



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2025 – 01:07 PM EST

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:

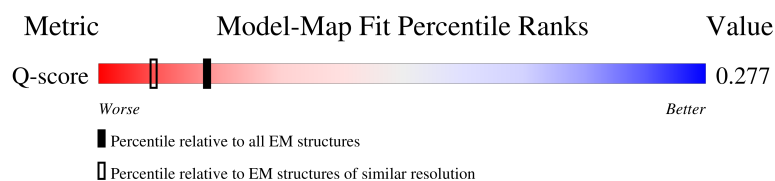
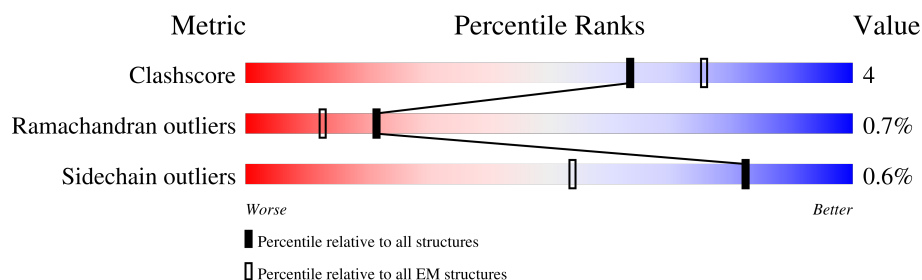
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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	
1	B	836	
1	C	836	
1	D	836	

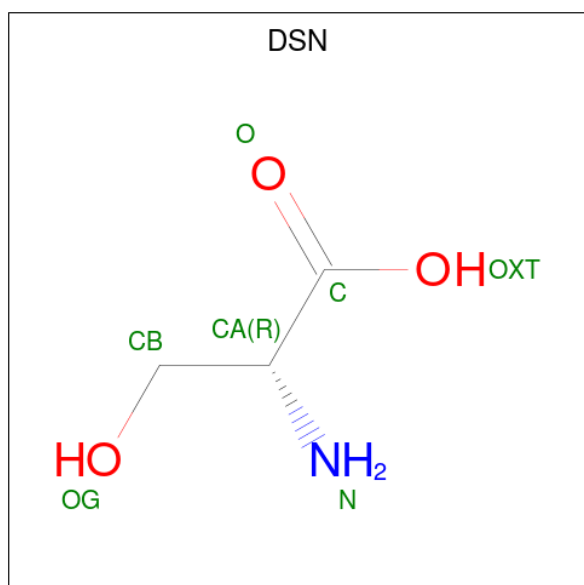


In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor ionotropic, delta-2.

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

- Molecule 2 is D-SERINE (CCD ID: DSN) (formula:  $\text{C}_3\text{H}_7\text{NO}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

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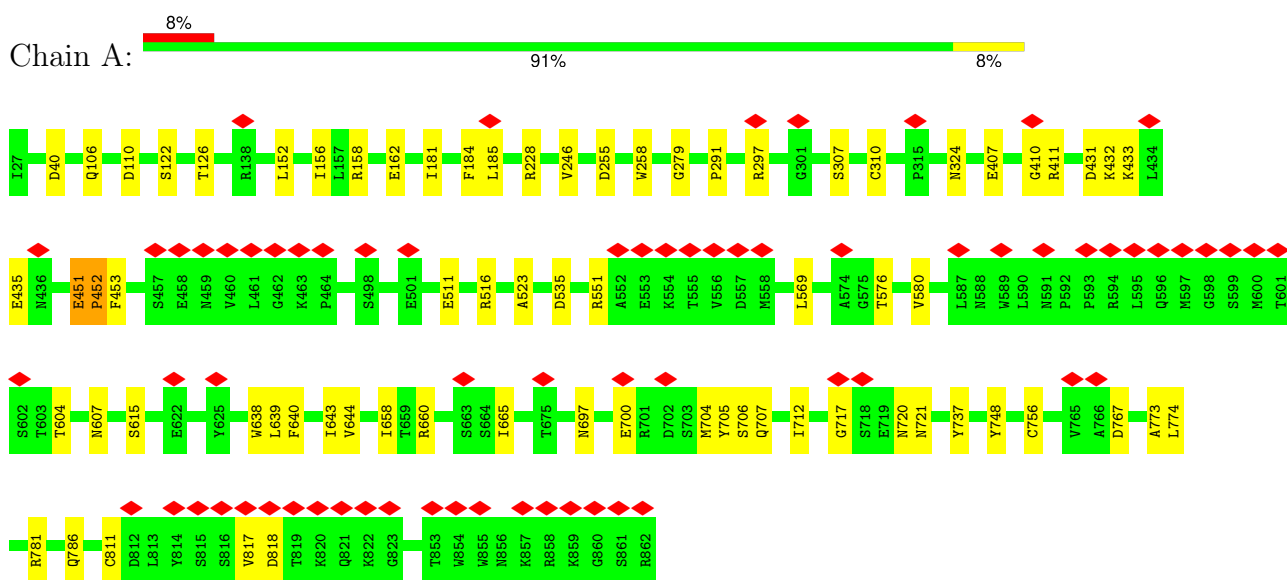
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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			7	3	1	3	
2	D	1	Total	C	N	O	0
			7	3	1	3	

