



Full wwPDB EM Validation Report ⓘ

Aug 19, 2026 – 12:57 PM EDT

PDB ID : 9OEO / pdb_00009oeo
EMDB ID : EMD-70405
Title : GluN1/GluN3A in complex with glycine, LBD-TMD focused, in desensitized conformation
Authors : Kim, J.; Gouaux, E.
Deposited on : 2025-04-29
Resolution : 4.21 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.50

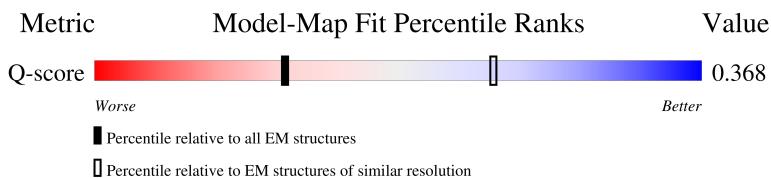
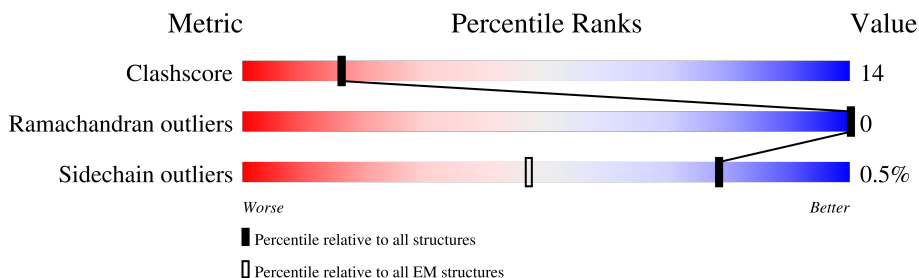
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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	4806 (3.71 - 4.71)

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	870	
1	C	870	
2	B	993	
2	D	993	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10884 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 Isoform E of Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	385	Total	C	N	O	S	0	0
			2618	1679	451	473	15		
1	C	385	Total	C	N	O	S	0	0
			2642	1695	455	477	15		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	LEU	-	expression tag	UNP P35439
A	849	VAL	-	expression tag	UNP P35439
A	850	PRO	-	expression tag	UNP P35439
A	851	ARG	-	expression tag	UNP P35439
A	852	GLY	-	expression tag	UNP P35439
A	853	SER	-	expression tag	UNP P35439
A	854	ALA	-	expression tag	UNP P35439
A	855	ALA	-	expression tag	UNP P35439
A	856	ALA	-	expression tag	UNP P35439
A	857	ALA	-	expression tag	UNP P35439
A	858	SER	-	expression tag	UNP P35439
A	859	GLY	-	expression tag	UNP P35439
A	860	LEU	-	expression tag	UNP P35439
A	861	ARG	-	expression tag	UNP P35439
A	862	SER	-	expression tag	UNP P35439
A	863	HIS	-	expression tag	UNP P35439
A	864	HIS	-	expression tag	UNP P35439
A	865	HIS	-	expression tag	UNP P35439
A	866	HIS	-	expression tag	UNP P35439
A	867	HIS	-	expression tag	UNP P35439
A	868	HIS	-	expression tag	UNP P35439
A	869	HIS	-	expression tag	UNP P35439
A	870	HIS	-	expression tag	UNP P35439
C	848	LEU	-	expression tag	UNP P35439
C	849	VAL	-	expression tag	UNP P35439
C	850	PRO	-	expression tag	UNP P35439

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	851	ARG	-	expression tag	UNP P35439
C	852	GLY	-	expression tag	UNP P35439
C	853	SER	-	expression tag	UNP P35439
C	854	ALA	-	expression tag	UNP P35439
C	855	ALA	-	expression tag	UNP P35439
C	856	ALA	-	expression tag	UNP P35439
C	857	ALA	-	expression tag	UNP P35439
C	858	SER	-	expression tag	UNP P35439
C	859	GLY	-	expression tag	UNP P35439
C	860	LEU	-	expression tag	UNP P35439
C	861	ARG	-	expression tag	UNP P35439
C	862	SER	-	expression tag	UNP P35439
C	863	HIS	-	expression tag	UNP P35439
C	864	HIS	-	expression tag	UNP P35439
C	865	HIS	-	expression tag	UNP P35439
C	866	HIS	-	expression tag	UNP P35439
C	867	HIS	-	expression tag	UNP P35439
C	868	HIS	-	expression tag	UNP P35439
C	869	HIS	-	expression tag	UNP P35439
C	870	HIS	-	expression tag	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			2755	1762	470	506	17		
2	D	396	Total	C	N	O	S	0	0
			2729	1748	468	498	15		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	971	LEU	-	expression tag	UNP Q9R1M7
B	972	VAL	-	expression tag	UNP Q9R1M7
B	973	PRO	-	expression tag	UNP Q9R1M7
B	974	ARG	-	expression tag	UNP Q9R1M7
B	975	GLY	-	expression tag	UNP Q9R1M7
B	976	SER	-	expression tag	UNP Q9R1M7
B	977	ALA	-	expression tag	UNP Q9R1M7
B	978	ALA	-	expression tag	UNP Q9R1M7
B	979	ALA	-	expression tag	UNP Q9R1M7
B	980	ALA	-	expression tag	UNP Q9R1M7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	981	SER	-	expression tag	UNP Q9R1M7
B	982	GLY	-	expression tag	UNP Q9R1M7
B	983	LEU	-	expression tag	UNP Q9R1M7
B	984	ARG	-	expression tag	UNP Q9R1M7
B	985	SER	-	expression tag	UNP Q9R1M7
B	986	TRP	-	expression tag	UNP Q9R1M7
B	987	SER	-	expression tag	UNP Q9R1M7
B	988	HIS	-	expression tag	UNP Q9R1M7
B	989	PRO	-	expression tag	UNP Q9R1M7
B	990	GLN	-	expression tag	UNP Q9R1M7
B	991	PHE	-	expression tag	UNP Q9R1M7
B	992	GLU	-	expression tag	UNP Q9R1M7
B	993	LYS	-	expression tag	UNP Q9R1M7
D	971	LEU	-	expression tag	UNP Q9R1M7
D	972	VAL	-	expression tag	UNP Q9R1M7
D	973	PRO	-	expression tag	UNP Q9R1M7
D	974	ARG	-	expression tag	UNP Q9R1M7
D	975	GLY	-	expression tag	UNP Q9R1M7
D	976	SER	-	expression tag	UNP Q9R1M7
D	977	ALA	-	expression tag	UNP Q9R1M7
D	978	ALA	-	expression tag	UNP Q9R1M7
D	979	ALA	-	expression tag	UNP Q9R1M7
D	980	ALA	-	expression tag	UNP Q9R1M7
D	981	SER	-	expression tag	UNP Q9R1M7
D	982	GLY	-	expression tag	UNP Q9R1M7
D	983	LEU	-	expression tag	UNP Q9R1M7
D	984	ARG	-	expression tag	UNP Q9R1M7
D	985	SER	-	expression tag	UNP Q9R1M7
D	986	TRP	-	expression tag	UNP Q9R1M7
D	987	SER	-	expression tag	UNP Q9R1M7
D	988	HIS	-	expression tag	UNP Q9R1M7
D	989	PRO	-	expression tag	UNP Q9R1M7
D	990	GLN	-	expression tag	UNP Q9R1M7
D	991	PHE	-	expression tag	UNP Q9R1M7
D	992	GLU	-	expression tag	UNP Q9R1M7
D	993	LYS	-	expression tag	UNP Q9R1M7

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

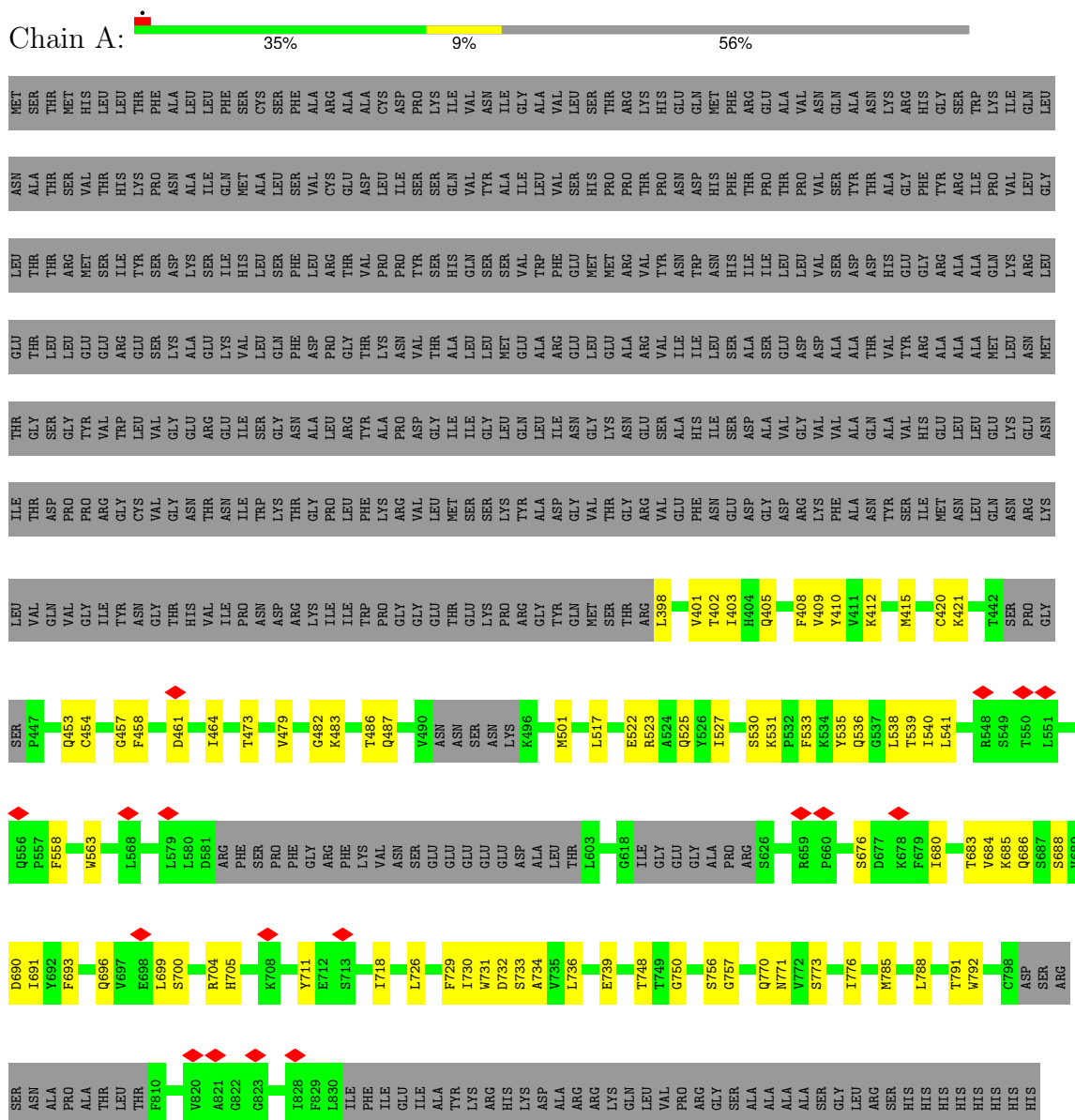


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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: Isoform E of Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Isoform E of Glutamate receptor ionotropic, NMDA 1

HIS	Q742	A640	R523	PRO	LEU	ILE	THR	THR	GLU	LEU	THR	ASN	MET
	K743	A524	R524		GLN	VAL	GLY	THR	ALA	THR	SER		
	T749	I643	R526		ASP	ASP	GLY	THR	SER	THR	SER		
	G750	Y647	R527		GLY	PRO	VAL	MET	VAL	SER	HIS		
	F753	D658	R528		ILE	ARG	VAL	SER	THR	THR	LEU		
	GLN	F529	F529		ASN	GLY	TRP	ILE	HIS	HIS	LEU		
		LEU	K534		Q453	CYS	LEU	GLU	THR	THR	LEU		
			G535		Q456	VAL	VAL	GLU	ALA	ALA	LEU		
			Y535		G457	HIS	GLY	GLY	LYS	LEU	LEU		
			Q536		Q457	THR	VAL	GLY	ASP	GLY	PHE		
PRO	F758	T667	Q537	L463	ASN	THR	GLU	GLN	ILE	LEU			
	GLY	P675	L538	ILE	ASN	GLU	ILE	GLN	GLN	PHE			
		R763	S676	PRO	ASP	ILE	VAL	HIS	MET	CYS			
		D677	D677	THR	THR	GLN	GLY	ALA	ALA	GLY			
		H780	K678	ASN	ASP	LYS	ASN	PHE	VAL	ARG			
ALA	SER	R548	Y476	ARG	GLY	ALA	ALA	ASP	ALA	ARG			
		T683	Y479	ILE	PRO	GLY	LEU	GLY	PRO	ARG			
		K790	L551	ILE	LEU	LEU	LEU	ALA	ALA	ALA			
		T791	K685	TRP	PHE	THR	THR	VAL	GLU	ALA			
	LEU	W792	F558	D481	PRO	LYS	ALA	LYS	ASP	ALA			
ARG	W793	Q686	Q482	K483	GLY	ARG	ASN	VAL	PRO	CYS			
	S687	Q559	VAL	ARG	VAL	VAL	ASP	ASN	ILE	ASP			
	R794	S560	GLU	GLY	LEU	GLY	THR	SER	PRO	PRO			
	Y795	R694	G485	F484	GLU	THR	SER	SER	LYS	LYS			
	Q796	R695	THR	G485	THR	MET	ILE	ILE	GLN	VAL			
HIS	E797	Q696	GLU	T486	GLU	SER	ILE	VAL	ASN	ASN			
	C798	V697	LYS	Q487	LYS	LYS	LEU	THR	TYR	ASN			
	ASP	E698	ARG	E488	PRO	LYS	LEU	ILE	ASN	ILE			
	SER	L699	PHE	R489	ARG	TYR	GLN	GLY	GLY	GLY			
	ARG	S700	SER	ASN	GLY	ALA	ALA	LEU	ARG	VAL			
HIS	SER	T701	PHE	ASN	TYR	ASP	ILE	ARG	VAL	VAL			
	ASN	W702	GLY	ASN	MET	GLY	GLY	GLU	SER	GLU			
	ALA	Y703	ARG	ASN	SER	THR	LYS	GLU	HIS	THR			
	ALA	R704	PHE	LYS	THR	GLY	ASN	ALA	PRO	ARG			
	THR	H705	LYS	ARG	ARG	GLY	GLU	VAL	THR	LYS			
LEU	THR	W706	VAL	E497	ARG	VAL	THR	VAL	THR	HIS			
	THR	E707	ASN	K398	L399	GLU	ALA	ILE	ASN	GLU			
	F810	K708	SER	I400	ASN	PHE	HIS	ILE	ASP	GLN			
	E811	H709	GLU	G500	V401	GLU	ILE	ASN	MET	PHE			
	N812	N710	GLU	M502	H404	ASP	SER	HIS	ASN	ARG			
LEU	V816	Y711	GLU	G503	H404	GLY	ASP	ALA	ILE	THR			
	F817	E712	GLU	E504	P407	GLY	GLU	SER	ALA	PRO			
	N818	E716	ASP	L505	K412	ARG	VAL	GLY	VAL	VAL			
	A821	Q719	ALA	S507	P413	LYS	VAL	ASP	VAL	ASN			
	T828	R722	THR	A510	T414	PHE	VAL	ALA	SER	GLN			
SER	F829	R729	THR	M415	M415	ALA	GLN	THR	THR	ASN			
	L830	F729	ILE	C420	C420	SER	VAL	VAL	ALA	LYS			
	ILE	W730	GLY	A515	A515	THR	THR	GLY	GLY	ARG			
	PHE	T731	GLY	P516	C436	HIS	ARG	ARG	GLY	HIS			
	ILE	D732	GLU	L517	T437	MET	GLU	ALA	TYR	GLY			
GLU	ILE	S733	GLU	L517	C436	LEU	LEU	ALA	ARG	TRP			
	ILE	A734	ALA	T518	T437	GLU	GLU	ALA	ILE	SER			
	ILE	W735	PRO	T519	N440	ASN	LYS	LEU	VAL	LYS			
	ALA	L736	ARG	N520	D441	ASN	LYS	LEU	VAL	VAL			
	THR	T736	ARG	N521	N442	ASN	ASN	GLU	LEU	GLN			

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.590	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/2677	0.30	0/3669
1	C	0.20	0/2699	0.35	0/3693
2	B	0.14	0/2823	0.27	0/3862
2	D	0.14	0/2795	0.26	0/3823
All	All	0.16	0/10994	0.30	0/15047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2618	0	2143	72	0
1	C	2642	0	2182	88	0
2	B	2755	0	2275	64	0
2	D	2729	0	2250	64	0
3	A	28	0	24	1	0
3	B	42	0	39	1	0
3	C	28	0	26	0	0
3	D	42	0	39	1	0
All	All	10884	0	8978	282	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 14.

