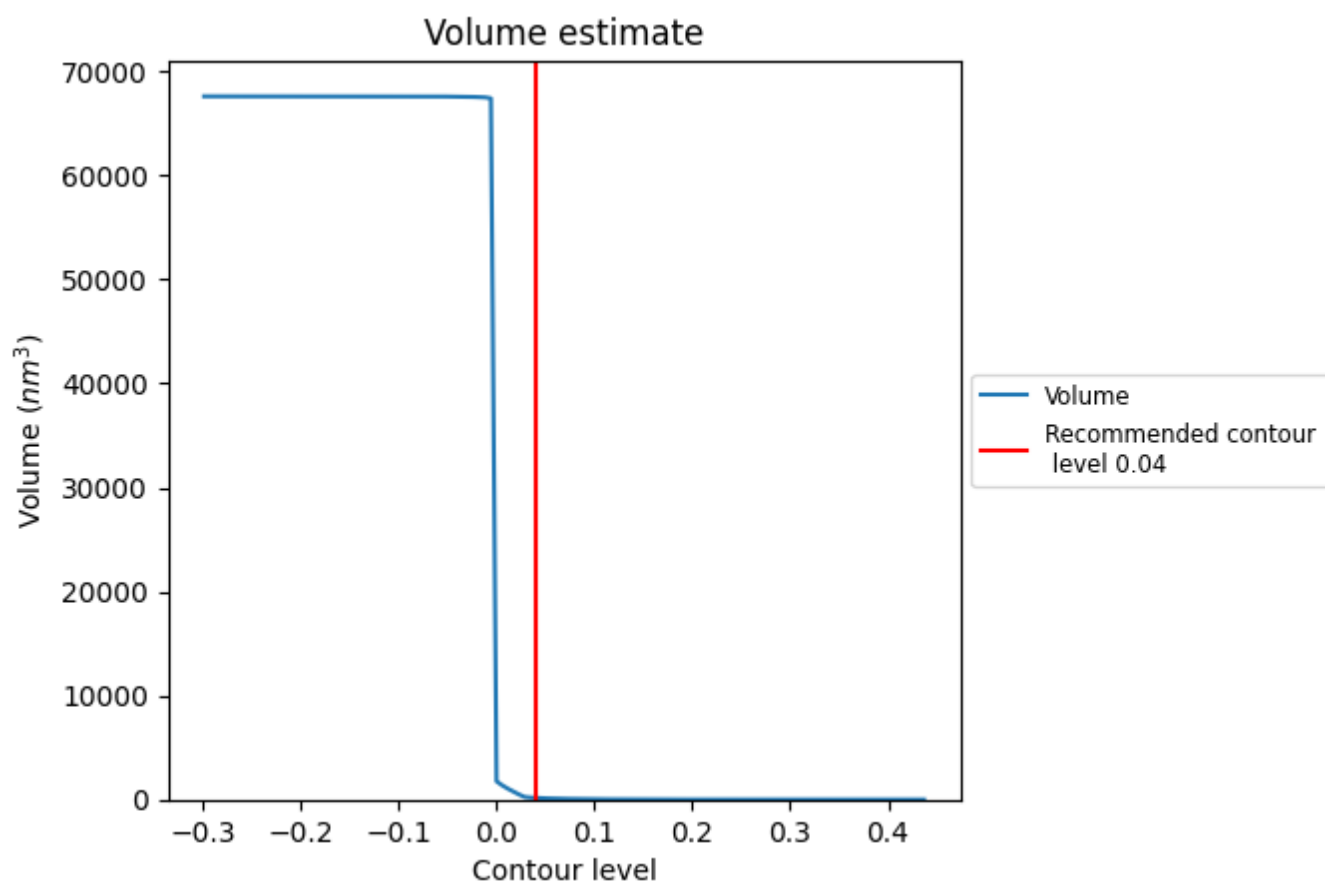
This section contains the results of statistical analysis of the map.