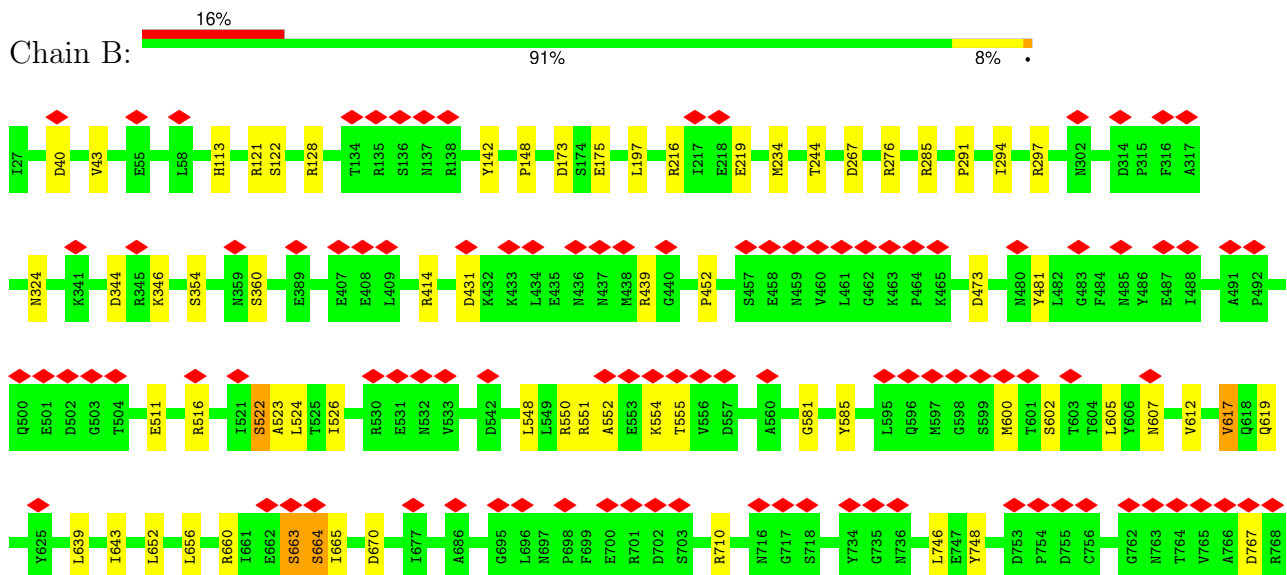
### 3 Residue-property plots

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





Q810	Y606	M459	F387	I327	D267	M207	R147	N87
Q811	N607	V460	G388	Y328	V268	I208	P148	Q88
L813	V612	L461	E389	D329	D269	T209	P149	G89
W817	V617	G462	N390	T330	V270	T210	V150	I90
D818	M634	K463	G391	V331	Q271	L211	Y151	L91
T819	Q634	P464	G392	L332	E272	F212	L152	A92
K820	M638	K465	N393	L333	L273	D213	H153	L93
Q821	M639	F484	P394	L334	Y274	T214	D154	V94
K822	F640	E487	N395	A335	R275	M215	V155	S95
G823	T643	E495	V396	N336	R276	R216	I156	S96
S845	V644	K496	H397	A337	S277	I217	L157	I97
C846	A654	E501	F398	N338	I278	E218	R158	G98
F847	T657	D502	H399	H339	Q279	E219	V159	C99
I848	T658	G503	E399	K340	R280	L220	V160	T100
A849	R660	L401	I400	K341	L281	N221	T161	S101
M850	A517	G402	G402	L342	T282	R222	E162	A102
W854	D518	T403	T403	E343	I283	Y223	Y163	G103
M855	I519	M404	M404	D344	I284	R224	A164	S104
W856	T518	Y405	Y405	R345	R285	D225	W165	L105
M857	E662	D529	G406	K346	Q286	T226	Q166	Q106
K857	S663	R530	E407	W347	T287	L227	K167	S107
M858	S664	E531	E408	H348	F288	R228	F168	L108
R858	T665	V534	L409	S349	P289	R229	I169	A109
K859	Q666	D535	G410	M350	V290	A230	I170	D110
G860	L671	F536	R411	K351	P291	I231	F171	A111
S861	Q674	C412	G412	S352	Q292	L232	Y172	M112
R862	D684	V413	V413	L353	N293	L232	D173	H113
		D642	R414	S354	I294	M234	S174	I114
		E553	K415	C355	S295	N235	E175	P115
		K554	L416	I356	Q296	P236	Y176	H116
			G417	R357	R297	A237	D177	L117
			C418	K358	C298	T238	I178	F118
			M419	N359	F299	A239	R179	I119
			N420	S360	R300	K240	G180	Q120
			P421	K361	G301	I181	I181	R121
			V422	P362	N302	F242	Q182	S122
			T423	W363	H303	I243	E183	T123
			G424	Q364	R304	T244	F184	A124
			L425	G365	I305	E245	L185	G125
			M426	G366	S306	V246	D186	T126
			R594	G367	S307	V247	K187	P127
			L595	R367	T308	E248	V188	R128
			S428	S368	L309	T249	S189	S129
			L429	M369	C310	N250	Q190	G130
			T430	L370	D311	L251	Q191	C131
			D431	E371	P312	V252	G192	G132
			K432	T372	K313	A253	M193	L133
			R433	I373	D314	F254	D194	T134
			L434	K374	P315	D255	V195	R135
			E435	K375	F316	C256	A196	S136
			M436	G376	A317	H257	L197	N137
			N437	G377	Q318	W258	Q198	R138
			M438	V378	N319	I259	K199	R139
			R439	S379	M320	V260	V200	D140
			G440	G380	E321	I261	E201	D141
			V441	L381	I322	N262	N202	Y142
			V442	T382	S323	E263	N203	T143
			R443	G383	N324	E264	L204	L144
			V445	E384	L325	N205	S145	S145
				F386	V326	N266	N206	V146

## 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

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	B	901	-	4,6,6	1.17	1 (25%)	2,7,7	1.93	1 (50%)
2	DSN	D	901	-	4,6,6	1.17	1 (25%)	2,7,7	1.98	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	B	901	-	-	0/6/6/6	-
2	DSN	D	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.

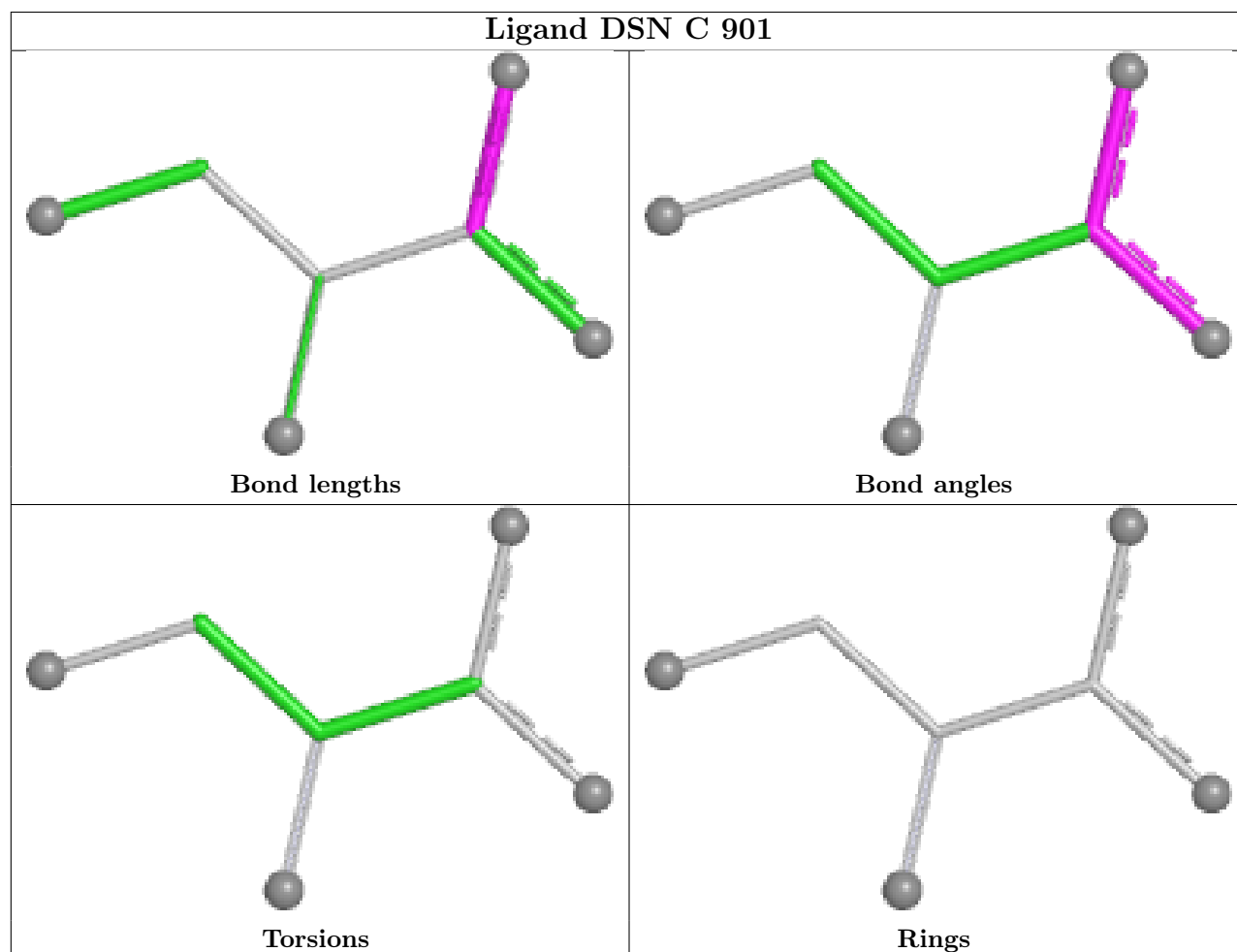
There are no torsion outliers.

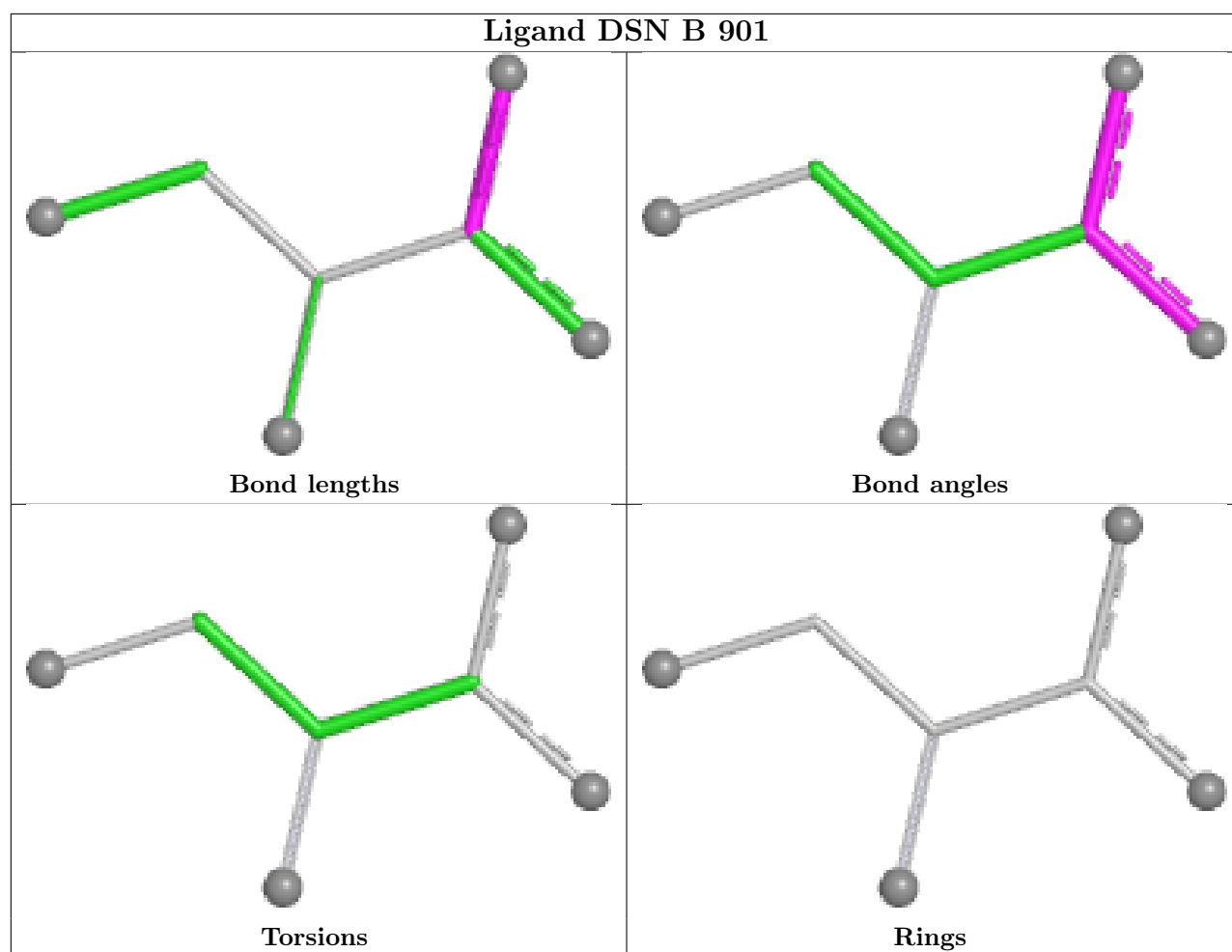
There are no ring outliers.