All (282) 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:736:LEU:HG	1:A:748:THR:HG22	1.26	1.17
1:A:736:LEU:HG	1:A:748:THR:CG2	1.80	1.11
1:C:400:ILE:CD1	1:C:463:LEU:HD11	2.04	0.88
1:A:736:LEU:CG	1:A:748:THR:HG22	2.05	0.86
1:A:517:LEU:HD12	1:A:517:LEU:O	1.76	0.85
1:C:400:ILE:HD11	1:C:463:LEU:HD11	1.61	0.82
2:D:629:VAL:HG12	2:D:875:ILE:HD12	1.63	0.81
1:C:400:ILE:HD13	1:C:463:LEU:CD1	2.11	0.80
1:C:398:LEU:N	1:C:473:THR:O	2.17	0.77
2:D:621:LEU:HD11	2:D:641:VAL:CG1	2.17	0.74
1:C:487:GLN:HA	1:C:497:GLU:O	1.88	0.73
2:B:635:ASN:HD22	2:B:638:ARG:HE	1.37	0.72
1:A:533:PHE:HB3	1:A:776:ILE:HD11	1.72	0.72
1:C:400:ILE:CD1	1:C:463:LEU:CD1	2.68	0.72
1:A:684:VAL:O	1:A:711:TYR:N	2.15	0.71
2:D:558:PHE:O	2:D:562:HIS:ND1	2.24	0.69
1:C:400:ILE:HD13	1:C:463:LEU:HD13	1.74	0.69
2:D:656:LEU:HB3	2:D:849:LEU:HD13	1.75	0.68
1:C:536:GLN:OE1	1:C:733:SER:N	2.26	0.68
2:B:728:PHE:O	2:B:730:ARG:NH1	2.25	0.68
1:A:536:GLN:OE1	1:A:733:SER:N	2.23	0.68
1:A:401:VAL:HG13	1:A:501:MET:HE2	1.76	0.67
1:A:680:ILE:HG13	1:A:726:LEU:HD12	1.76	0.67
2:D:514:HIS:NE2	2:D:596:ASP:OD2	2.28	0.66
1:C:485:GLY:HA3	1:C:499:ASN:O	1.95	0.66
1:C:527:ILE:HD11	1:C:763:ARG:HA	1.78	0.66
2:D:517:VAL:HG23	2:D:627:MET:HG3	1.78	0.66
2:D:621:LEU:HD11	2:D:641:VAL:HG12	1.78	0.65
2:B:813:MET:HB3	2:B:817:MET:HE2	1.78	0.65
2:D:656:LEU:HD13	2:D:849:LEU:HD22	1.78	0.65
1:C:794:ARG:NH2	2:B:788:PRO:O	2.24	0.65
2:B:652:SER:O	2:B:846:LYS:N	2.30	0.64
2:D:803:GLU:HA	2:D:806:VAL:HG22	1.79	0.64
1:C:485:GLY:HA2	1:C:499:ASN:ND2	2.13	0.63
1:C:437:THR:OG1	1:C:476:VAL:O	2.17	0.63
1:C:684:VAL:HG23	1:C:685:LYS:H	1.63	0.63
2:B:815:GLU:HA	2:B:818:ARG:HD2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:HB3	1:A:736:LEU:HD21	1.82	0.62
2:B:612:HIS:NE2	3:B:1002:NAG:O7	2.32	0.62
2:B:628:ALA:HB3	2:B:876:GLY:HA3	1.81	0.62
1:C:551:LEU:O	1:C:812:ASN:ND2	2.27	0.62
1:C:750:GLY:O	2:B:787:HIS:NE2	2.32	0.62
1:A:539:THR:OG1	1:A:540:ILE:N	2.31	0.62
2:B:580:CYS:HB3	2:B:629:VAL:HG12	1.81	0.62
2:B:630:THR:HG22	2:B:631:SER:H	1.65	0.62
1:C:731:TRP:CD1	1:C:732:ASP:H	2.19	0.61
1:C:485:GLY:HA2	1:C:499:ASN:CG	2.25	0.61
2:B:531:VAL:HA	2:B:537:CYS:HB2	1.83	0.61
1:A:517:LEU:HD12	1:A:517:LEU:C	2.25	0.61
2:D:529:ARG:N	2:D:575:CYS:O	2.34	0.61
1:C:538:LEU:HA	1:C:732:ASP:HA	1.83	0.60
1:A:736:LEU:HG	1:A:748:THR:HG21	1.76	0.60
1:C:664:ILE:O	1:C:749:THR:OG1	2.19	0.60
2:B:546:PRO:HG3	2:B:554:LEU:HD21	1.83	0.60
1:A:540:ILE:HG22	1:A:730:ILE:HG12	1.83	0.59
1:C:513:ILE:HD12	1:C:517:LEU:HD22	1.84	0.59
2:B:519:THR:OG1	2:B:629:VAL:O	2.18	0.59
2:D:796:THR:OG1	2:D:797:VAL:N	2.36	0.59
2:B:797:VAL:O	2:B:800:SER:OG	2.20	0.58
1:A:558:PHE:HB2	1:A:563:TRP:NE1	2.18	0.58
1:C:414:THR:HA	1:C:420:CYS:HB3	1.86	0.58
1:C:722:ARG:HH21	1:C:743:LYS:HE2	1.67	0.58
2:D:598:TYR:OH	2:D:619:ASP:OD2	2.16	0.58
2:B:831:TYR:HB3	2:B:839:LEU:HD13	1.86	0.58
2:D:547:MET:HA	2:D:601:GLY:HA2	1.86	0.57
1:A:398:LEU:N	1:A:473:THR:O	2.38	0.57
1:A:683:THR:HG21	1:A:690:ASP:HB2	1.86	0.57
1:C:486:THR:HA	1:C:498:TRP:CE3	2.39	0.57
1:C:415:MET:H	1:C:420:CYS:HA	1.70	0.57
1:C:483:LYS:NZ	1:C:712:GLU:O	2.37	0.56
1:C:536:GLN:N	1:C:756:SER:O	2.35	0.56
2:D:792:PHE:O	2:D:816:TYR:OH	2.19	0.56
2:D:831:TYR:HB3	2:D:839:LEU:HD13	1.88	0.56
1:A:535:TYR:CG	2:D:811:PRO:HB2	2.41	0.55
2:B:545:ASP:N	2:B:572:PHE:O	2.36	0.55
2:D:532:ASP:N	2:D:536:LEU:O	2.35	0.55
1:A:486:THR:HG22	1:A:487:GLN:N	2.20	0.55
2:D:817:MET:HB3	2:D:821:ASN:HD21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:THR:OG1	1:A:684:VAL:N	2.38	0.55
1:A:684:VAL:HG23	1:A:685:LYS:H	1.71	0.55
2:B:532:ASP:OD1	2:B:533:ASP:N	2.40	0.54
2:B:629:VAL:HG22	2:B:875:ILE:HD12	1.89	0.54
1:C:401:VAL:HG23	1:C:501:MET:HE3	1.88	0.54
2:D:605:TYR:HA	2:D:616:LEU:HD23	1.89	0.54
1:A:483:LYS:HE2	1:A:684:VAL:HG23	1.89	0.54
1:C:412:LYS:NZ	1:C:456:TYR:OH	2.40	0.54
1:A:523:ARG:O	1:A:527:ILE:N	2.39	0.54
2:D:514:HIS:HA	2:D:594:ASP:HB2	1.91	0.53
1:C:558:PHE:HB2	1:C:563:TRP:NE1	2.24	0.53
2:B:587:LEU:HD21	2:B:887:ILE:HD12	1.91	0.53
2:B:586:GLN:NE2	2:B:589:GLU:OE2	2.42	0.53
2:B:598:TYR:OH	2:B:619:ASP:OD2	2.18	0.53
1:A:483:LYS:HE3	1:A:686:GLN:H	1.74	0.52
1:C:486:THR:HA	1:C:498:TRP:CZ3	2.44	0.52
1:C:675:PRO:HB3	1:C:705:HIS:CE1	2.44	0.52
2:B:806:VAL:O	2:B:810:PHE:N	2.40	0.52
1:A:458:PHE:CE2	1:A:788:LEU:HB3	2.44	0.52
1:A:731:TRP:CD1	1:A:732:ASP:H	2.28	0.52
2:D:650:SER:HA	2:D:872:GLY:HA2	1.91	0.52
2:B:635:ASN:ND2	2:B:638:ARG:HE	2.06	0.52
2:D:806:VAL:HG23	2:D:814:HIS:HB2	1.92	0.52
2:D:856:ASP:HB2	2:D:859:CYS:HA	1.91	0.51
1:C:683:THR:OG1	1:C:684:VAL:N	2.41	0.51
1:C:762:MET:SD	1:C:762:MET:N	2.83	0.51
1:C:742:GLN:OE1	1:C:743:LYS:NZ	2.44	0.51
1:A:403:ILE:HG22	1:A:405:GLN:H	1.77	0.50
2:B:587:LEU:HD11	2:B:887:ILE:HD12	1.94	0.50
1:C:560:SER:HA	1:C:563:TRP:HD1	1.75	0.50
2:D:645:THR:OG1	2:D:875:ILE:N	2.40	0.50
2:B:530:GLU:OE1	2:B:530:GLU:N	2.40	0.50
2:B:883:LEU:O	2:B:887:ILE:HG12	2.12	0.50
1:A:541:LEU:HD21	1:A:729:PHE:HB3	1.94	0.50
1:C:791:THR:HG23	1:C:792:TRP:CD1	2.46	0.50
1:A:412:LYS:O	1:A:454:CYS:N	2.45	0.50
1:A:696:GLN:OE1	1:A:699:LEU:N	2.45	0.50
1:A:408:PHE:HA	1:A:458:PHE:HB3	1.94	0.49
1:C:499:ASN:HD21	1:C:686:GLN:HE21	1.57	0.49
2:B:517:VAL:HG12	2:B:627:MET:HB3	1.95	0.49
2:B:645:THR:OG1	2:B:875:ILE:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:621:LEU:HD11	2:D:641:VAL:HG11	1.92	0.49
1:A:676:SER:H	1:A:705:HIS:HE1	1.59	0.49
1:C:735:VAL:HG13	1:C:736:LEU:HD23	1.94	0.49
1:A:541:LEU:HD21	1:A:729:PHE:HD2	1.77	0.49
1:C:719:GLN:OE1	1:C:722:ARG:NH1	2.46	0.49
2:D:546:PRO:HA	2:D:572:PHE:CD2	2.48	0.49
1:A:402:THR:HG21	1:A:409:VAL:HG11	1.94	0.49
1:A:750:GLY:O	2:D:787:HIS:NE2	2.40	0.49
2:D:544:LEU:HA	2:D:573:LYS:HA	1.95	0.49
1:A:486:THR:OG1	1:A:686:GLN:O	2.27	0.48
1:C:504:GLU:O	1:C:507:SER:OG	2.23	0.48
2:B:641:VAL:HG23	2:B:642:ILE:HG23	1.95	0.48
2:B:803:GLU:HA	2:B:806:VAL:HG22	1.95	0.48
2:D:628:ALA:HB3	2:D:876:GLY:HA3	1.95	0.48
2:D:520:LEU:HD23	2:D:522:GLU:HB2	1.95	0.48
2:B:516:ARG:O	2:B:627:MET:N	2.44	0.48
1:A:704:ARG:HA	1:A:704:ARG:HH11	1.79	0.48
2:D:522:GLU:OE1	2:D:605:TYR:OH	2.27	0.48
1:A:700:SER:O	1:A:704:ARG:HG2	2.14	0.48
2:B:522:GLU:H	2:B:526:VAL:HB	1.79	0.48
1:A:538:LEU:HA	1:A:732:ASP:HA	1.95	0.47
1:C:521:ASN:OD1	1:C:695:ARG:NH2	2.47	0.47
2:B:516:ARG:NH1	2:B:555:ASP:OD1	2.42	0.47
2:B:586:GLN:O	2:B:589:GLU:HG3	2.14	0.47
2:D:529:ARG:O	2:D:575:CYS:N	2.43	0.47
2:D:542:LEU:HD21	2:D:561:LEU:HD11	1.96	0.47
2:B:828:GLY:HA3	2:B:842:PHE:HE2	1.80	0.47
1:C:712:GLU:N	1:C:716:GLU:OE2	2.48	0.47
2:D:726:LEU:HD21	2:D:750:ALA:HB2	1.96	0.47
1:A:483:LYS:NZ	1:A:686:GLN:HG2	2.29	0.47
2:D:797:VAL:O	2:D:800:SER:OG	2.20	0.46
2:D:796:THR:HG22	2:D:817:MET:HE3	1.97	0.46
1:C:404:HIS:CG	1:C:404:HIS:O	2.68	0.46
2:B:678:TRP:O	2:B:681:ILE:HG22	2.15	0.46
2:D:524:PRO:HB3	2:D:851:TYR:CZ	2.51	0.46
1:A:538:LEU:HD23	1:A:538:LEU:H	1.81	0.46
2:B:715:SER:O	2:B:719:ALA:N	2.47	0.46
2:B:560:SER:O	2:B:566:ASP:HA	2.15	0.46
1:A:533:PHE:O	1:A:785:MET:HE2	2.16	0.46
1:C:499:ASN:OD1	1:C:686:GLN:HG3	2.15	0.46
1:A:791:THR:HG23	1:A:792:TRP:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:PHE:HE1	1:C:647:TYR:HD1	1.63	0.46
2:B:792:PHE:O	2:B:816:TYR:OH	2.27	0.46
1:C:535:TYR:CG	2:B:811:PRO:HB2	2.51	0.46
1:C:536:GLN:HG2	1:C:758:PHE:CZ	2.51	0.46
1:C:684:VAL:HA	1:C:711:TYR:O	2.16	0.45
1:A:483:LYS:HZ1	1:A:686:GLN:C	2.25	0.45
2:B:669:PHE:CD1	2:B:933:GLY:HA3	2.51	0.45
1:C:541:LEU:HD11	1:C:729:PHE:HB3	1.99	0.45
2:D:793:ARG:HB2	2:D:820:TYR:CD2	2.51	0.45
1:C:791:THR:O	1:C:795:TYR:OH	2.29	0.45
2:B:634:ILE:HG12	2:B:872:GLY:O	2.16	0.45
2:D:851:TYR:CZ	2:D:855:ILE:HG21	2.52	0.45
2:B:848:LEU:HD13	2:B:848:LEU:HA	1.84	0.45
1:C:400:ILE:HG22	1:C:401:VAL:N	2.31	0.45
1:C:401:VAL:CG2	1:C:513:ILE:HG22	2.47	0.45
2:D:842:PHE:CE1	2:D:844:MET:HB2	2.52	0.45
1:C:517:LEU:HD11	1:C:523:ARG:NH1	2.31	0.45
2:B:650:SER:HA	2:B:872:GLY:HA2	1.99	0.45
2:D:517:VAL:HG11	2:D:584:LEU:HD21	1.98	0.45
2:D:626:ASN:O	2:D:878:PRO:HD3	2.16	0.45
1:C:407:PRO:HG3	1:C:738:PHE:CG	2.52	0.45
1:C:479:VAL:HG11	1:C:482:GLY:HA2	1.99	0.45
1:C:756:SER:OG	1:C:757:GLY:N	2.49	0.45
2:D:612:HIS:CE1	3:D:1001:NAG:HO4	2.34	0.45
1:C:684:VAL:HG22	1:C:687:SER:HB3	1.99	0.44
2:D:844:MET:HG3	2:D:845:ASP:H	1.83	0.44
1:C:441:ASP:H	1:C:448:ARG:NH1	2.15	0.44
1:C:534:LYS:HB2	1:C:534:LYS:HE3	1.78	0.44
1:C:731:TRP:CD1	1:C:732:ASP:N	2.85	0.44
2:D:525:PHE:HB3	2:D:580:CYS:SG	2.58	0.44
1:C:448:ARG:NH2	1:C:449:HIS:O	2.47	0.44
1:C:481:ASP:OD1	1:C:481:ASP:N	2.47	0.44
2:B:851:TYR:HB2	2:B:908:TYR:HE1	1.81	0.44
2:D:602:ASP:OD1	2:D:604:LYS:N	2.37	0.44
1:A:420:CYS:SG	1:A:421:LYS:N	2.91	0.44
1:A:536:GLN:O	1:A:756:SER:N	2.40	0.44
1:C:522:GLU:O	1:C:525:GLN:HG3	2.18	0.44
1:C:640:ALA:HA	1:C:643:ILE:HG22	2.00	0.44
1:C:696:GLN:CD	1:C:698:GLU:H	2.26	0.44
2:D:853:VAL:HA	2:D:856:ASP:OD2	2.18	0.44
1:A:486:THR:CG2	1:A:487:GLN:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:HIS:O	1:C:709:HIS:ND1	2.30	0.43
1:A:688:SER:HA	1:A:691:ILE:HG22	2.00	0.43
2:D:587:LEU:HD22	2:D:887:ILE:HD13	1.99	0.43
1:C:538:LEU:H	1:C:538:LEU:HD23	1.83	0.43
2:B:570:ILE:HD12	2:B:570:ILE:H	1.82	0.43
2:B:638:ARG:O	2:B:642:ILE:HG12	2.19	0.43
1:A:461:ASP:O	1:A:464:ILE:HG22	2.18	0.43
1:C:694:ARG:HA	1:C:703:TYR:OH	2.18	0.43
1:A:483:LYS:HG2	1:A:686:GLN:NE2	2.34	0.43
1:A:756:SER:OG	1:A:757:GLY:N	2.51	0.43
1:C:519:ILE:HG12	1:C:529:PHE:CE2	2.54	0.43
1:C:719:GLN:CD	1:C:722:ARG:HH12	2.26	0.43
2:B:517:VAL:HG23	2:B:597:LEU:HA	2.01	0.43
1:A:408:PHE:O	1:A:409:VAL:HG23	2.19	0.43
1:A:479:VAL:HG13	1:A:482:GLY:HA2	2.01	0.43
1:C:487:GLN:HB2	1:C:497:GLU:N	2.34	0.43
2:B:514:HIS:NE2	2:B:596:ASP:OD2	2.46	0.43
1:A:693:PHE:O	1:A:696:GLN:NE2	2.52	0.42
2:B:525:PHE:HB3	2:B:580:CYS:SG	2.59	0.42
2:B:895:LYS:HA	2:B:900:MET:SD	2.59	0.42
1:C:436:CYS:O	1:C:453:GLN:N	2.30	0.42
1:C:536:GLN:O	1:C:756:SER:N	2.43	0.42
1:A:483:LYS:HG2	1:A:686:GLN:HE21	1.85	0.42
1:A:718:ILE:HG21	1:A:739:GLU:OE1	2.19	0.42
2:D:645:THR:HG21	2:D:875:ILE:HB	2.00	0.42
2:D:652:SER:OG	2:D:653:LEU:N	2.53	0.42
1:A:536:GLN:NE2	1:A:734:ALA:H	2.17	0.42
2:B:842:PHE:HE1	2:B:844:MET:HB2	1.85	0.42
2:D:669:PHE:CD1	2:D:933:GLY:HA3	2.54	0.42
1:A:771:ASN:HD21	3:A:902:NAG:H2	1.84	0.42
2:D:796:THR:HB	2:D:843:ILE:HG23	2.02	0.42
1:A:409:VAL:HA	1:A:457:GLY:HA3	2.02	0.42
1:A:415:MET:H	1:A:420:CYS:HA	1.85	0.42
1:C:457:GLY:HA2	1:C:792:TRP:CZ3	2.55	0.42
1:C:560:SER:HA	1:C:563:TRP:CD1	2.54	0.42
1:C:732:ASP:O	1:C:736:LEU:HG	2.20	0.42
2:B:729:GLY:C	2:B:730:ARG:HD2	2.45	0.42
2:D:634:ILE:HG22	2:D:872:GLY:O	2.20	0.42
1:A:522:GLU:O	1:A:525:GLN:HG3	2.20	0.42
1:C:504:GLU:HG3	1:C:510:ALA:HB3	2.01	0.42
1:A:402:THR:CG2	1:A:409:VAL:HG11	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:SER:OG	1:A:531:LYS:N	2.53	0.41
1:C:675:PRO:HB3	1:C:705:HIS:HE1	1.84	0.41
1:C:789:ASP:OD1	2:B:819:ARG:NH2	2.53	0.41
2:D:851:TYR:CE2	2:D:855:ILE:HD13	2.55	0.41
2:B:856:ASP:HB2	2:B:859:CYS:HA	2.02	0.41
2:D:634:ILE:HD13	2:D:644:PHE:CD2	2.54	0.41
1:C:401:VAL:HG23	1:C:513:ILE:HG22	2.02	0.41
2:B:598:TYR:OH	2:B:625:ALA:HB2	2.21	0.41
2:B:793:ARG:O	2:B:840:ASP:HB2	2.20	0.41
2:D:795:GLY:HA3	2:D:820:TYR:O	2.20	0.41
1:A:539:THR:HG23	1:A:736:LEU:HD23	2.01	0.41
2:B:520:LEU:HD13	2:B:603:GLY:HA2	2.02	0.41
2:D:798:ARG:HD3	2:D:821:ASN:HB2	2.03	0.41
1:A:412:LYS:O	1:A:453:GLN:HB2	2.20	0.41
1:C:515:ALA:O	1:C:517:LEU:N	2.54	0.41
2:D:569:PRO:HG2	2:D:572:PHE:CD1	2.56	0.41
2:D:656:LEU:HD12	2:D:861:LEU:HD13	2.02	0.41
2:D:853:VAL:HG12	2:D:861:LEU:HD12	2.03	0.41
1:C:667:ILE:HB	1:C:753:PHE:CE2	2.55	0.41
2:B:524:PRO:HB3	2:B:851:TYR:CZ	2.55	0.41
1:C:731:TRP:HB3	1:C:736:LEU:HD21	2.03	0.41
2:B:606:GLY:HA2	2:B:614:THR:HG23	2.02	0.41
2:D:822:VAL:HG11	2:D:828:GLY:HA2	2.03	0.41
1:A:410:TYR:HB3	1:A:412:LYS:NZ	2.36	0.41
1:A:788:LEU:HA	1:A:791:THR:HG22	2.03	0.40
1:A:770:GLN:O	1:A:773:SER:OG	2.26	0.40
1:C:400:ILE:CG2	1:C:401:VAL:N	2.83	0.40
1:C:463:LEU:HD13	1:C:514:VAL:HG21	2.03	0.40
1:C:502:MET:O	1:C:505:LEU:HG	2.22	0.40
1:A:731:TRP:CG	1:A:732:ASP:H	2.39	0.40
1:A:736:LEU:CD2	1:A:748:THR:HG22	2.51	0.40
2:B:621:LEU:HD23	2:B:621:LEU:HA	1.94	0.40
1:A:408:PHE:C	1:A:409:VAL:HG23	2.46	0.40
2:B:520:LEU:HD23	2:B:605:TYR:CE1	2.56	0.40
2:B:630:THR:O	2:B:632:PHE:N	2.54	0.40
1:A:541:LEU:HD21	1:A:729:PHE:CD2	2.56	0.40
1:C:513:ILE:HD13	1:C:513:ILE:HG21	1.85	0.40
2:D:570:ILE:HD12	2:D:570:ILE:HA	1.92	0.40
2:D:632:PHE:O	2:D:873:TYR:HA	2.22	0.40
2:D:671:TRP:N	2:D:672:PRO:HD2	2.37	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	373/870 (43%)	348 (93%)	25 (7%)	0	100	100
1	C	373/870 (43%)	343 (92%)	30 (8%)	0	100	100
2	B	387/993 (39%)	372 (96%)	15 (4%)	0	100	100
2	D	386/993 (39%)	367 (95%)	19 (5%)	0	100	100
All	All	1519/3726 (41%)	1430 (94%)	89 (6%)	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	201/747 (27%)	201 (100%)	0	100	100
1	C	204/747 (27%)	202 (99%)	2 (1%)	68	75
2	B	226/861 (26%)	226 (100%)	0	100	100
2	D	219/861 (25%)	217 (99%)	2 (1%)	70	76
All	All	850/3216 (26%)	846 (100%)	4 (0%)	78	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	499	ASN
1	C	780	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	543	CYS
2	D	799	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	C	686	GLN
2	B	610	ASN
2	B	635	ASN
2	D	781	HIS
2	D	821	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](#)