### 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.

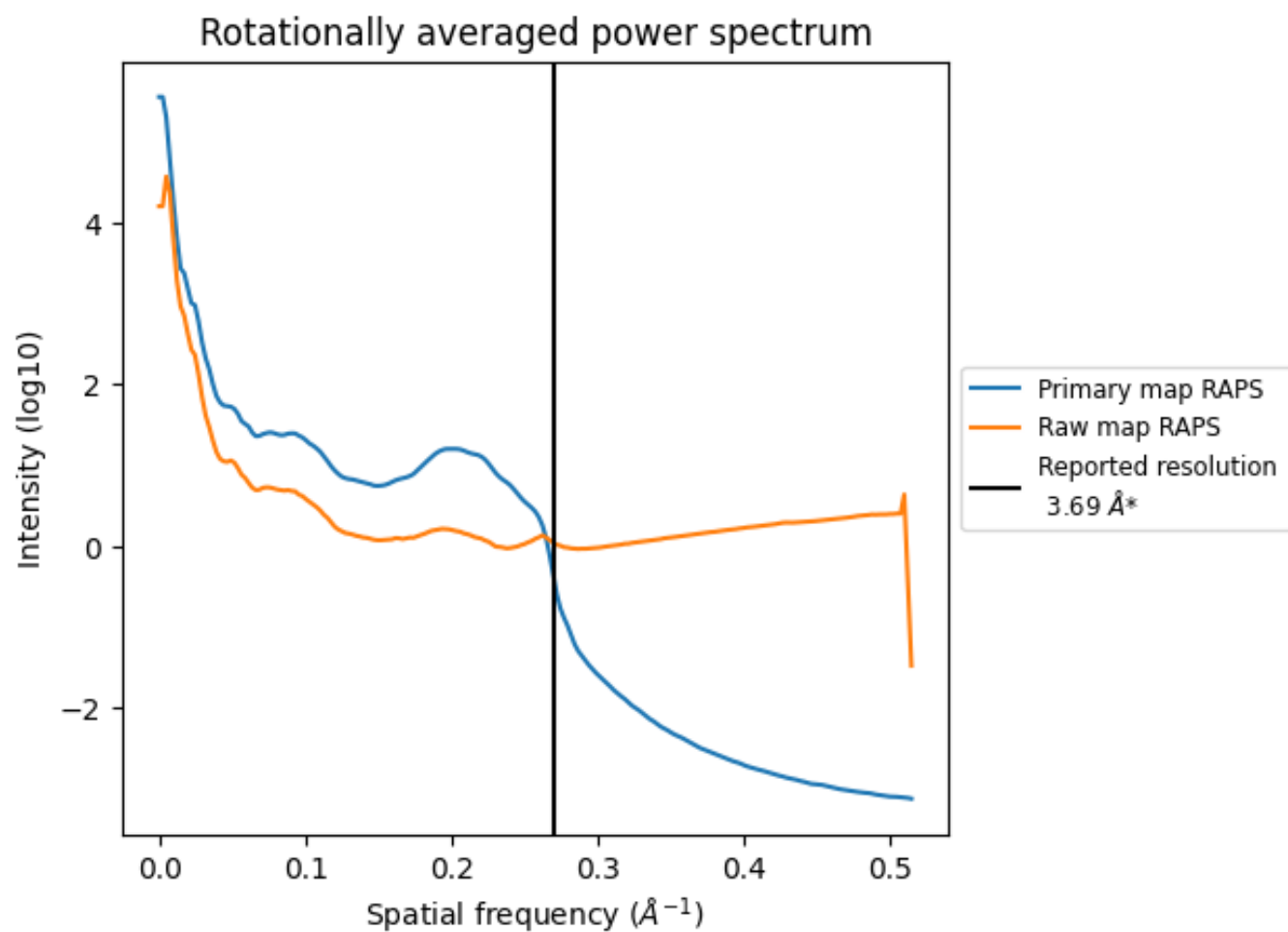
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm<sup>3</sup>; this corresponds to an approximate mass of 144 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 [i](#)

