



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:24 AM UTC

PDB ID : 9U62 / pdb_00009u62
EMDB ID : EMD-63895
Title : AP pathways C3 convertase C3bBbP and C3 complex
Authors : Yang, X.K.; Xiao, J.Y.
Deposited on : 2025-03-22
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

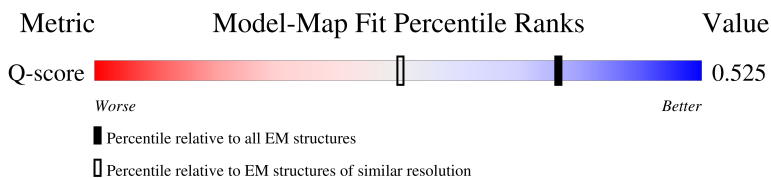
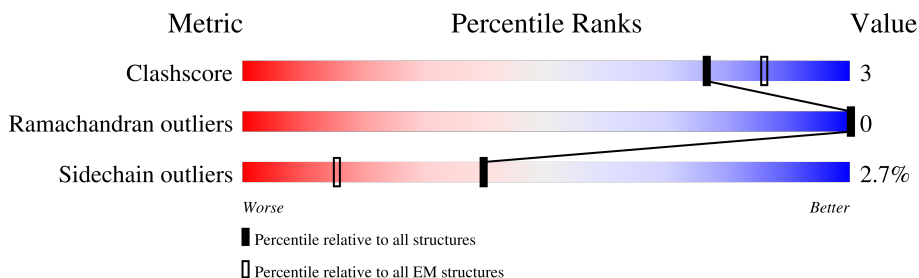
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	C	1663	
1	D	1663	
1	E	1663	
2	B	505	

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Mol	Chain	Length	Quality of chain
3	P	453	21%26%72%
4	A	2	100%100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29513 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 Complement C3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	970	Total	C	N	O	S	0	0
			7760	4911	1327	1477	45		
1	E	1474	Total	C	N	O	S	0	0
			11688	7426	1968	2243	51		
1	C	632	Total	C	N	O	S	0	0
			4922	3136	831	940	15		

- Molecule 2 is a protein called Complement factor B Bb.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			4012	2548	689	755	20		

- Molecule 3 is a protein called Properdin.

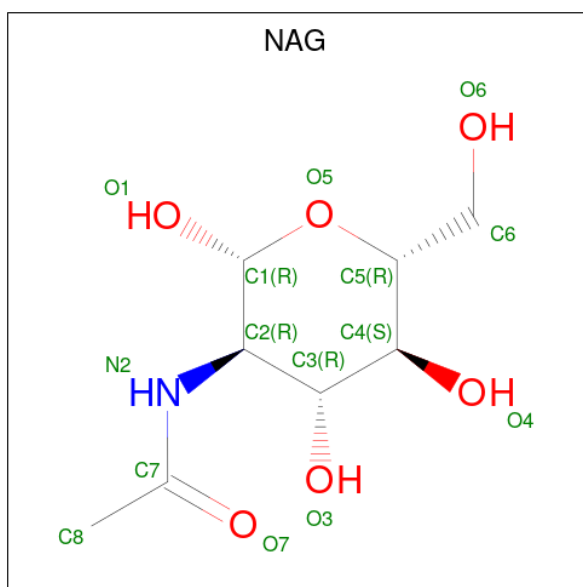
Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	127	Total	C	N	O	S	0	0
			1032	637	201	184	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