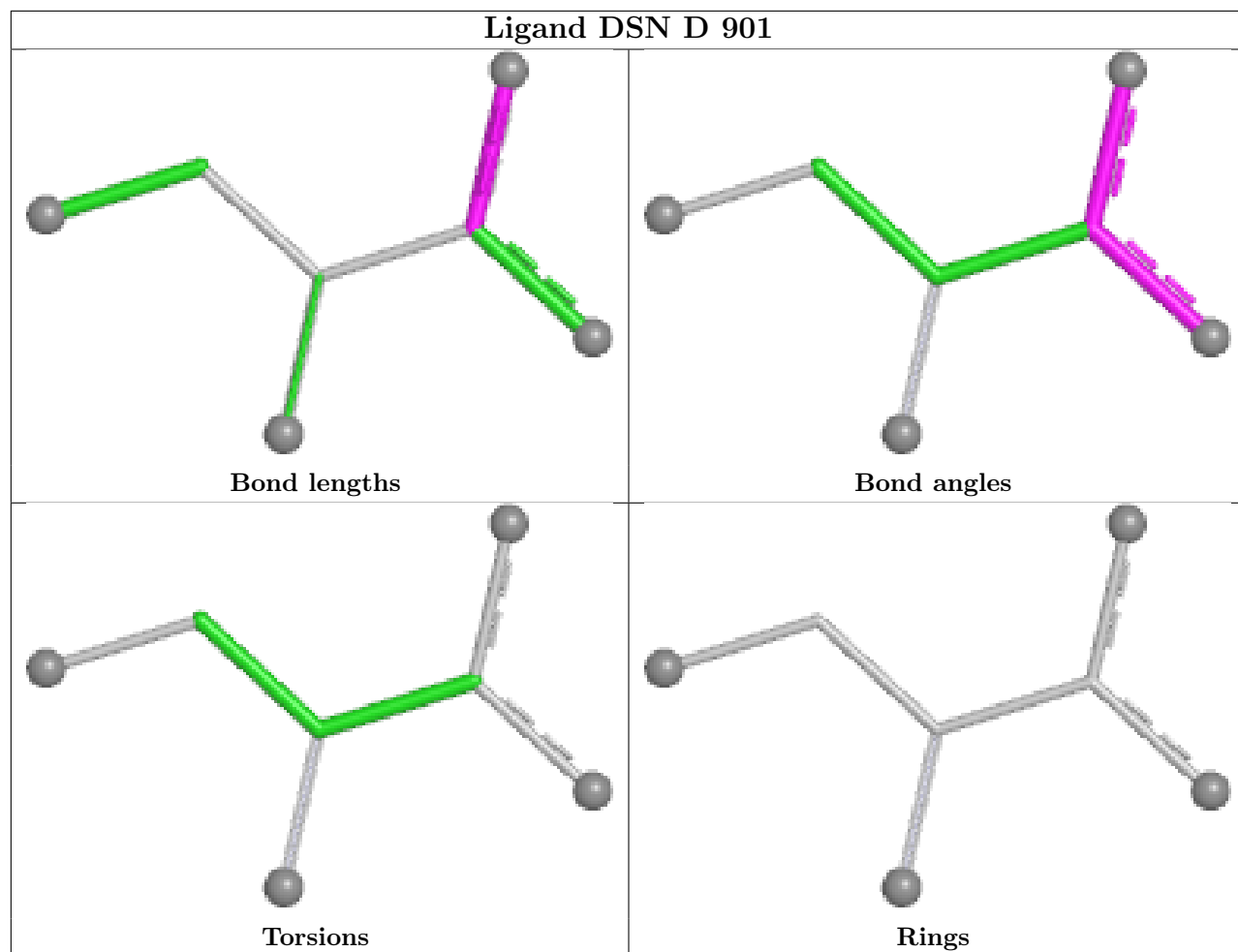
No monomer is involved in short contacts.

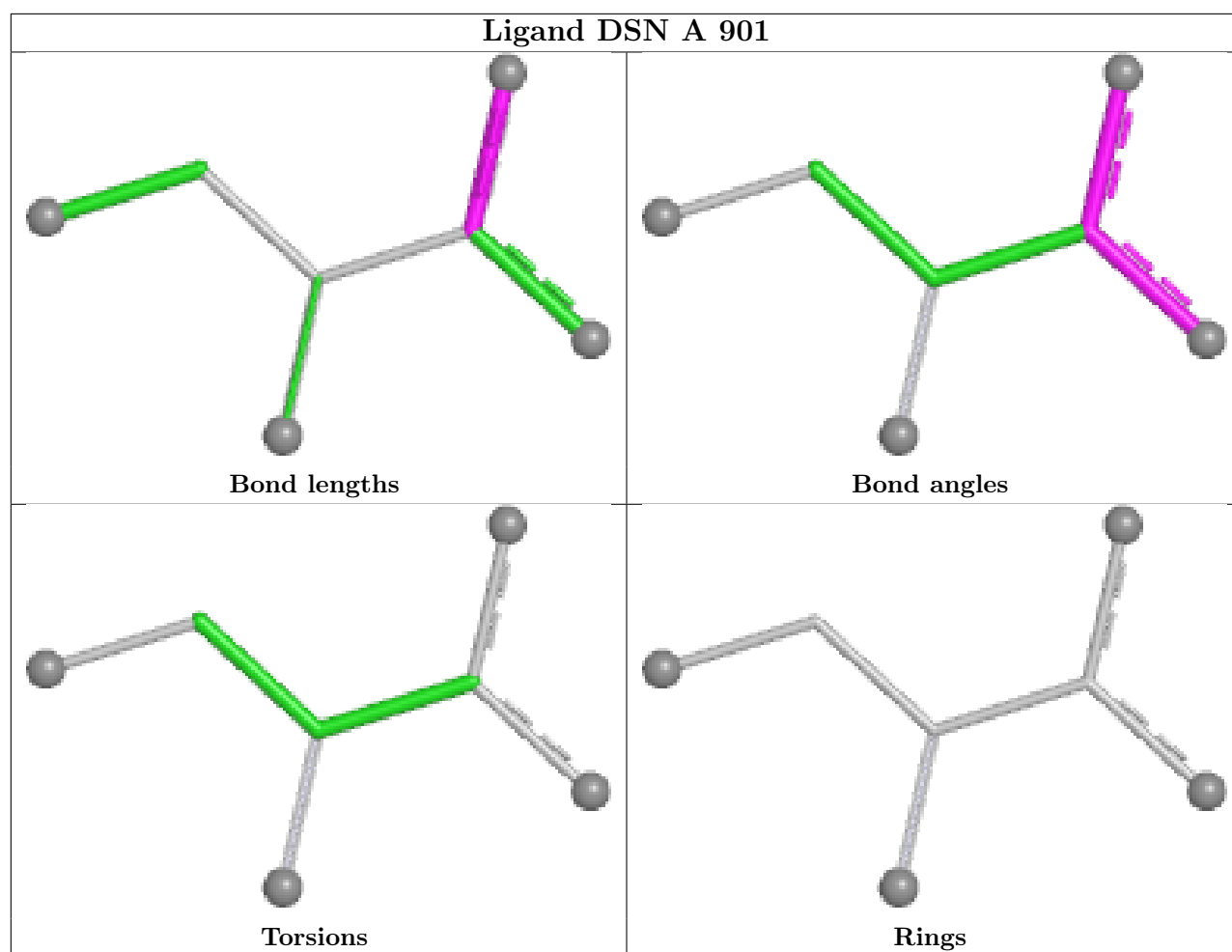
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

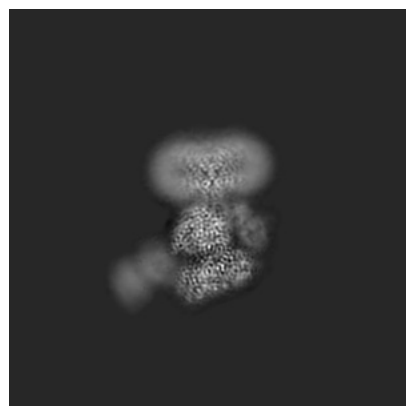
## 6 Map visualisation [i](#)

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.