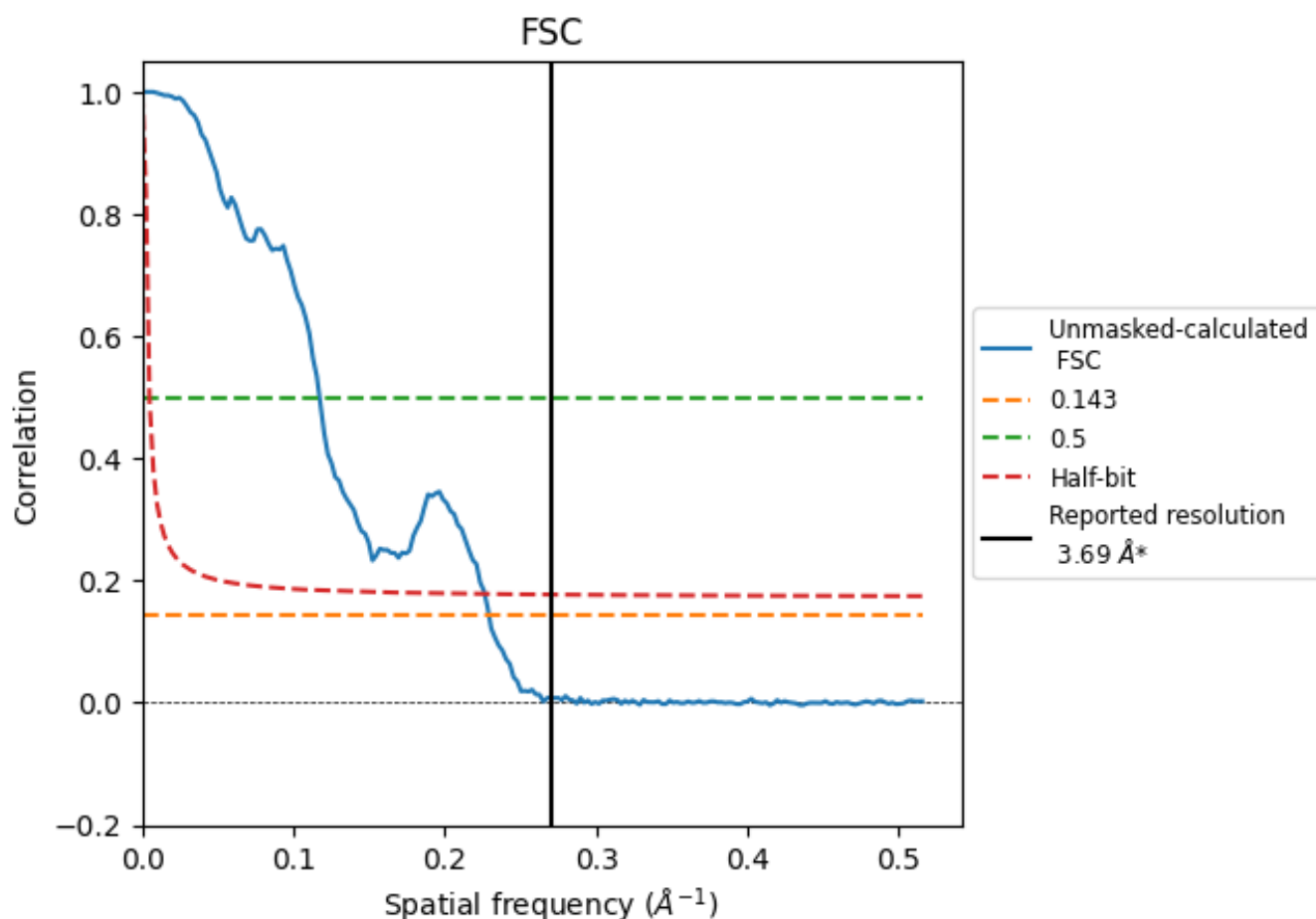


\*Reported resolution corresponds to spatial frequency of 0.271  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.271  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

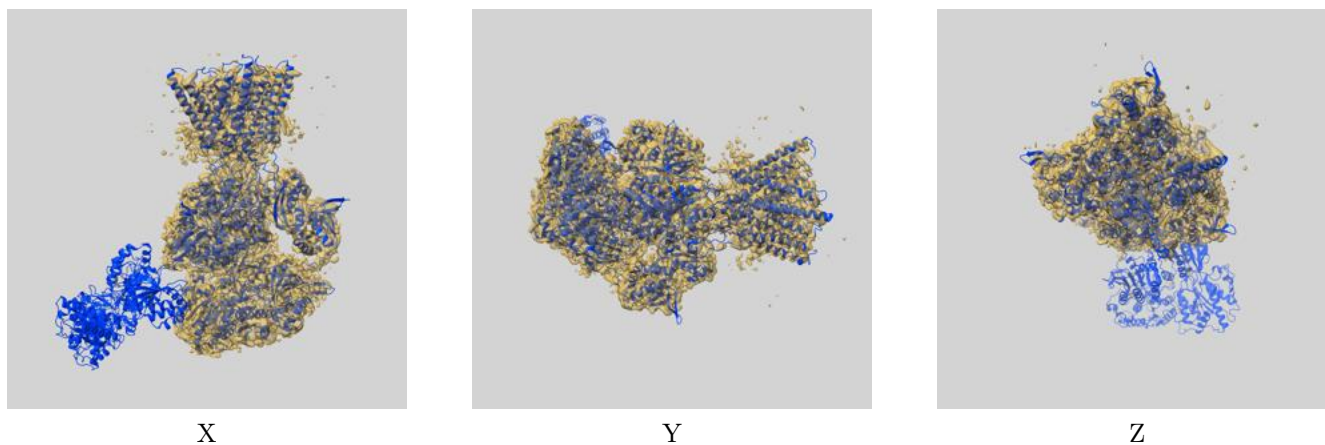
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	8.53	4.42