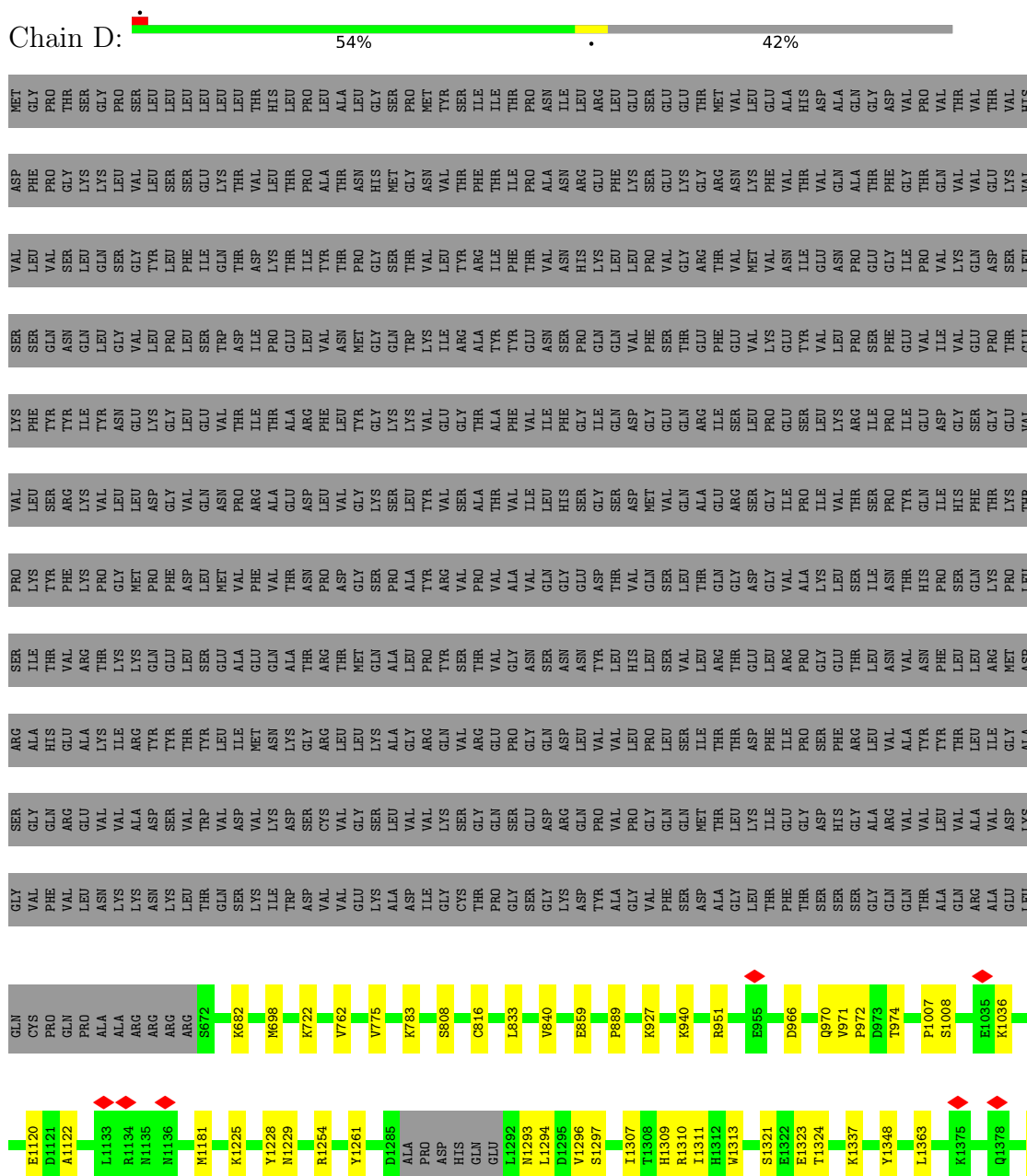
- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

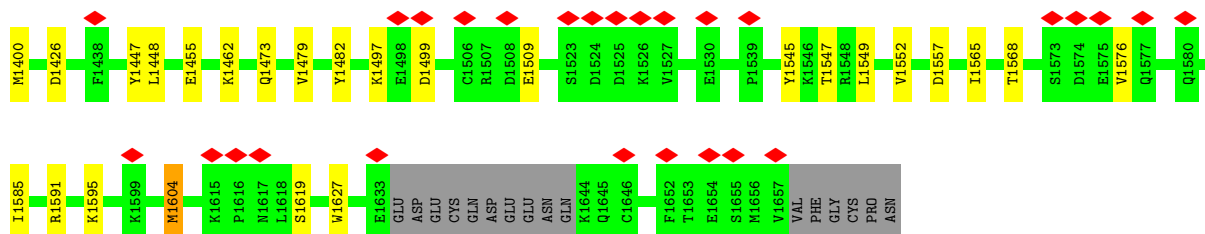
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ni	0
			1	1	