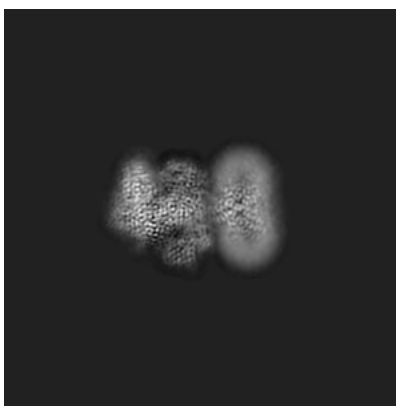
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

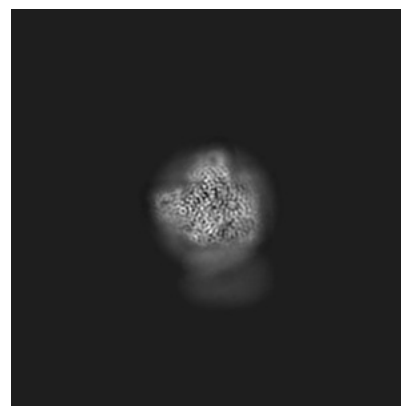
#### 6.1.1 Primary map



X

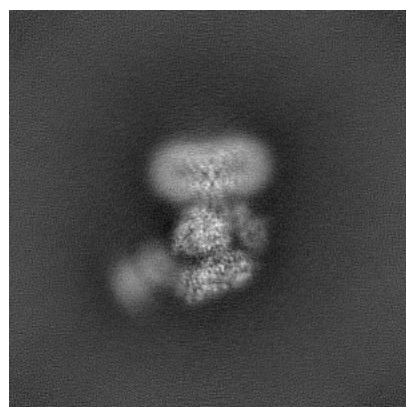


Y

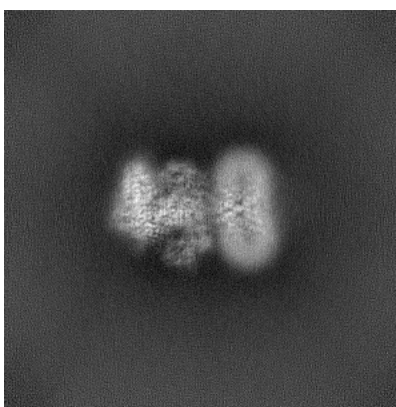


Z

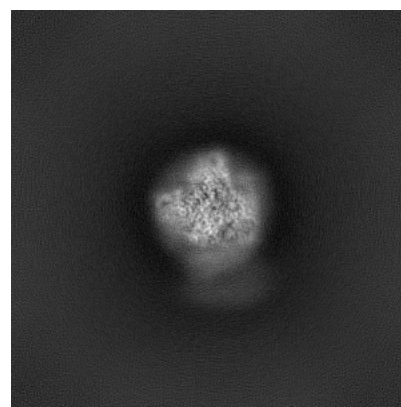
#### 6.1.2 Raw map



X



Y



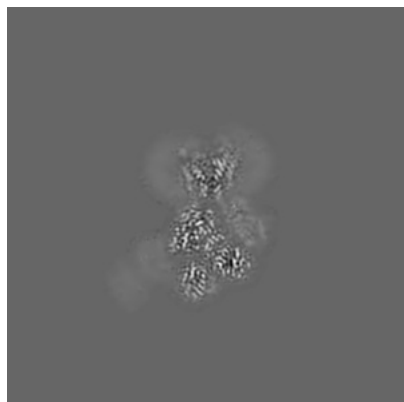
Z

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

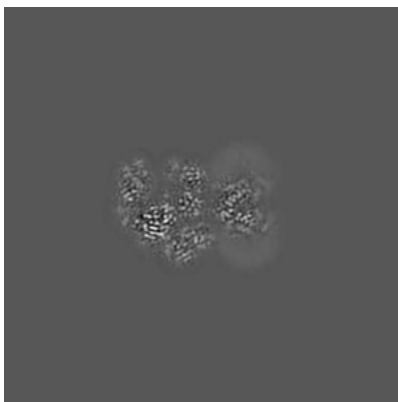


## 6.2 Central slices [i](#)

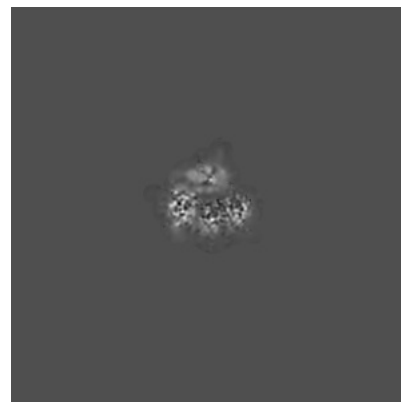
### 6.2.1 Primary map



X Index: 210

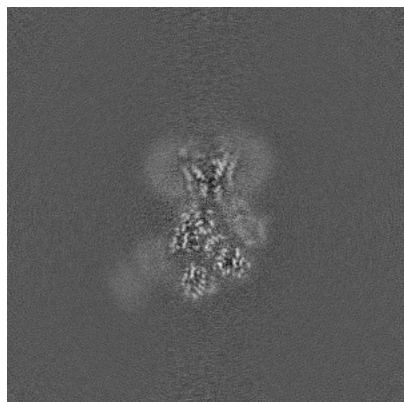


Y Index: 210

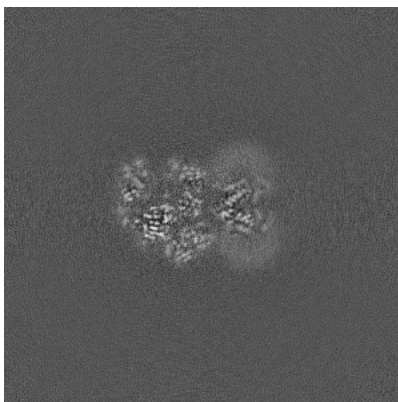


Z Index: 210

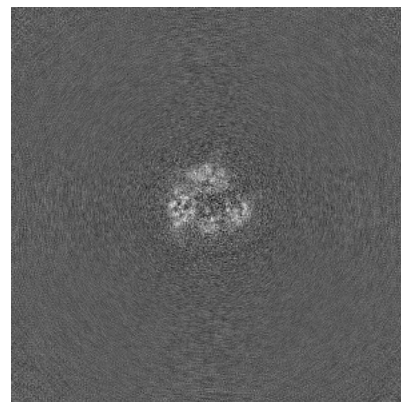
### 6.2.2 Raw map



X Index: 210



Y Index: 210

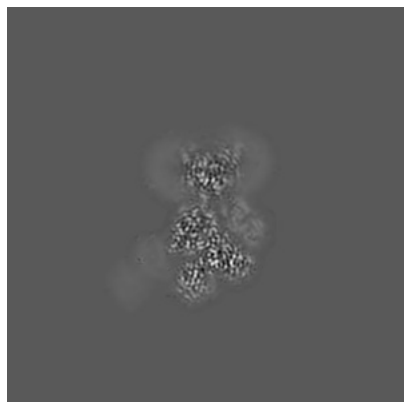


Z Index: 210

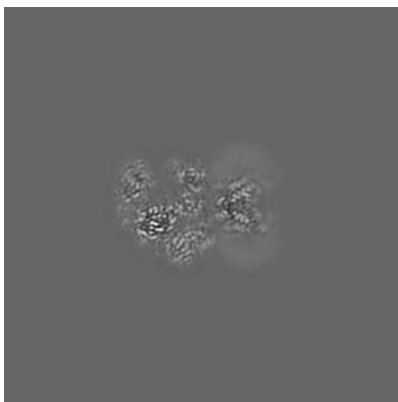
The images above show central slices of the map in three orthogonal directions.