10 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	NAG	B	1002	-	14,14,15	0.27	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	901	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1001	2	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	A	902	-	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	D	1001	2	14,14,15	0.25	0	17,19,21	0.36	0
3	NAG	D	1002	-	14,14,15	0.24	0	17,19,21	0.56	0
3	NAG	B	1003	2	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	A	901	1	14,14,15	0.96	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	D	1003	2	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	C	902	1	14,14,15	0.21	0	17,19,21	0.55	0

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
3	NAG	B	1002	-	-	4/6/23/26	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	A	902	-	-	2/6/23/26	0/1/1/1
3	NAG	D	1001	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1002	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAG	O5-C1	2.60	1.48	1.43
3	A	901	NAG	C1-C2	2.28	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAG	C1-O5-C5	3.34	116.66	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1003	NAG	C4-C5-C6-O6
3	A	902	NAG	C4-C5-C6-O6
3	B	1003	NAG	C4-C5-C6-O6
3	B	1001	NAG	O5-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6
3	D	1003	NAG	O5-C5-C6-O6
3	B	1003	NAG	O5-C5-C6-O6
3	A	901	NAG	C8-C7-N2-C2
3	A	901	NAG	O7-C7-N2-C2
3	C	901	NAG	C8-C7-N2-C2
3	C	901	NAG	O7-C7-N2-C2
3	B	1002	NAG	O5-C5-C6-O6
3	B	1002	NAG	C4-C5-C6-O6
3	B	1001	NAG	C4-C5-C6-O6
3	D	1001	NAG	O5-C5-C6-O6
3	C	902	NAG	C1-C2-N2-C7
3	B	1002	NAG	C1-C2-N2-C7
3	A	901	NAG	C4-C5-C6-O6
3	C	902	NAG	C4-C5-C6-O6
3	A	901	NAG	O5-C5-C6-O6
3	B	1002	NAG	C3-C2-N2-C7
3	D	1002	NAG	C3-C2-N2-C7
3	C	902	NAG	O5-C5-C6-O6
3	D	1002	NAG	C1-C2-N2-C7
3	C	902	NAG	C3-C2-N2-C7