3 Residue-property plots

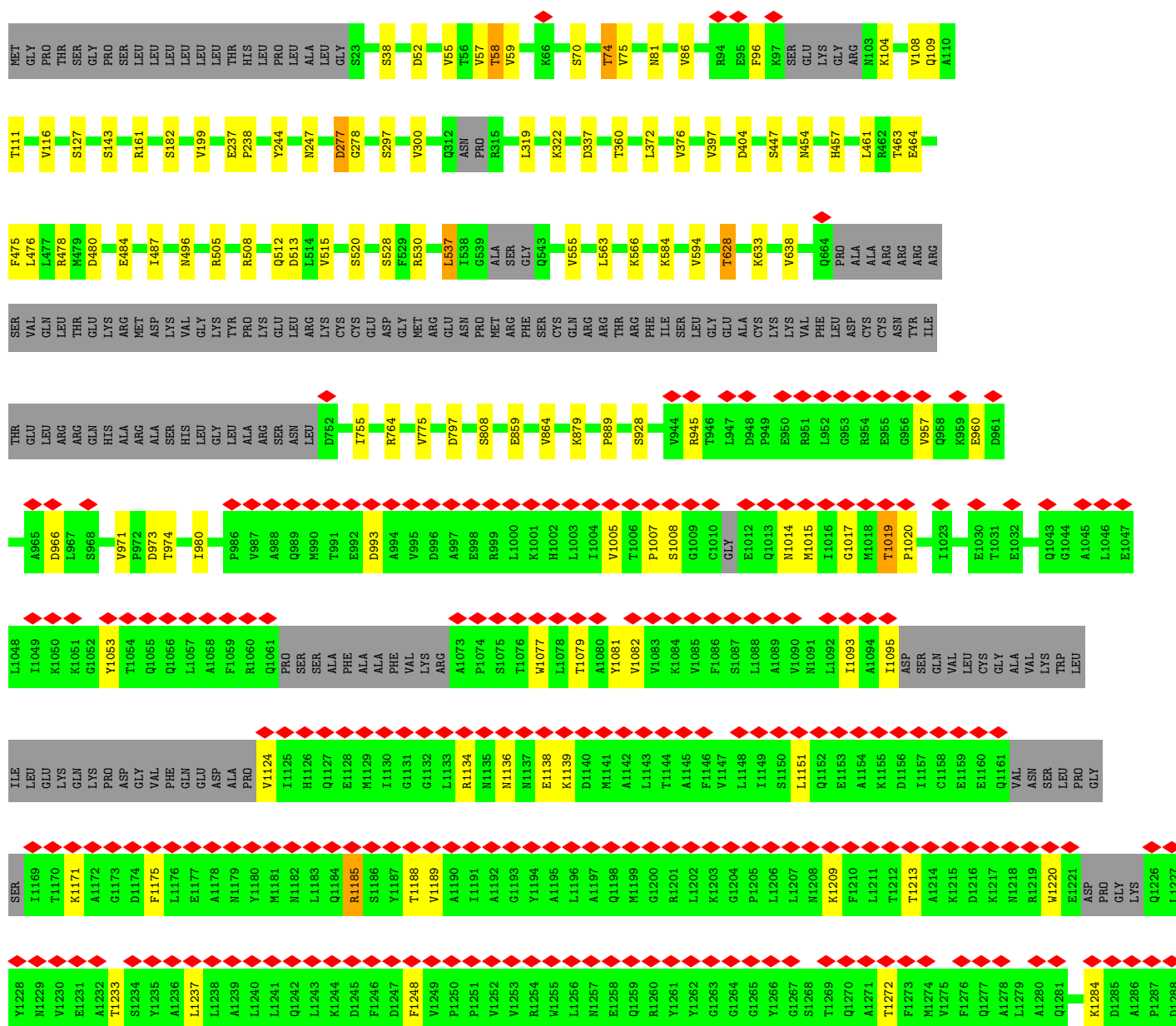
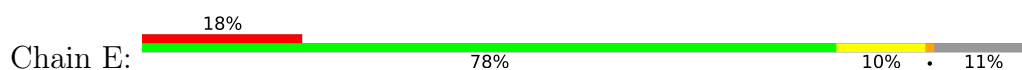
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Complement C3