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

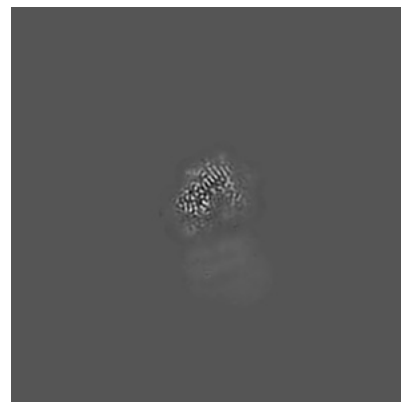
### 6.3.1 Primary map



X Index: 206

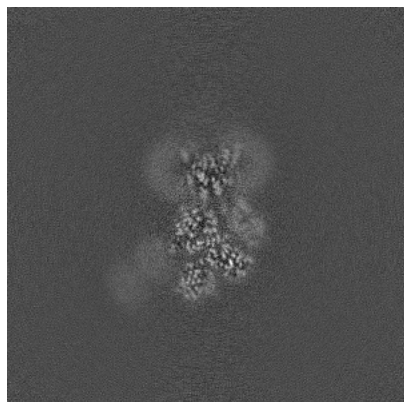


Y Index: 212

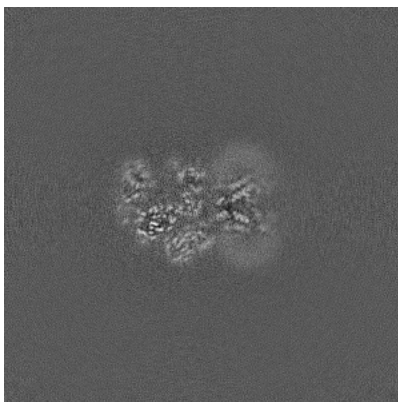


Z Index: 153

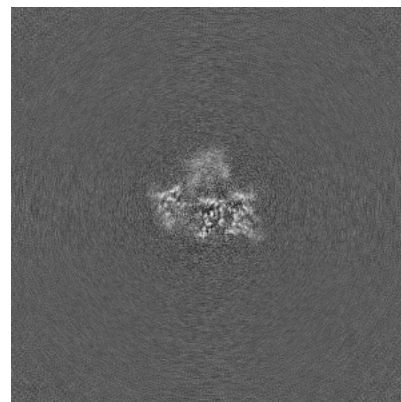
### 6.3.2 Raw map



X Index: 207



Y Index: 212

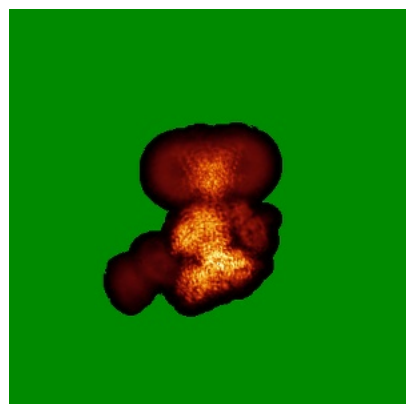


Z Index: 193

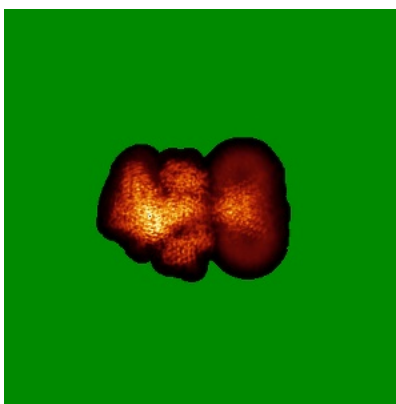
The images above show the largest variance slices of the map in three orthogonal directions.

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

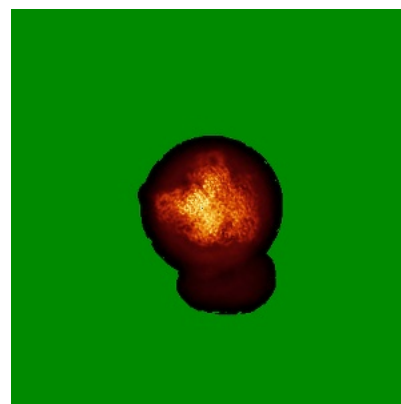
### 6.4.1 Primary map



X

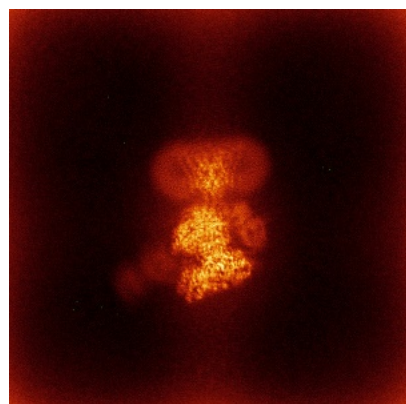


Y

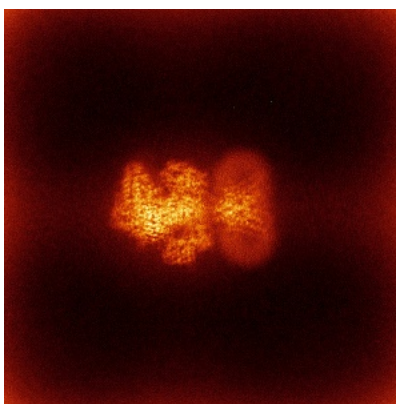


Z

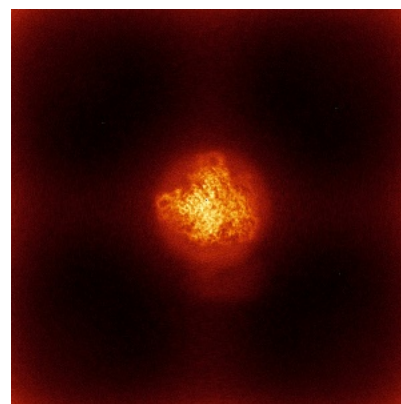
### 6.4.2 Raw map



X



Y

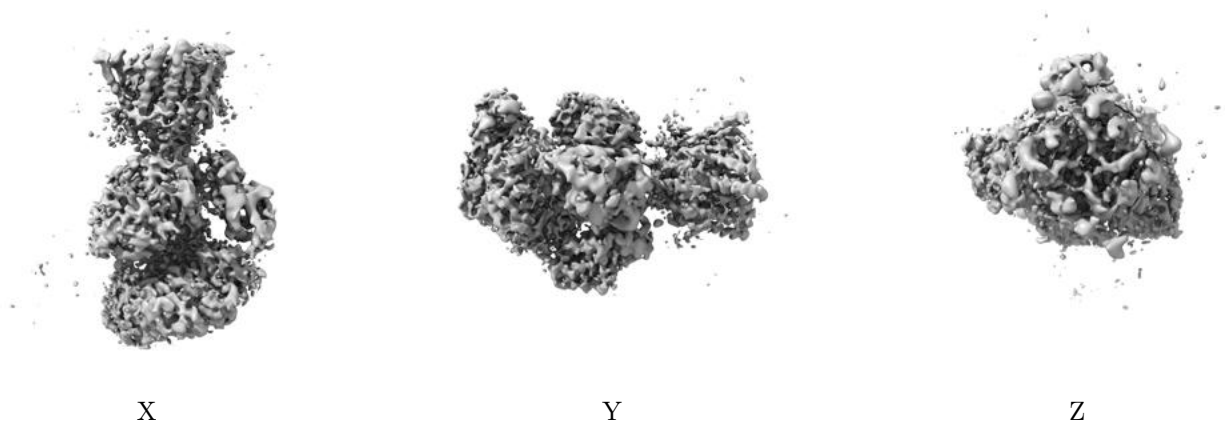


Z

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.