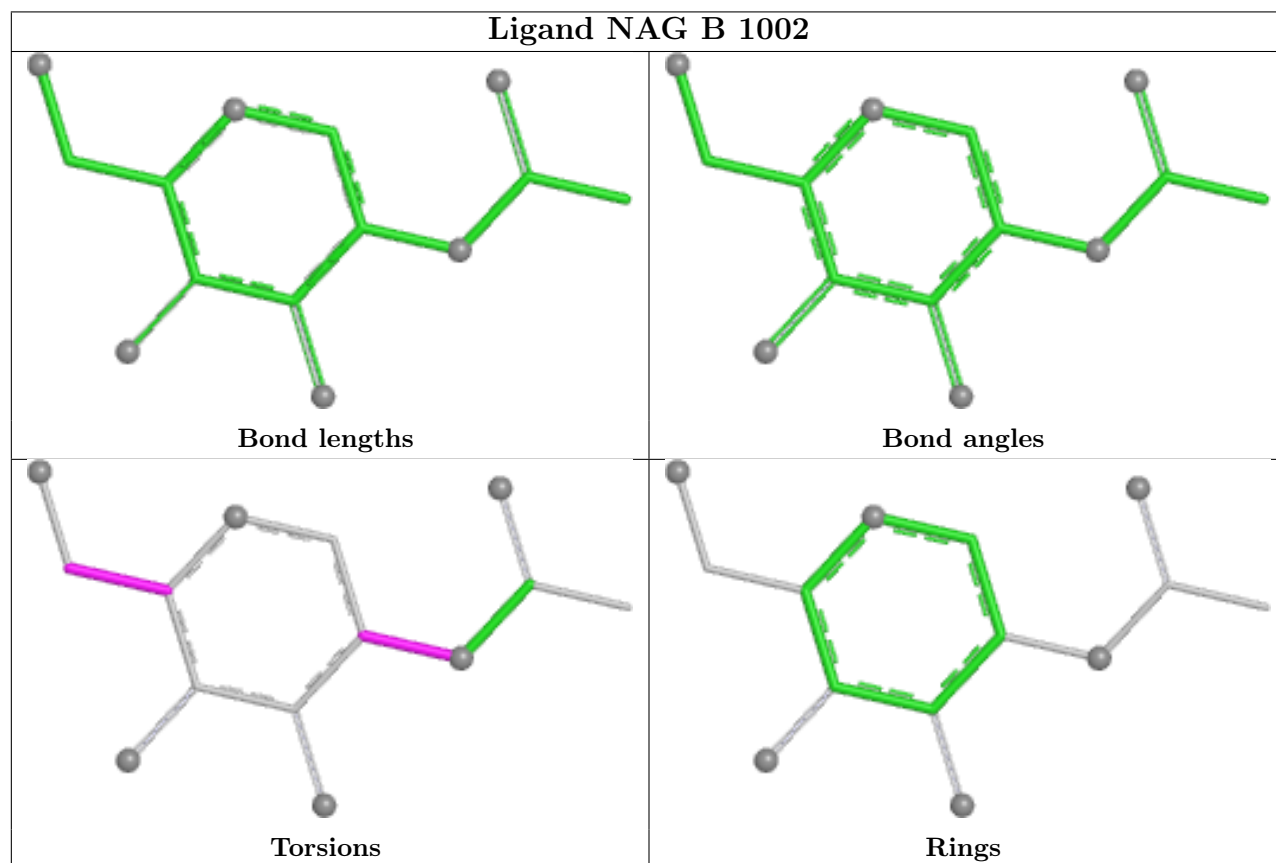
There are no ring outliers.

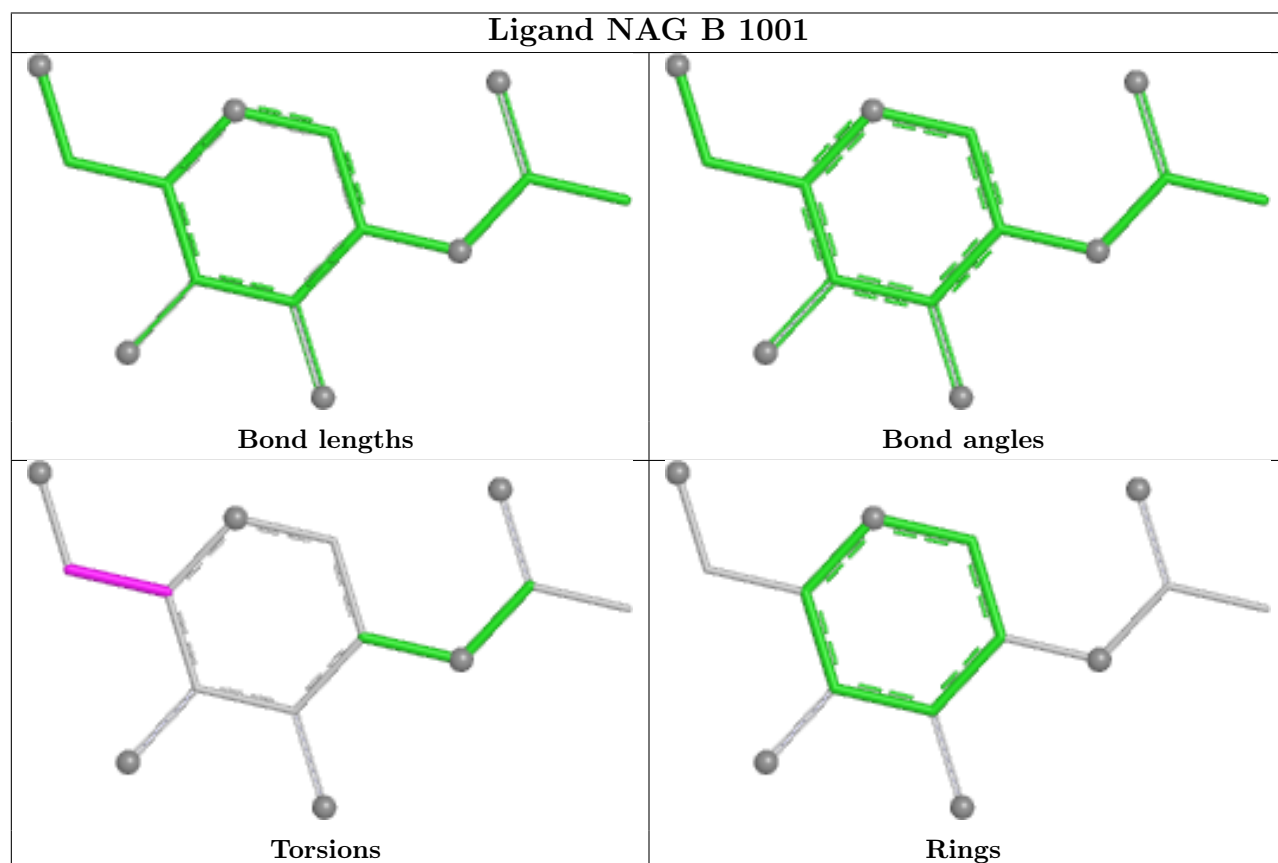
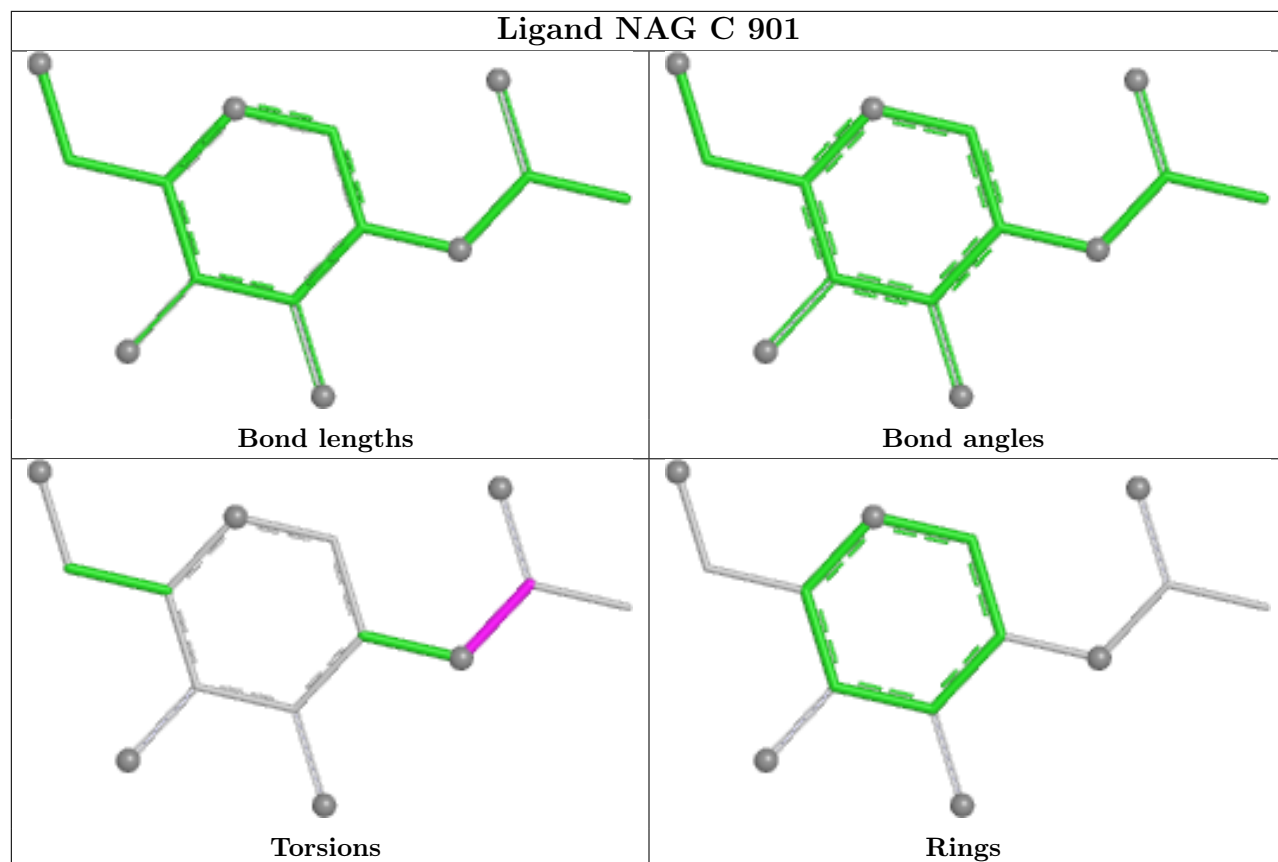
3 monomers are involved in 3 short contacts:

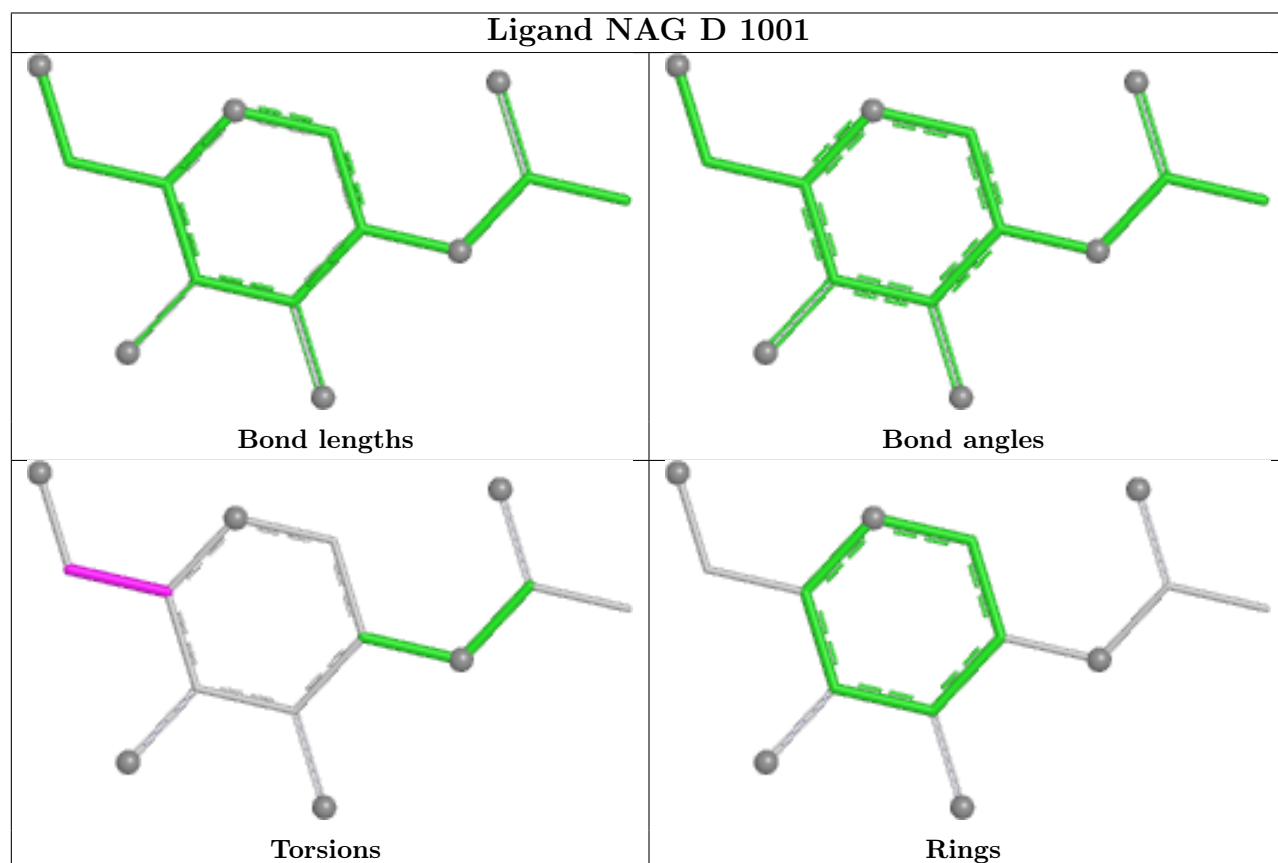
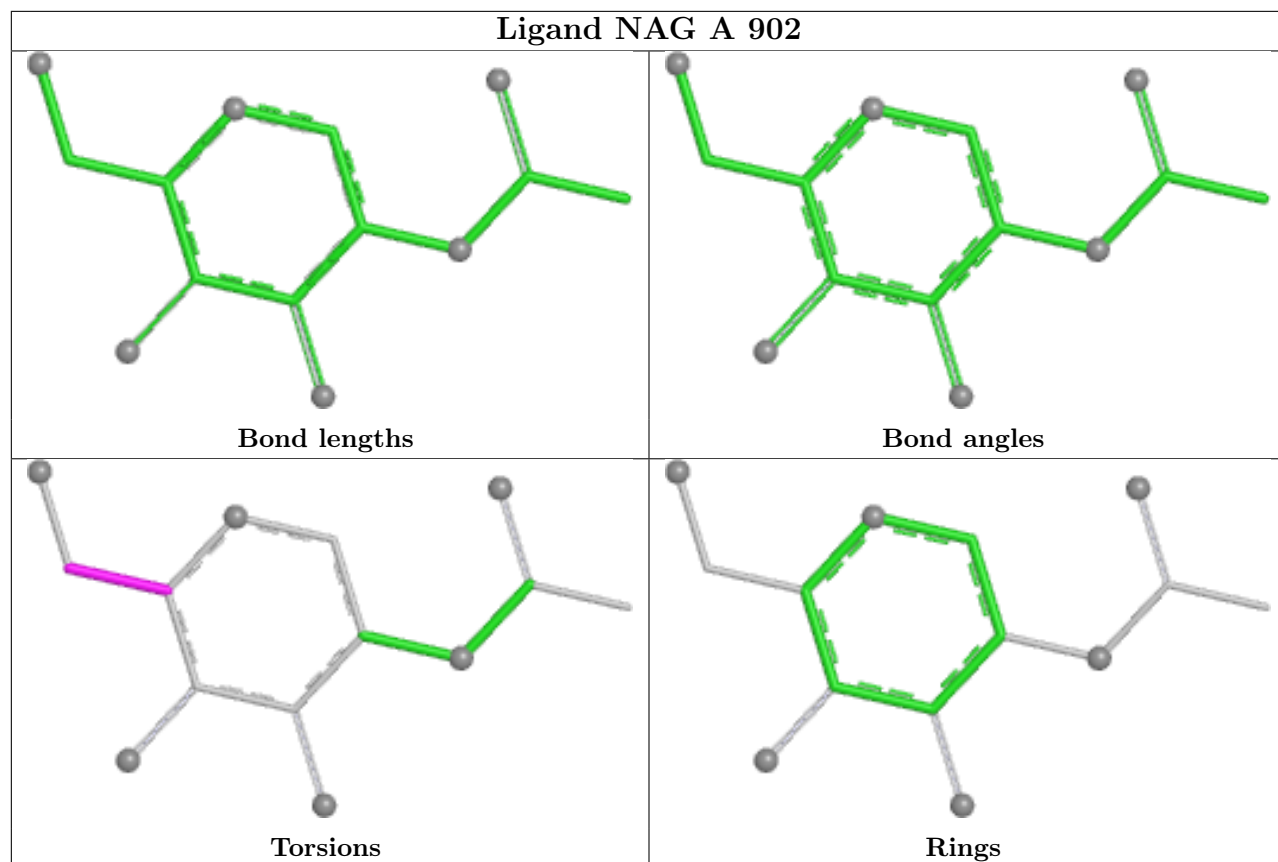
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	NAG	1	0
3	A	902	NAG	1	0
3	D	1001	NAG	1	0