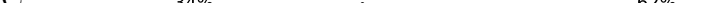


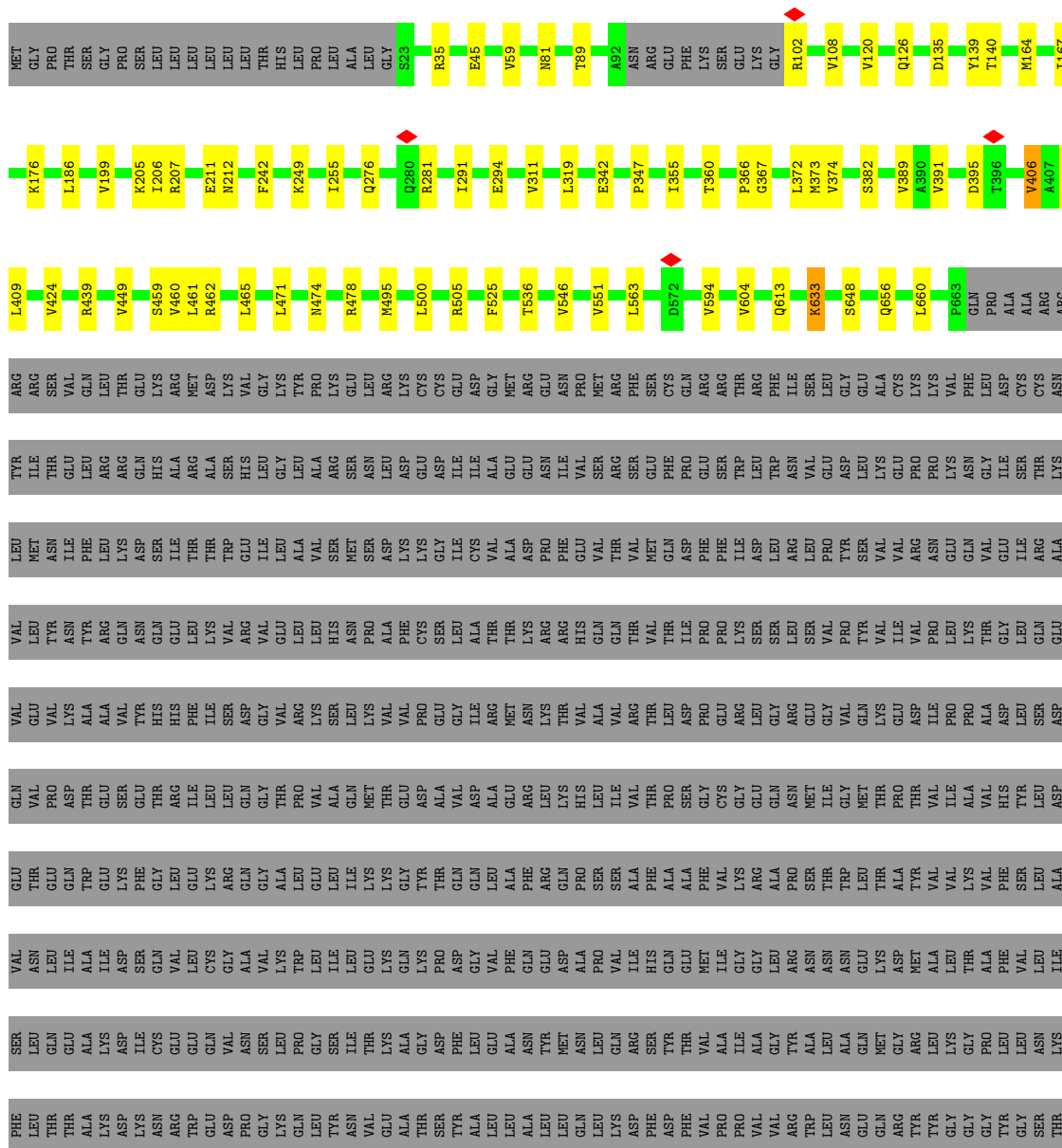


• Molecule 1: Complement C3



- Molecule 1: Complement C3

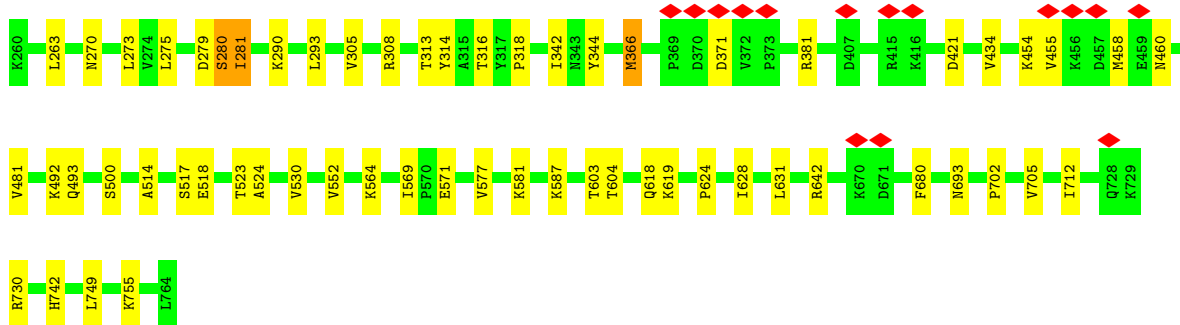
Chain C:  34% 1% 62%



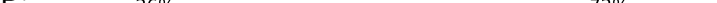
HIS	TRP	GLY	LEU	LYS	VAL	LEU	LYS	THR	THR	PHE	GLN
	PRO	SER	ARG	GLY	ARG	CYS	VAL	THR	VAL	THR	ALA
	GLU	SER	CYS	SER	CYS	CYS	HIS	ARG	THR	THR	PHE
	GLU	ASP	ALA	SER	ALA	GLU	SER	GLY	ASP	ALA	VAL
	ASP	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLN	GLY	VAL
	GLU	VAL	GLU	VAL	GLU	ASN	ASP	GLY	ASP	PHE	GLN
	CYS	GLN	GLN	VAL	GLN	GLN	CYS	ALA	GLY	GLY	ALA
	ASP	GLY	GLY	GLY	ILE	ILE	ALA	MET	THR	ALA	LEU
	GLU	GLN	GLN	GLN	GLN	GLN	PHE	SER	THR	GLN	GLN
	ASN	ARG	LYS	LYS	LYS	LYS	LYS	ILE	LEU	TYR	ALA
GLN	LYS	THR	SER	THR	SER	SER	VAL	THR	SER	SER	GLN
	GLN	LYS	PHE	ILE	ASP	ASP	HIS	ASP	VAL	VAL	LYS
	GLN	ILE	ASP	GLN	GLN	GLN	ILE	ILE	VAL	ASP	ALA
	CYS	CYS	SER	SER	LYS	LYS	TYR	SER	THR	THR	PRO
	GLN	PRO	VAL	PHE	VAL	VAL	PHE	MET	MET	THR	ASP
	ASP	ILE	THR	ASN	THR	THR	ASN	MET	THR	THR	ASP