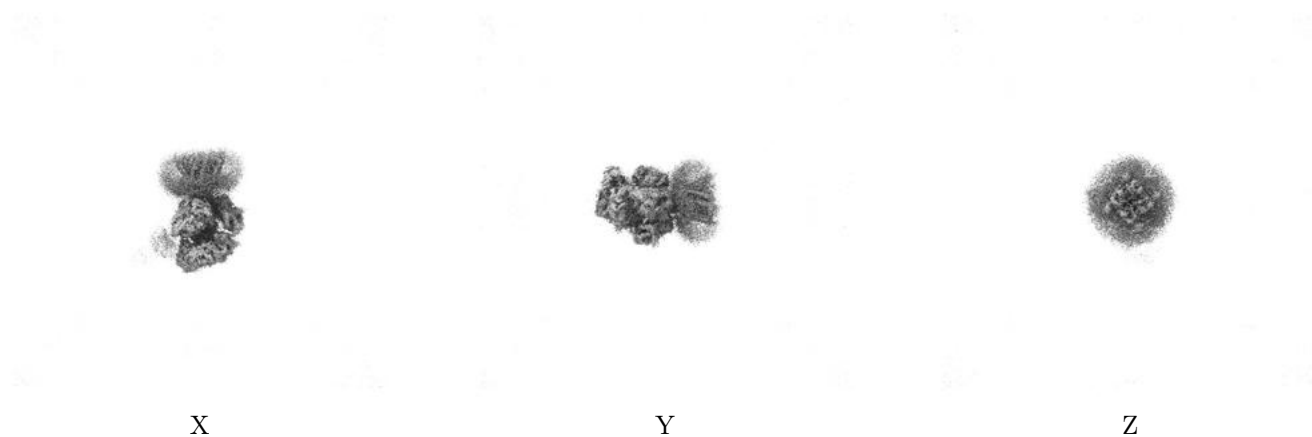
## 6.5 Orthogonal surface views [i](#)

### 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.

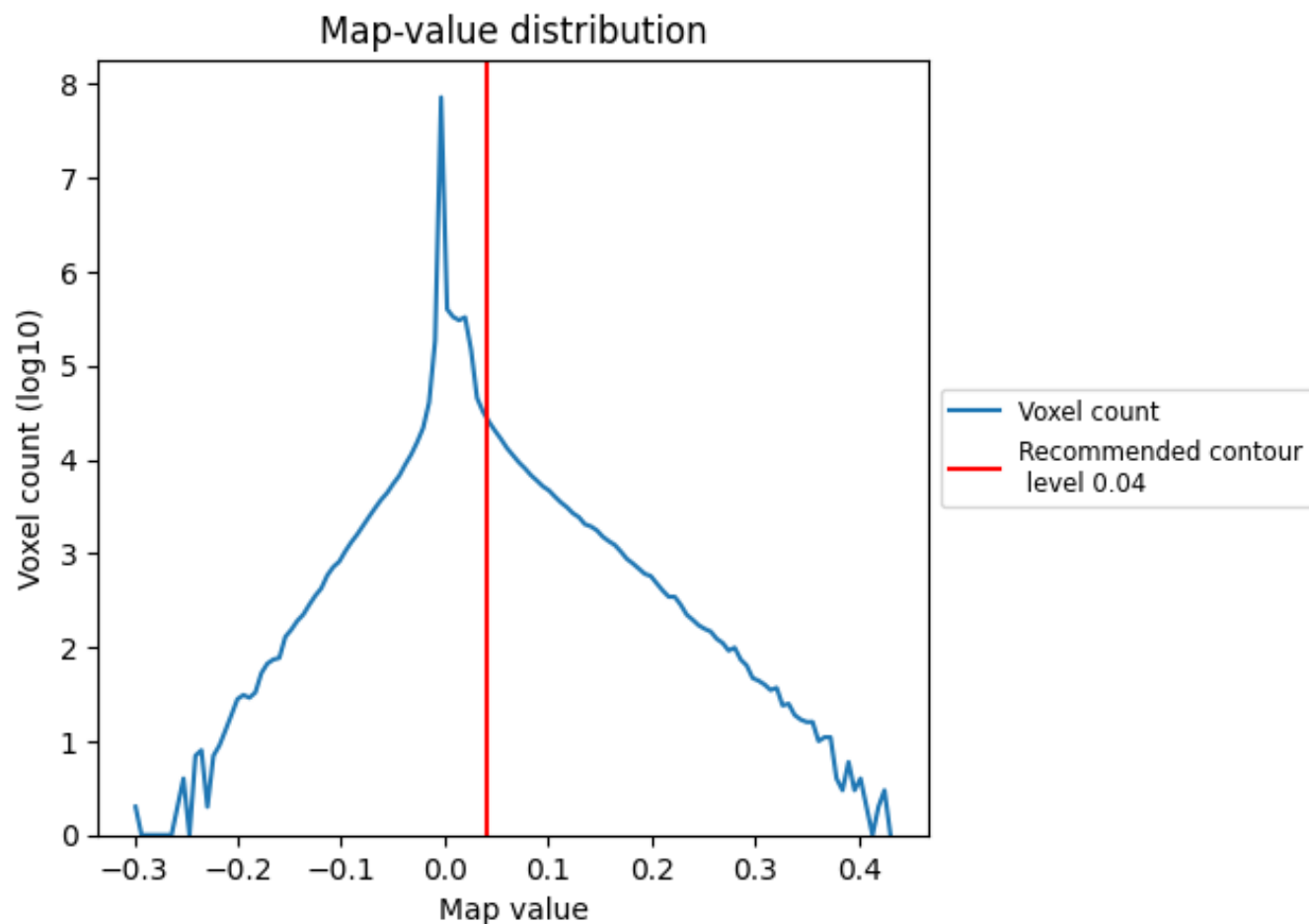
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

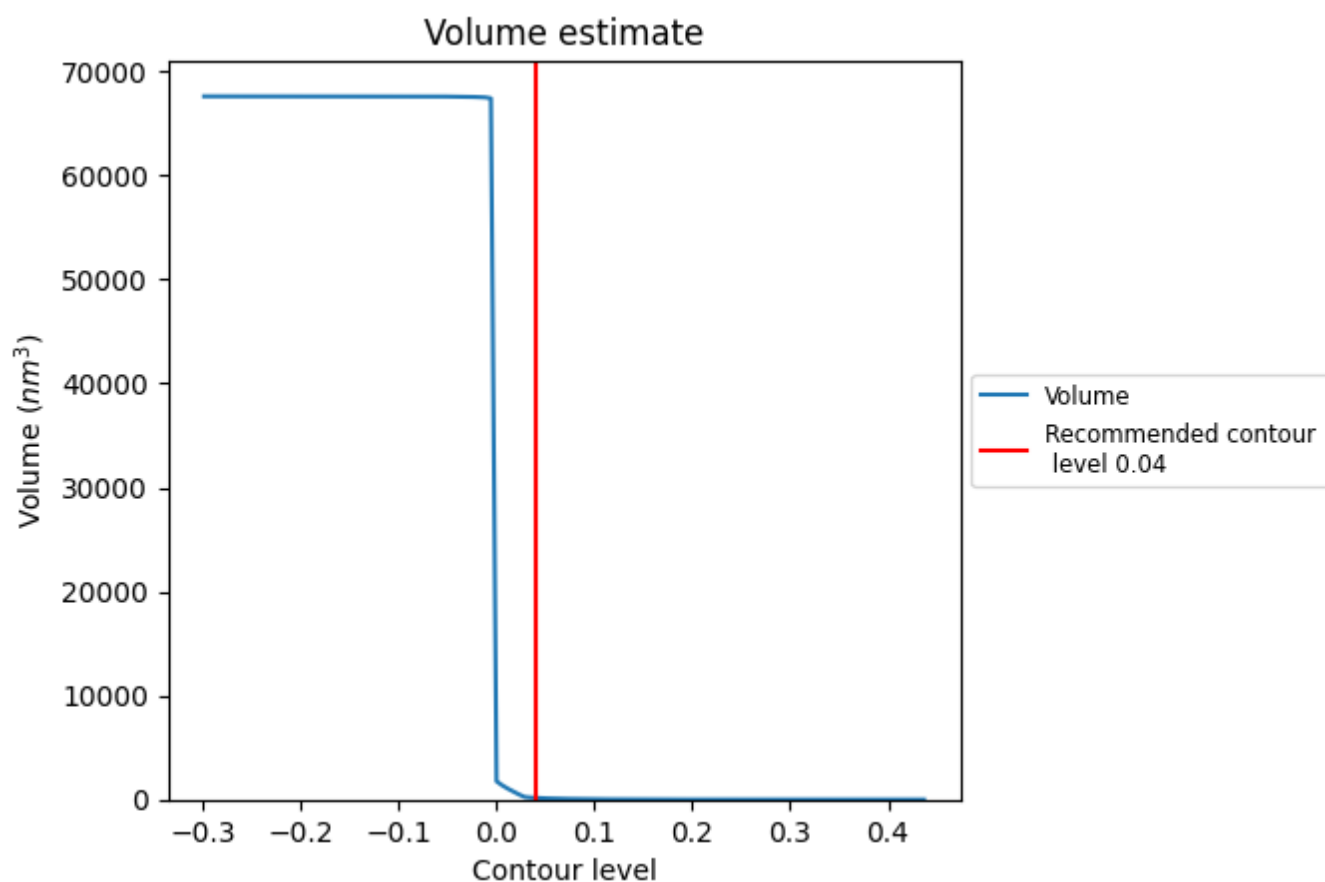
This section contains the results of statistical analysis of the map.