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

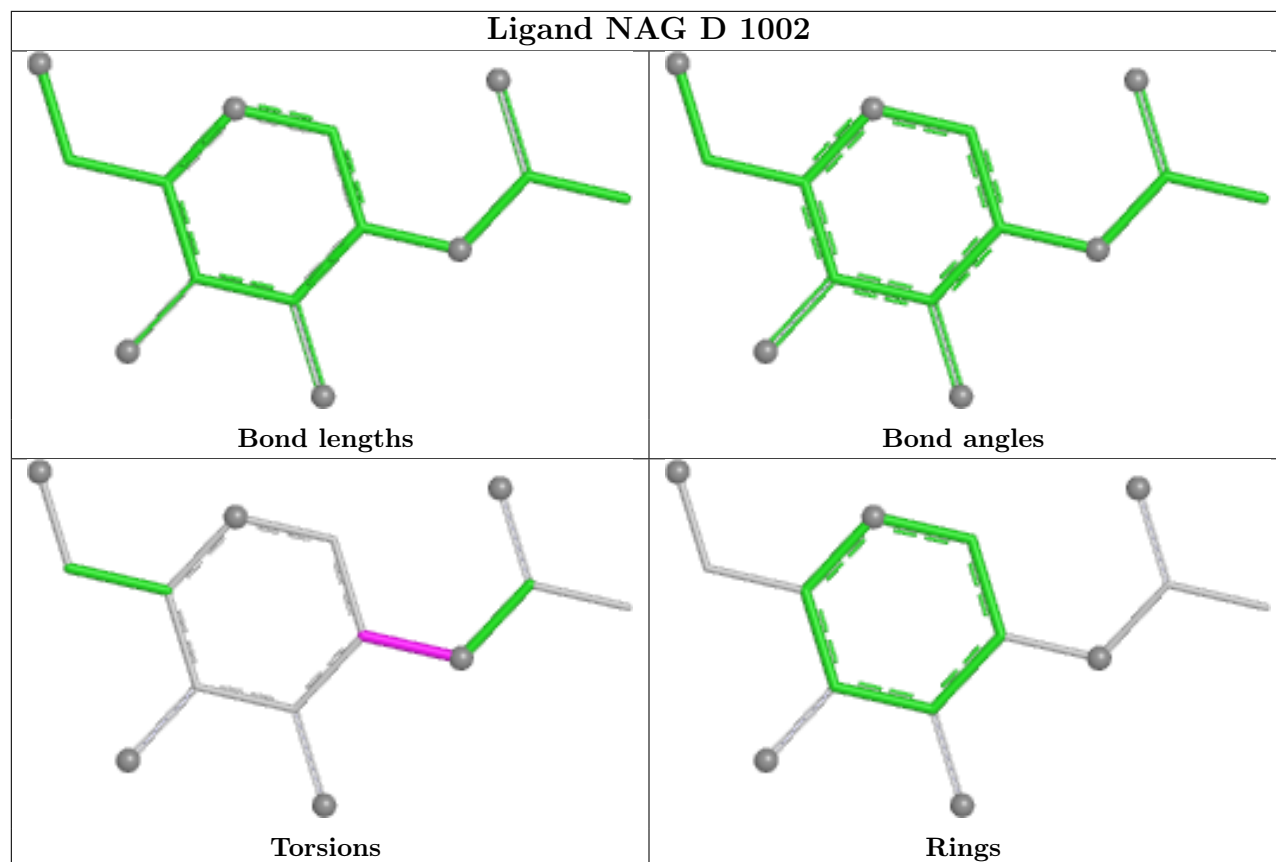
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



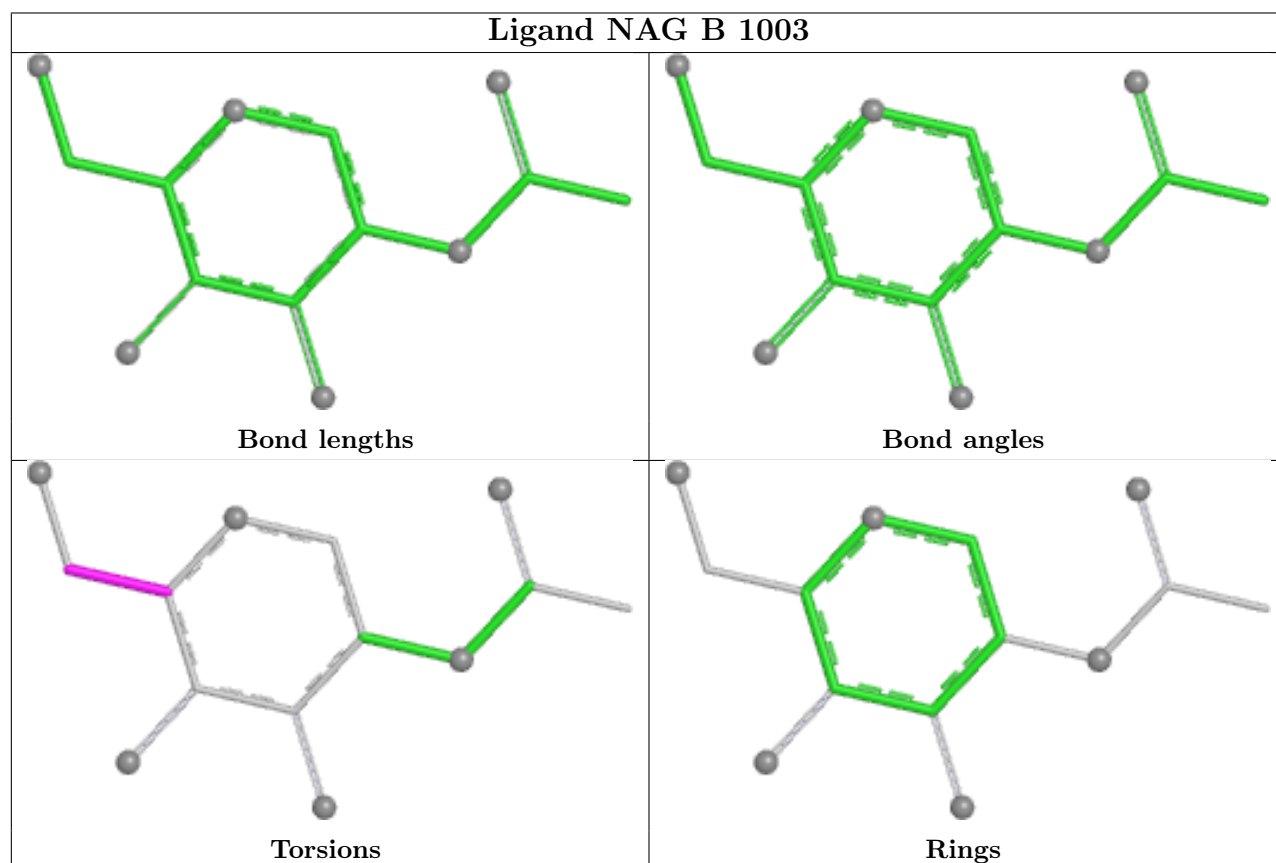


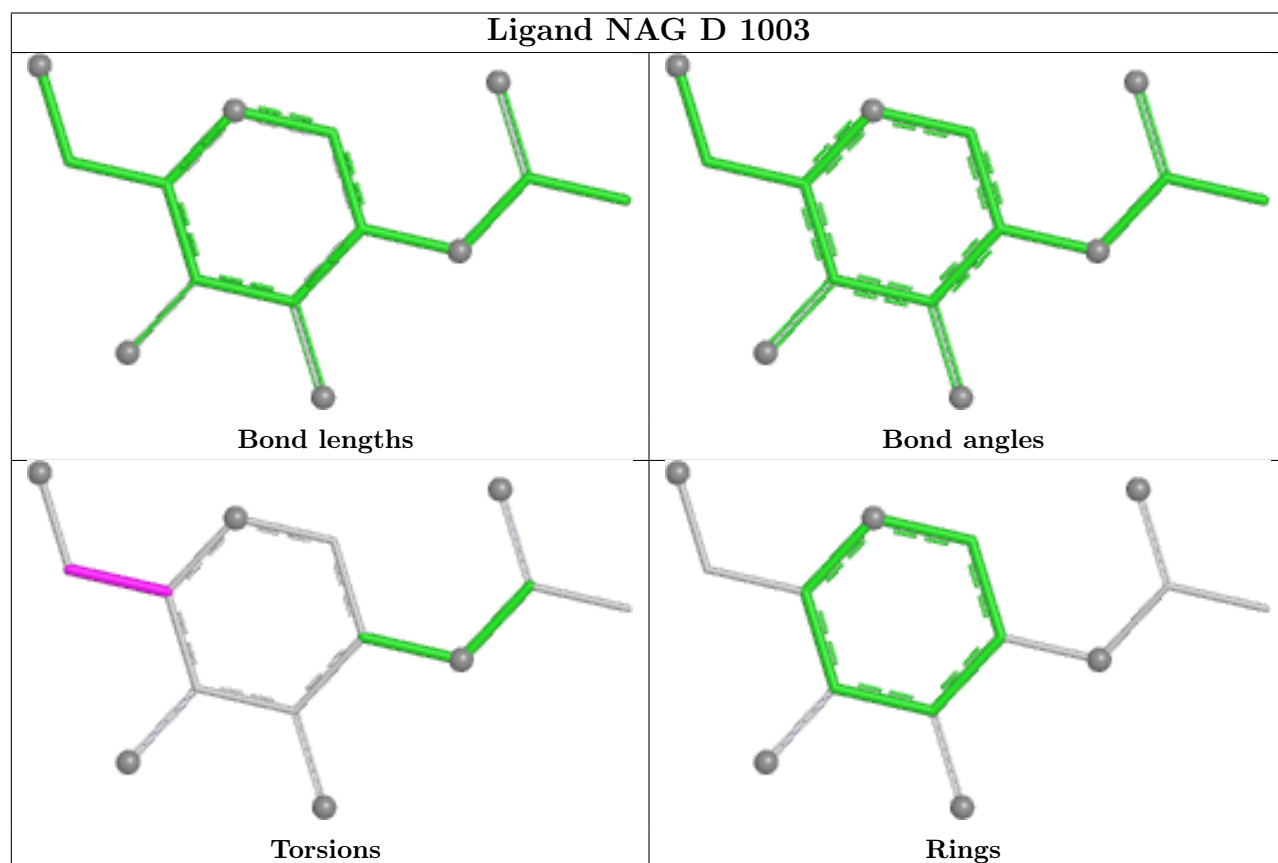
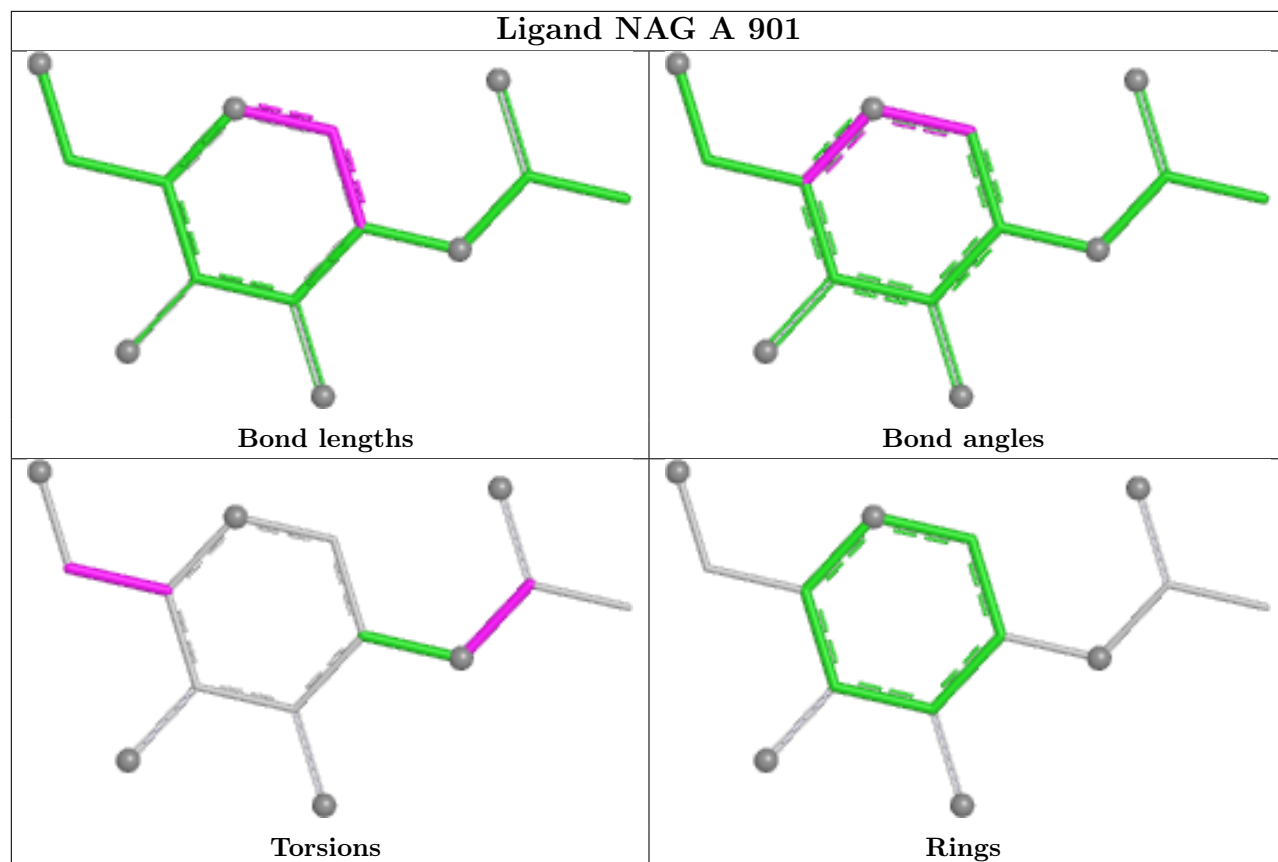