	LEU	LYS	LEU	VAL	LEU	VAL	HIS	THR	THR	HIS	GLN
	GLY	CYS	GLU	GLU	GLU	GLU	GLY	GLY	ALA	GLN	GLN
	ALA	ARG	ARG	ARG	ILE	ILE	ALA	ALA	ALA	LYS	LEU
	PHE	GLU	LEU	GLN	PRO	GLN	PRO	ALA	ALA	LYS	ASN
THR	GLU	LEU	ASP	LEU	ASP	LEU	PRO	ASP	ASP	ASP	LEU
	GLU	LEU	LYS	LYS	LYS	LYS	THR	THR	GLN	GLN	LEU
	SER	MET	LEU	ALA	ALA	ALA	ASP	ALA	LEU	LEU	ASP
	VAL	VAL	GLU	VAL	VAL	CYS	GLU	LEU	THR	THR	SER
	VAL	GLU	GLU	GLU	GLU	LYS	LEU	LEU	CYS	LEU	LEU
	PHE	LYS	PRO	VAL	VAL	VAL	LYS	LYS	ASN	ASN	GLN
	GLY	LYS	GLY	THR	THR	GLY	TYR	GLN	LYS	LYS	LEU
	CYS	HIS	VAL	ALA	ALA	VAL	TYR	ALA	ASP	PHE	PRO
	PRO	TYR	ASP	TYR	TYR	TYR	ASN	ASN	ASP	SER	ARG
	ASN	MET	VAL	MET	ASN	VAL	ASN	GLY	LYS	LYS	SER
SER	THR	GLY	TYR	PHE	LEU	TYR	VAL	VAL	VAL	VAL	SER
	GLY	GLY	LYS	GLY	GLU	LYS	GLU	ASP	THR	THR	LYS
	LEU	LEU	THR	ARG	GLU	THR	ARG	ARG	ILE	ILE	ILE
	SER	SER	SER	SER	LEU	CYS	ILE	SER	ILE	PRO	HIS
	ASP	ASP	VAL	THR	VAL	VAL	THR	SER	ALA	ARG	ARG
	PHE	THR	LYS	ARG	LYS	LYS	LYS	ARG	ALA	ILE	HIS
	THR	THR	VAL	PHE	THR	THR	TYR	GLU	GLU	GLU	THR
	TRP	THR	VAL	PHE	VAL	VAL	LYS	LYS	PRO	PRO	ILE