### 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.

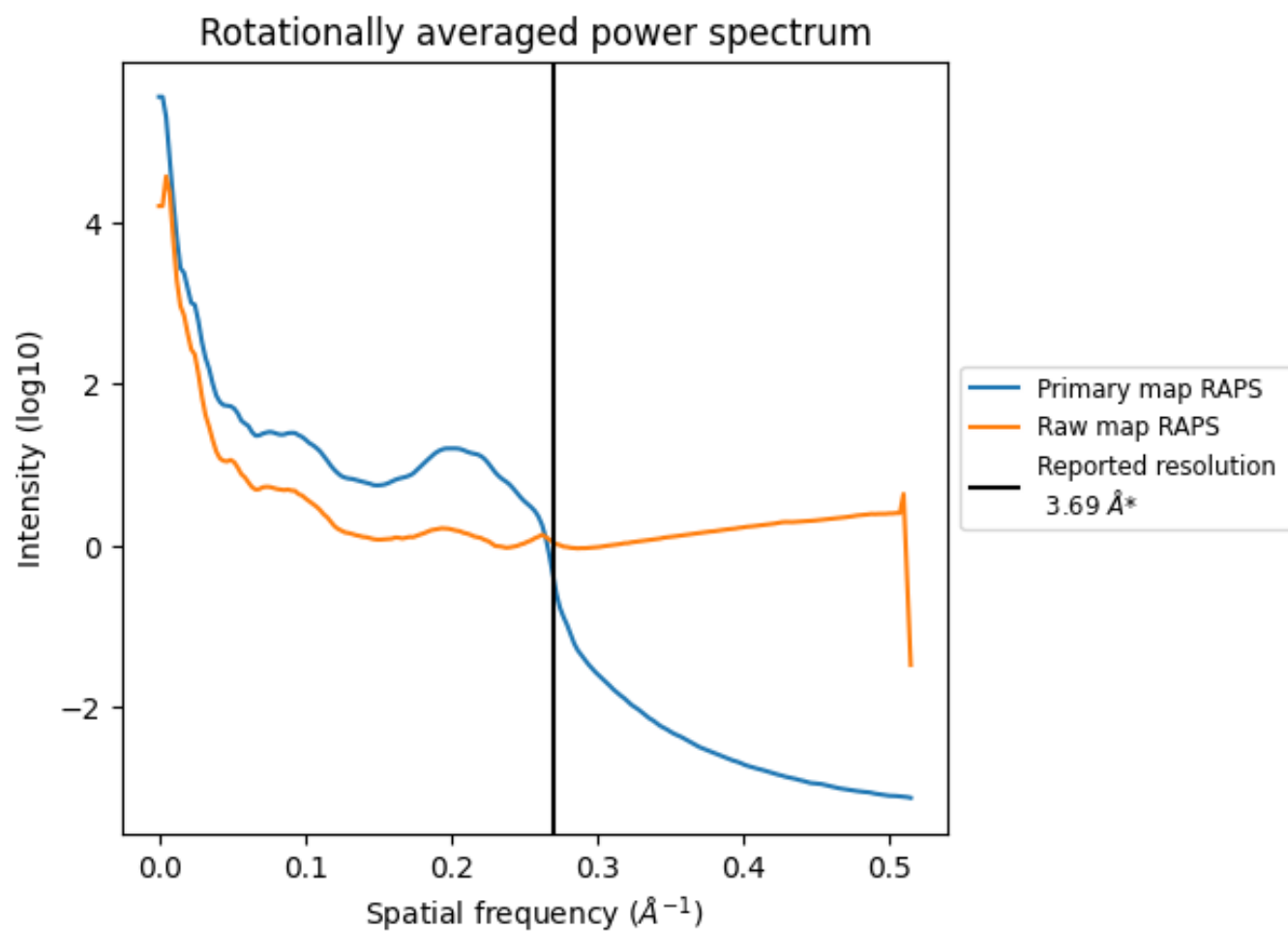
## 7.2 Volume estimate [i](#)



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 ⓘ

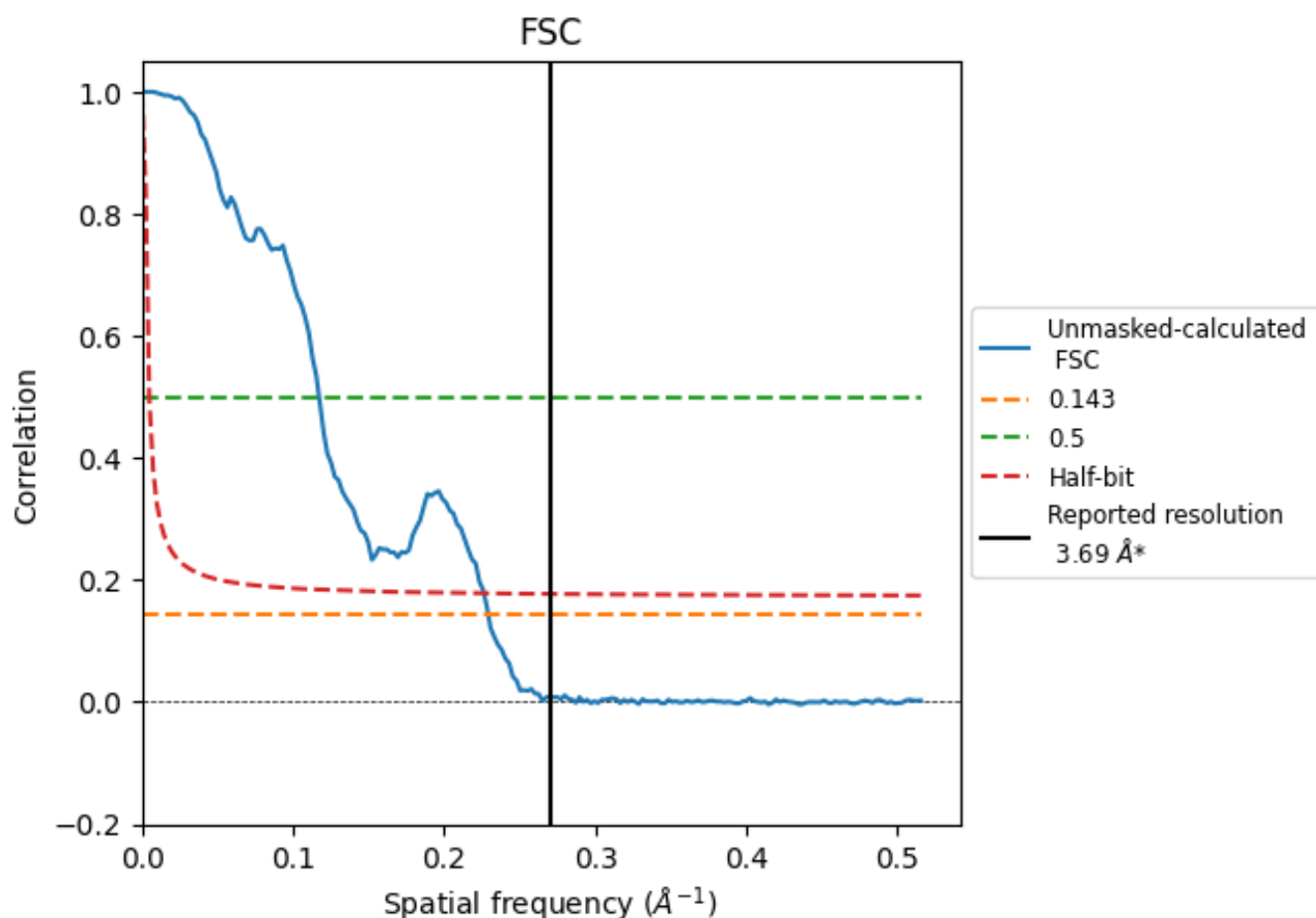


\*Reported resolution corresponds to spatial frequency of  $0.271 \text{ \AA}^{-1}$