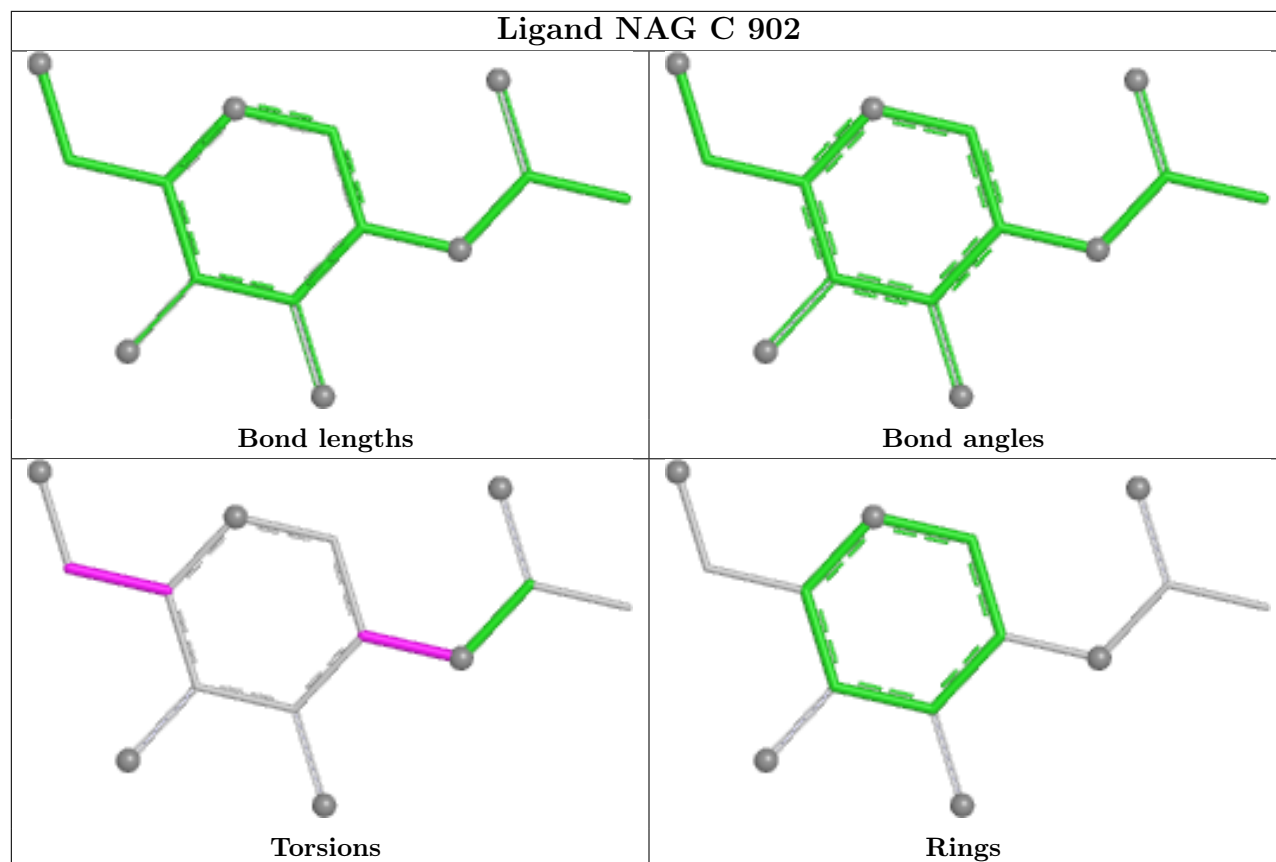
Ligand NAG D 1002



Ligand NAG B 1003







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.

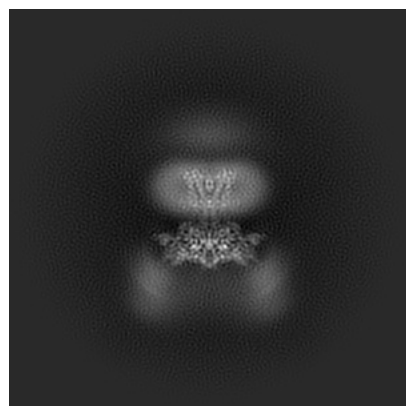
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70405. These allow visual inspection of the internal detail of the map and identification of artifacts.

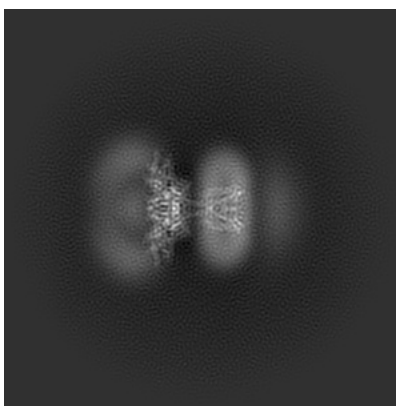
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

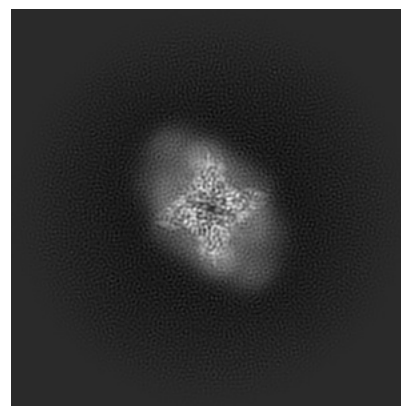
6.1.1 Primary map



X

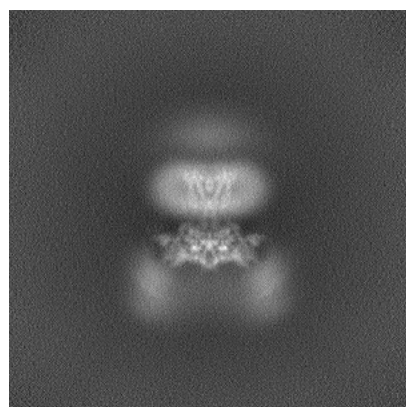


Y

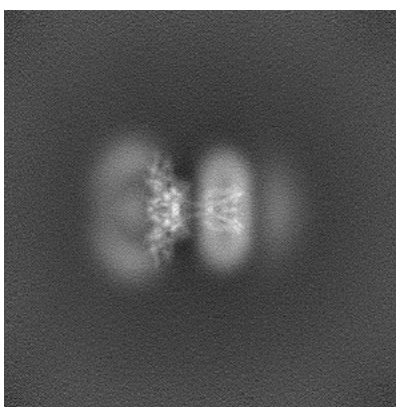


Z

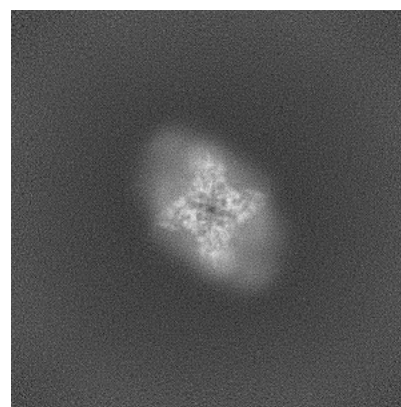
6.1.2 Raw map



X



Y

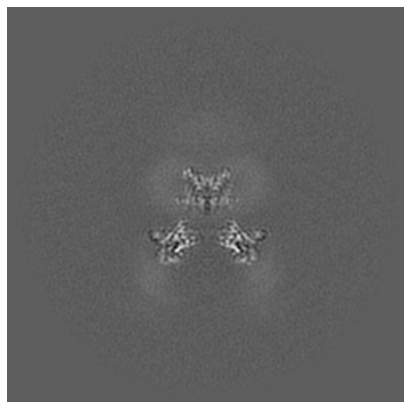


Z

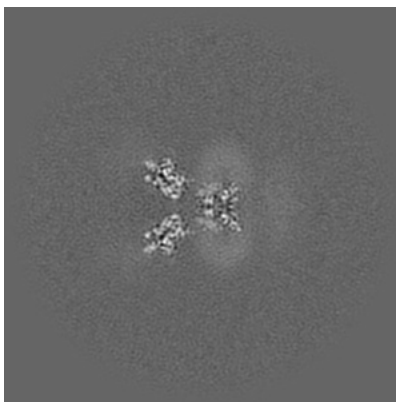
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

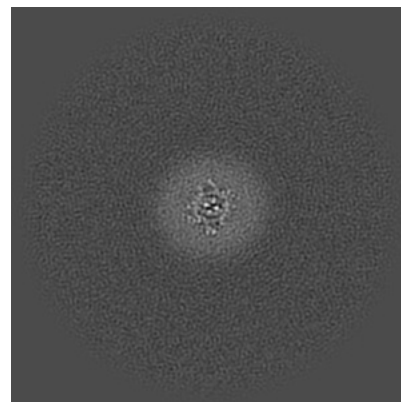
6.2.1 Primary map



X Index: 256

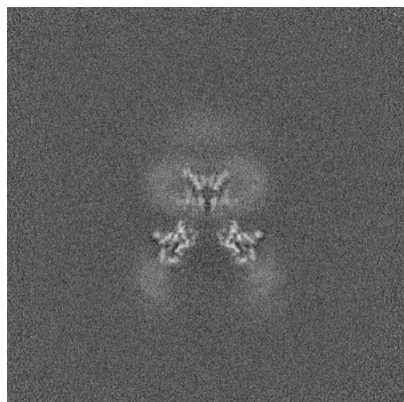


Y Index: 256

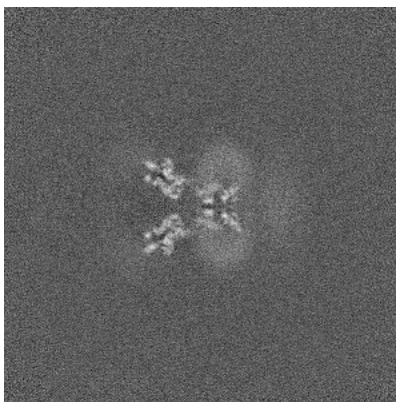


Z Index: 256

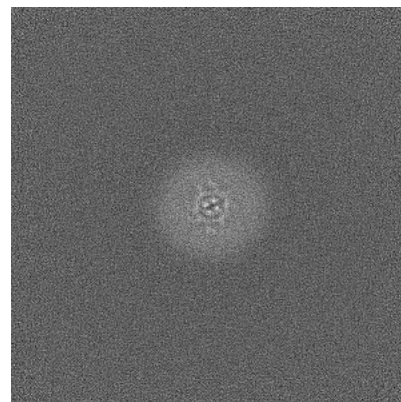
6.2.2 Raw map



X Index: 256



Y Index: 256

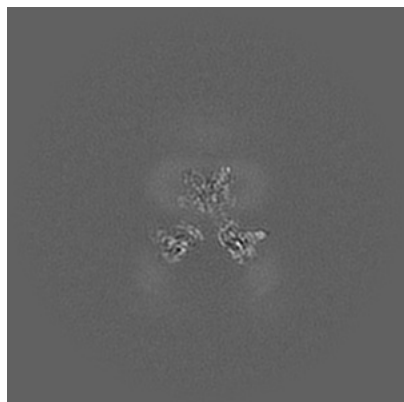


Z Index: 256

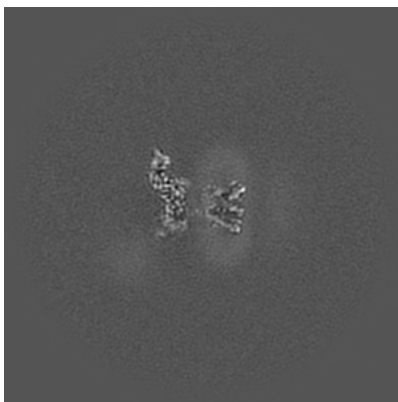
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

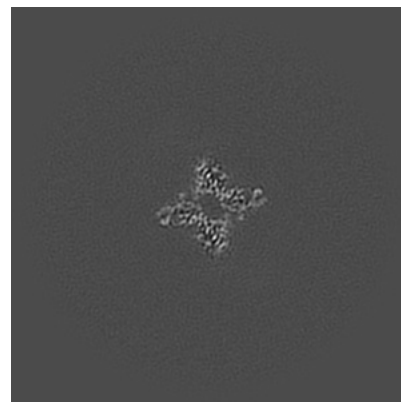
6.3.1 Primary map



X Index: 252

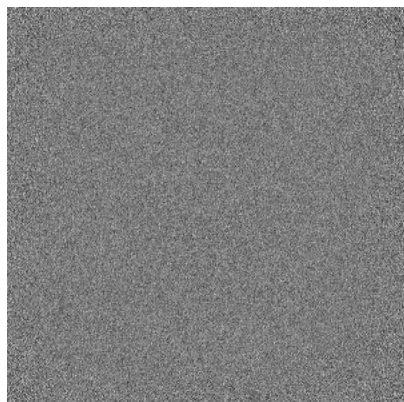


Y Index: 275

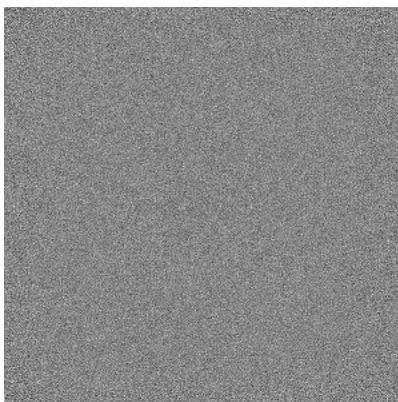


Z Index: 208

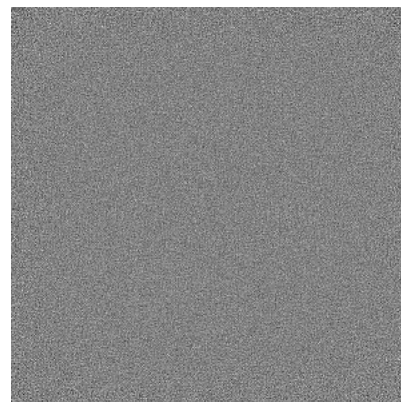
6.3.2 Raw map



X Index: 0



Y Index: 0

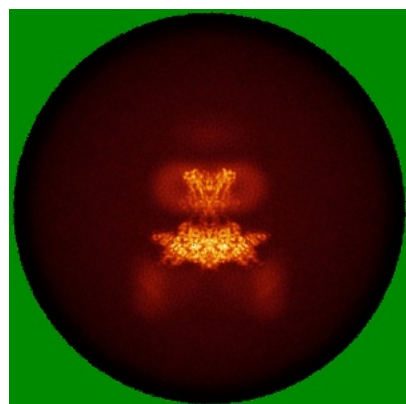


Z Index: 0

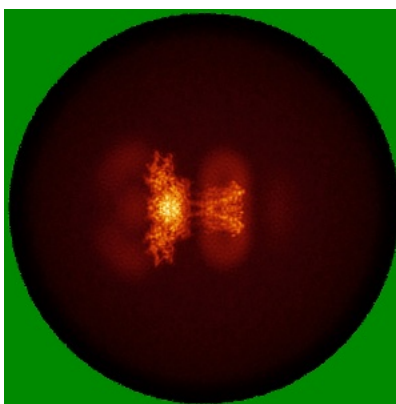
The images above show the largest variance slices of the map in three orthogonal directions.