\*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 4.36 differs from the reported value 3.69 by more than 10 %

## 9 Map-model fit [i](#)

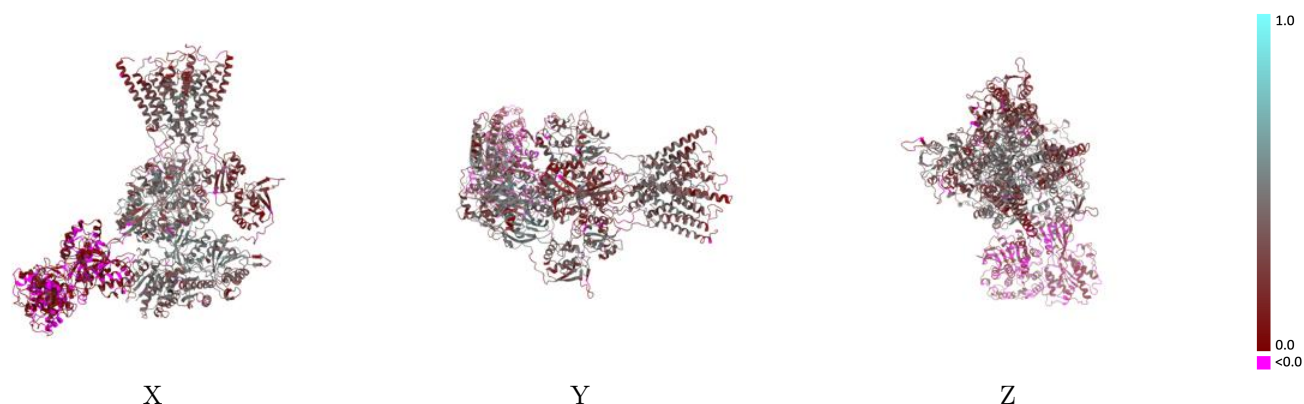
This section contains information regarding the fit between EMDB map EMD-49889 and PDB model 9NWP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

### 9.1 Map-model overlay [i](#)



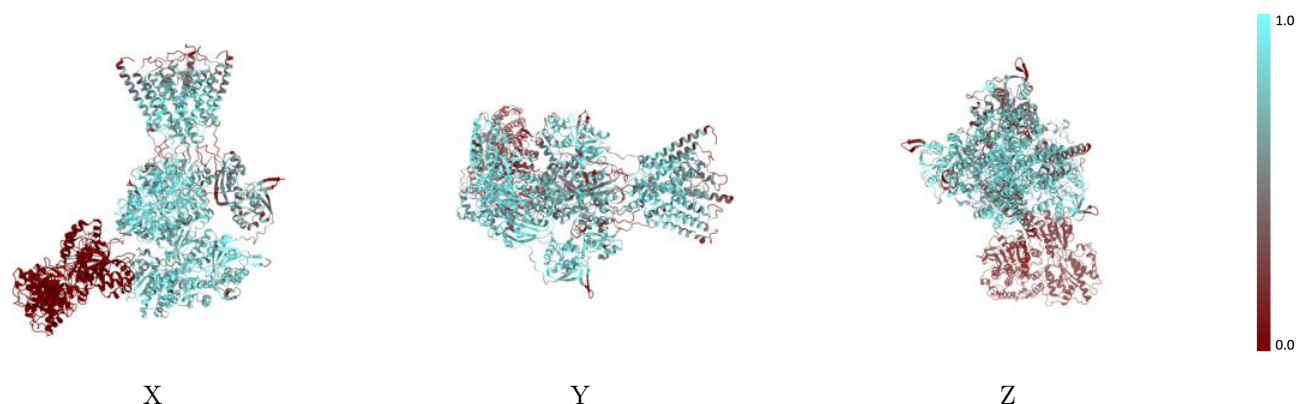
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