## 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](#)

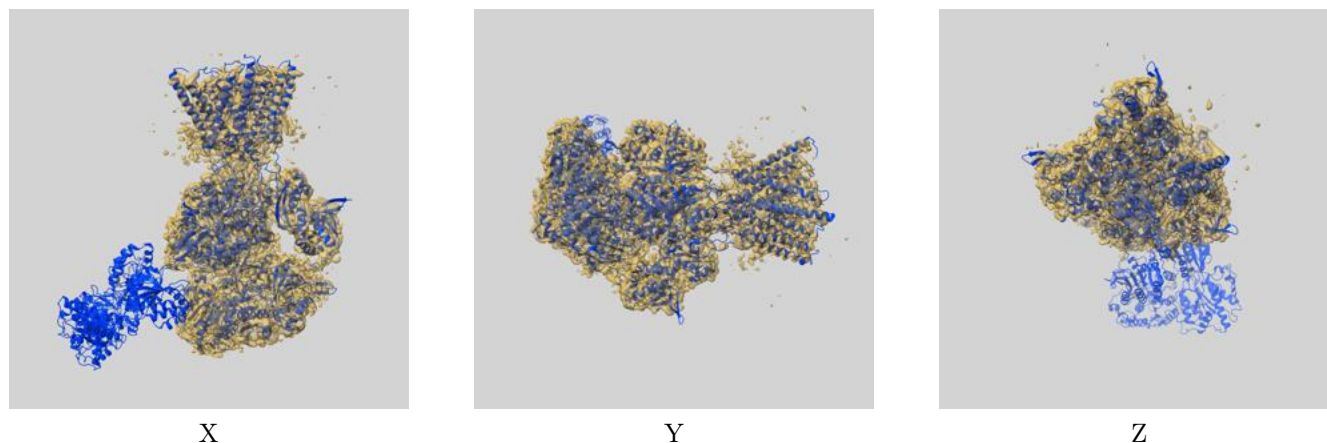
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	8.53	4.42

\*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](#)

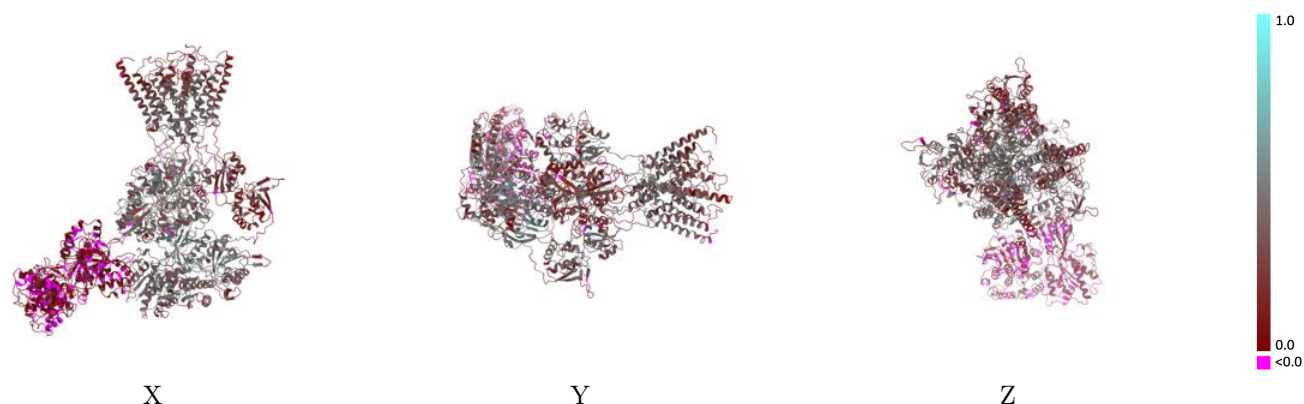
This section contains information regarding the fit between EMDB map EMD-49889 and PDB model 9NWP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



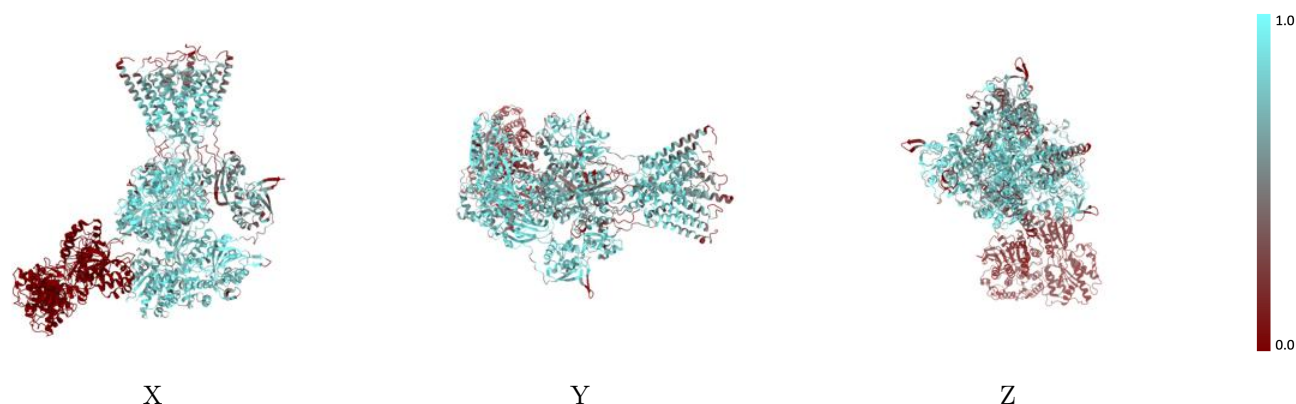
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



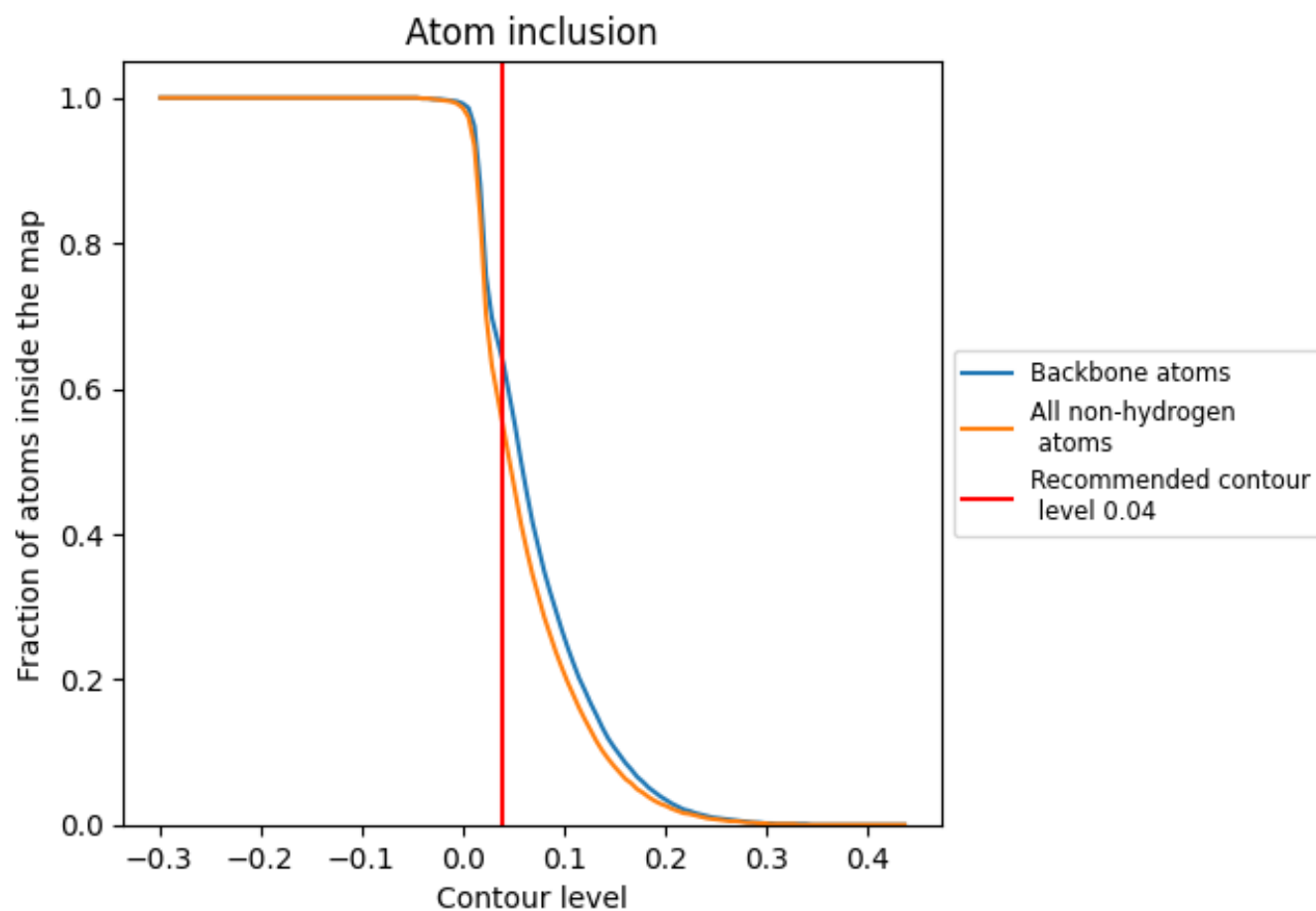
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