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

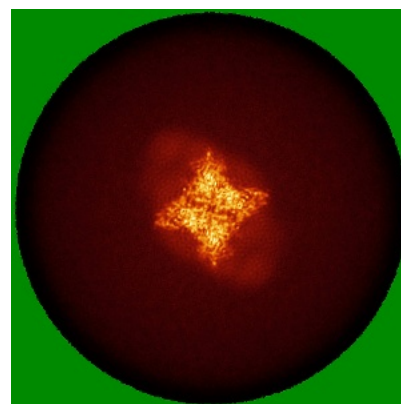
6.4.1 Primary map



X

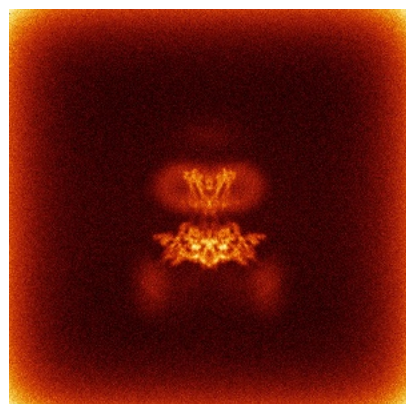


Y

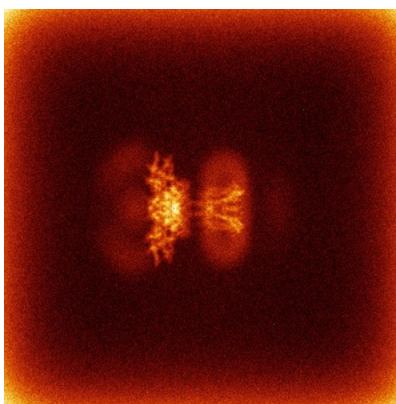


Z

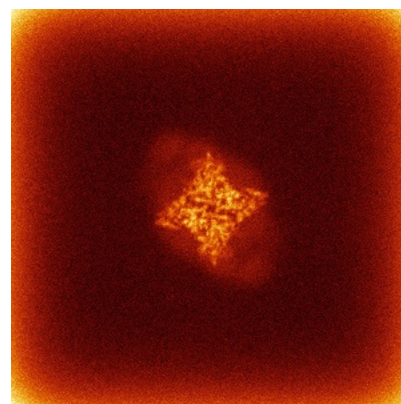
6.4.2 Raw map



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.

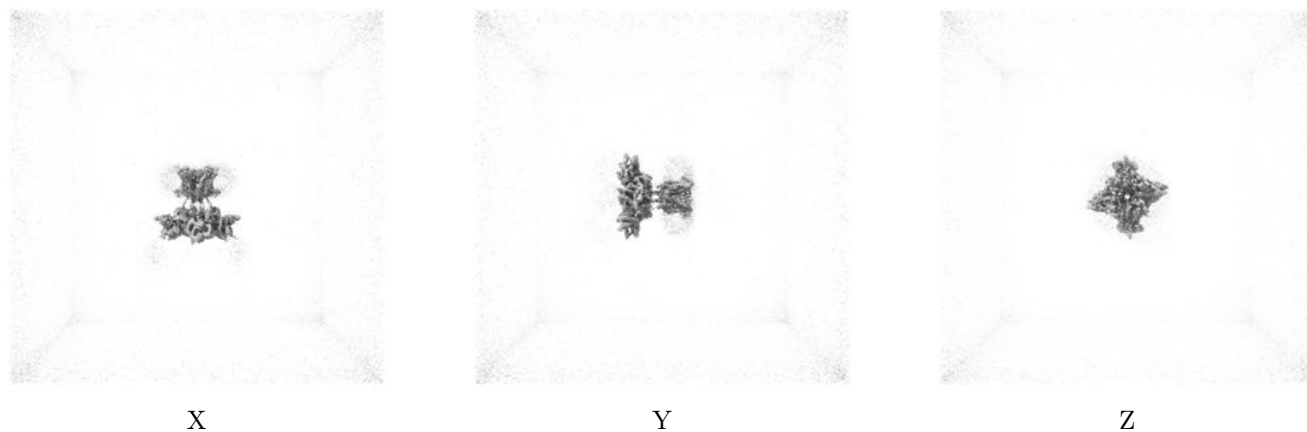
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

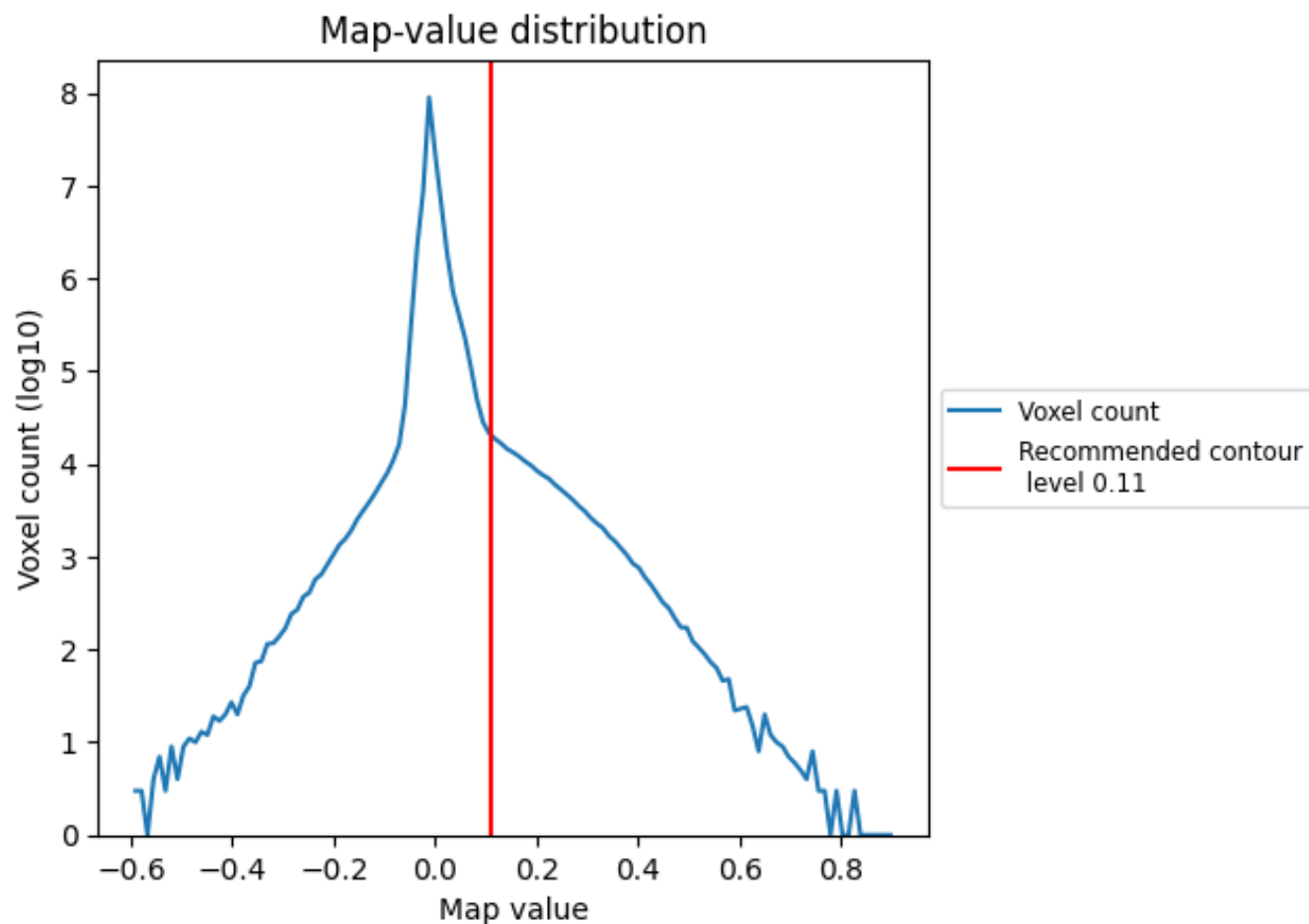
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

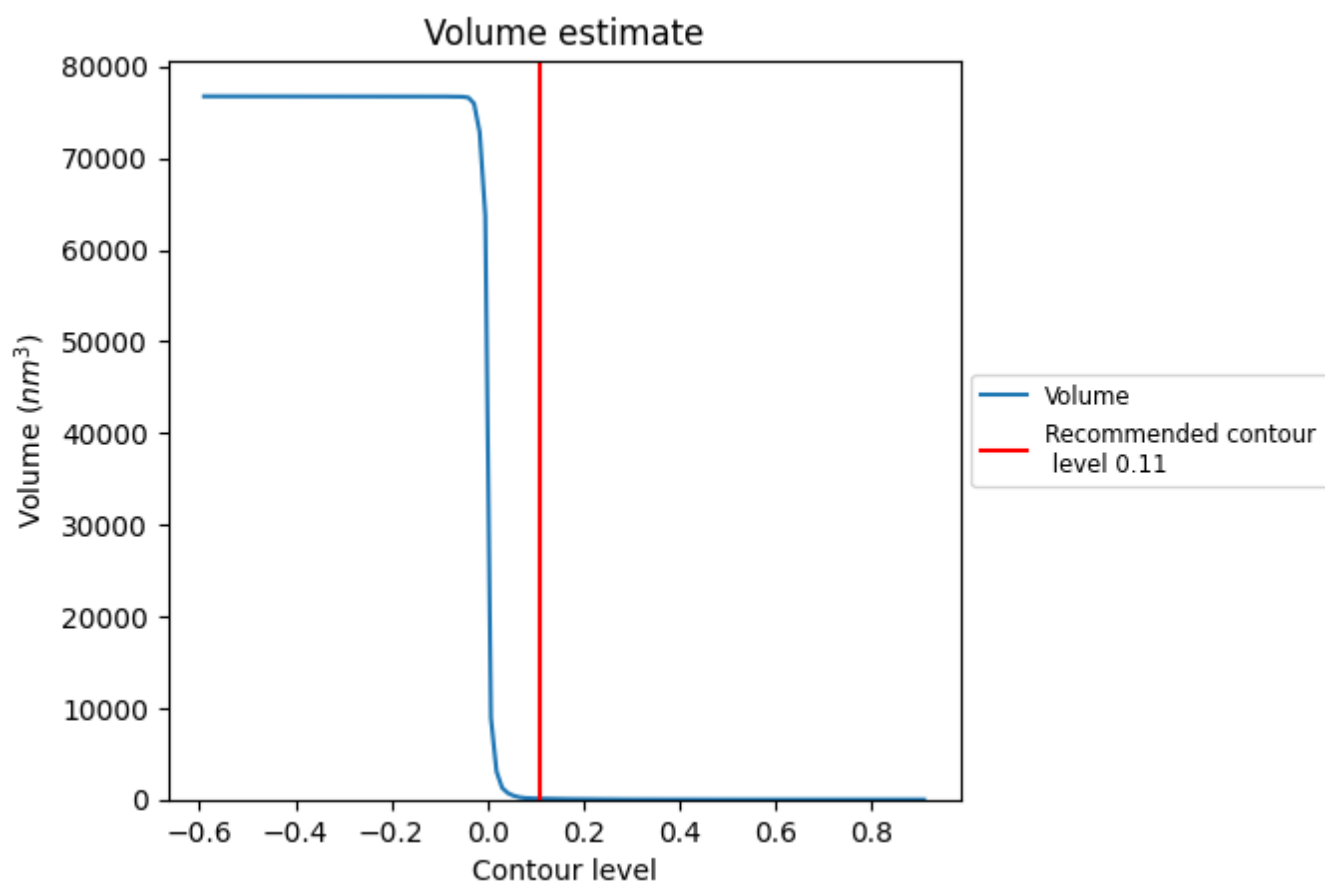
This section contains the results of statistical analysis of the map.

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.