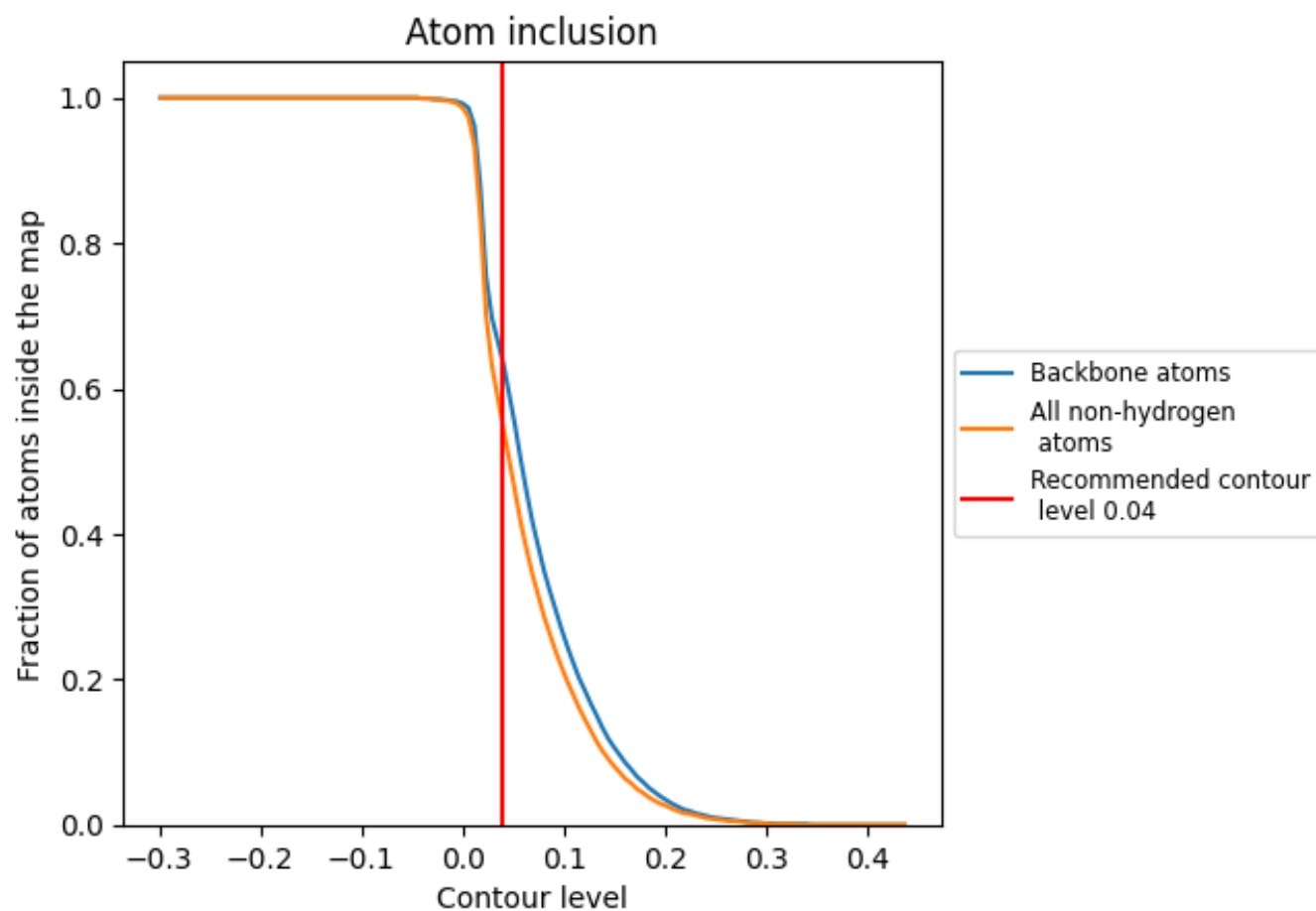
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5470	<div></div> 0.2770
A	<div></div> 0.7690	<div></div> 0.3820
B	<div></div> 0.6740	<div></div> 0.3130
C	<div></div> 0.3830	<div></div> 0.2130
D	<div></div> 0.3620	<div></div> 0.2010