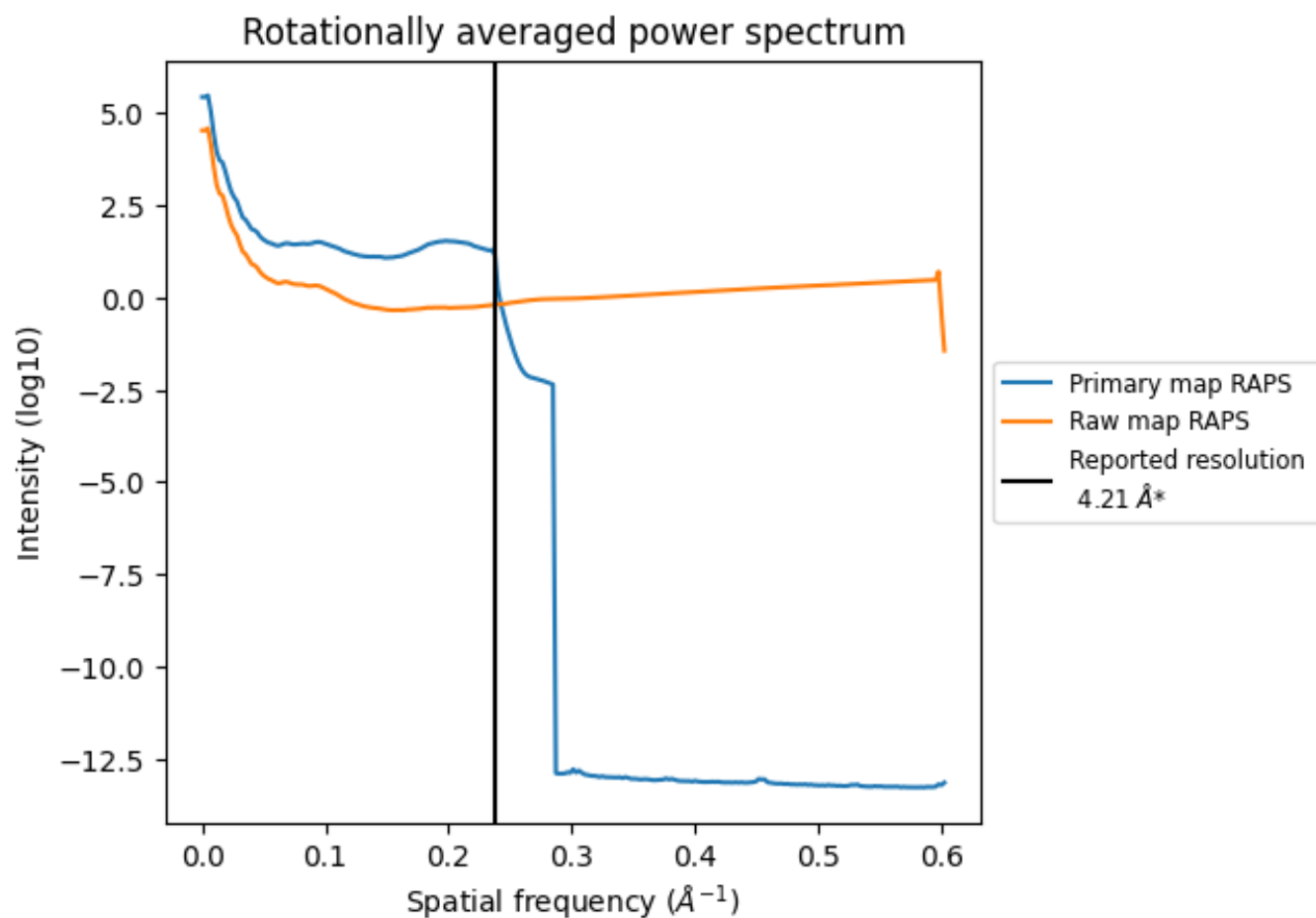
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 ⓘ

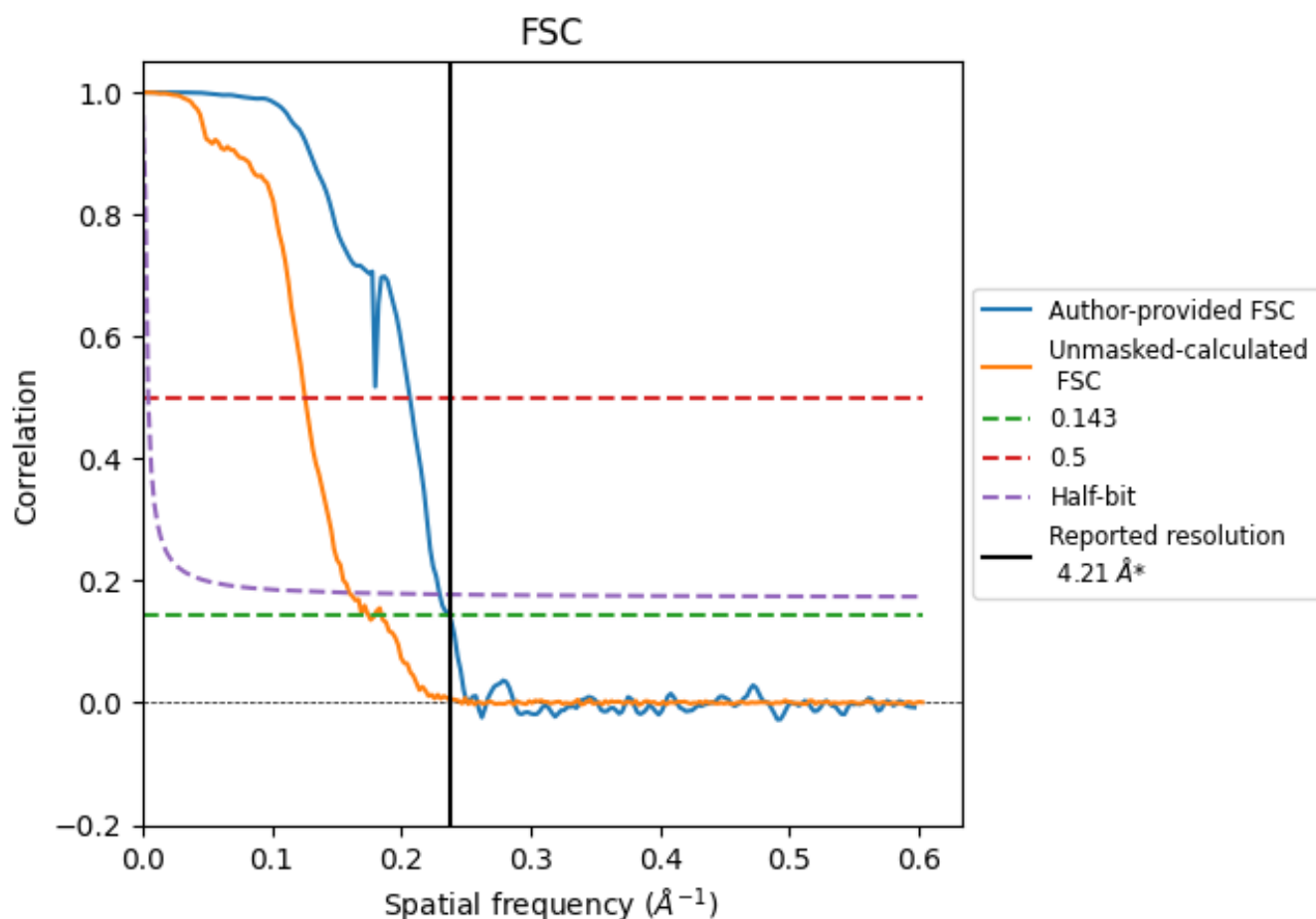


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

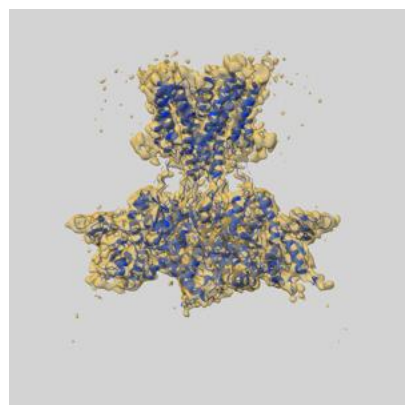
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	4.21	4.84	4.35
Unmasked-calculated*	5.72	7.96	6.25

*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 5.72 differs from the reported value 4.21 by more than 10 %

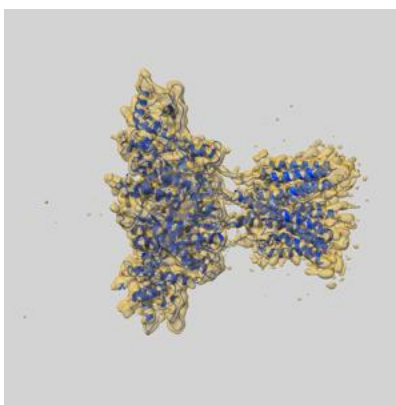
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70405 and PDB model 9OEO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

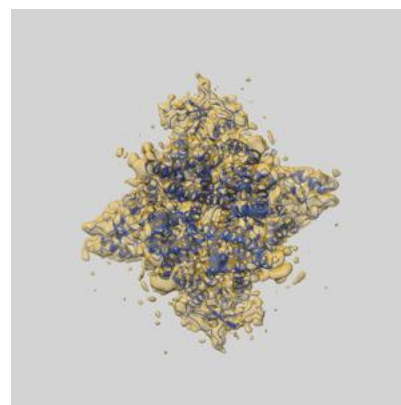
9.1 Map-model overlay [i](#)



X



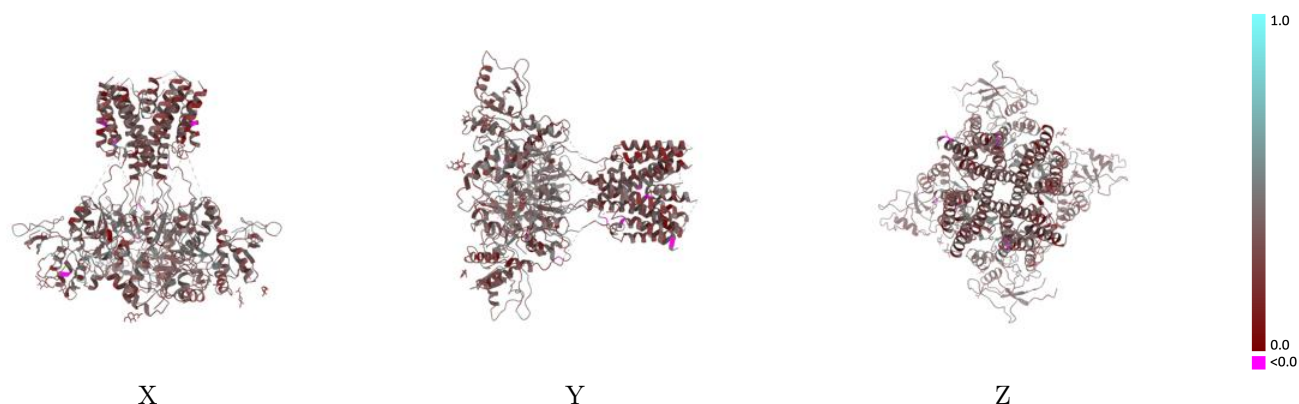
Y



Z

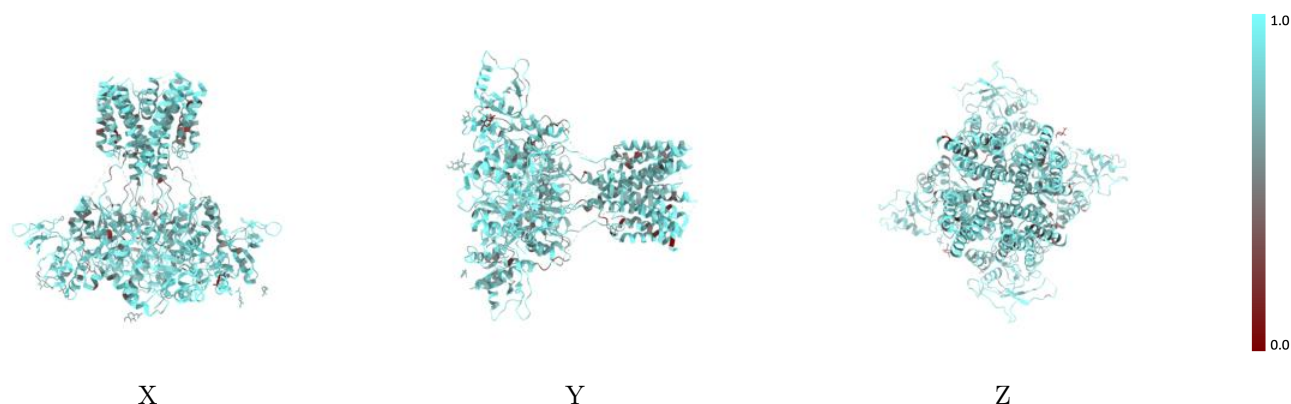
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



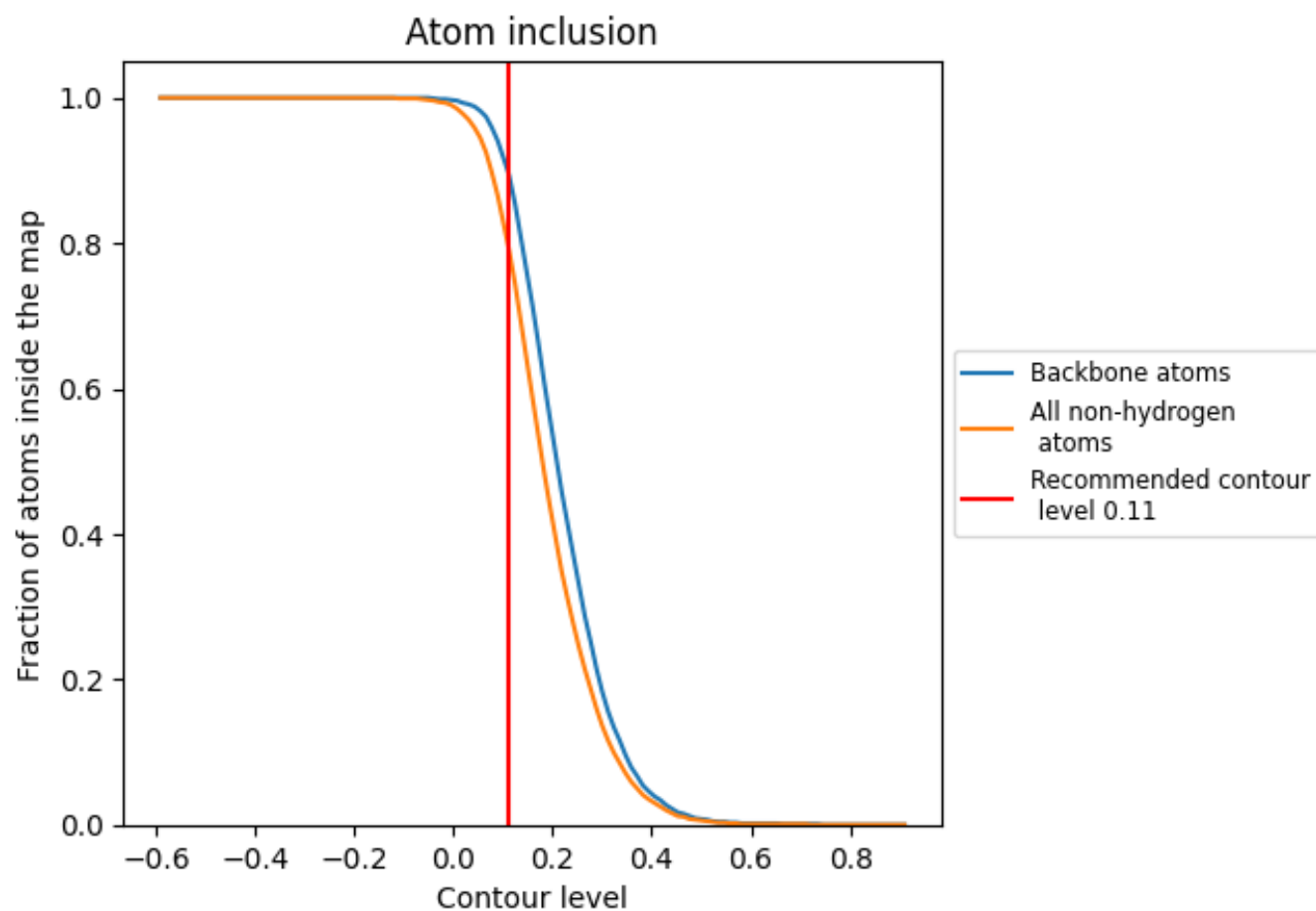
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.3680
A	0.7960	0.3650
B	0.8010	0.3690
C	0.7860	0.3640
D	0.8130	0.3740