	GLY	GLY	GLN	GLY	GLY	GLN	THR	TYR	THR	THR	THR
	GLU	GLU	LEU	GLY	GLY	LEU	HIS	LEU	LYS	GLY	GLY
VAL	GLU	GLU	GLU	GLU	GLU	ILE	ILE	ILE	ILE	ILE	ILE
	GLU	GLU	GLU	GLN	GLN	GLN	PHE	SER	GLY	GLY	GLY
	GLU	GLU	GLU	GLN	GLN	GLN	ASP	THR	THR	THR	THR
	ASN	ARG	LYS	ARG	LYS	LYS	LYS	ILE	THR	THR	THR
	GLN	THR	SER	THR	VAL	VAL	THR	THR	THR	THR	THR
	LYS	THR	PHE	ILE	ASP	ASP	HIS	ASP	VAL	VAL	LYS
	GLN	ILE	ASP	GLN	GLN	GLN	ILE	ILE	VAL	VAL	GLN
	CYS	CYS	SER	SER	LYS	LYS	TYR	SER	SER	SER	GLY
	GLN	PRO	VAL	PHE	VAL	VAL	PHE	MET	MET	THR	GLY
	ASP	ILE	THR	ASN	THR	THR	ASN	MET	THR	THR	GLY
PHE	LEU	GLY	GLU	ALA	ALA	GLU	GLY	GLY	ALA	ALA	ALA
	GLU	GLY	GLU	ARG	ARG	ARG	ILE	ALA	ALA	ALA	ALA
	GLU	GLU	GLU	GLN	GLN	GLN	PHE	SER	GLY	GLY	GLY
	GLU	GLU	GLU	GLN	GLN	GLN	ASP	GLN	GLN	GLN	GLN
	GLU	GLU	GLU	GLN	GLN	GLN	ASP	THR	THR	THR	THR
	ASN	ARG	LYS	ARG	LYS	LYS	LYS	ILE	THR	THR	THR
	GLN	THR	SER	THR	VAL	VAL	THR	THR	THR	THR	THR
	LYS	THR	PHE	ILE	ASP	ASP	HIS	ASP	VAL	VAL	LYS
	GLN	ILE	ASP	GLN	GLN	GLN	ILE	ILE	VAL	VAL	GLN
	CYS	CYS	SER	SER	LYS	LYS	TYR	SER	SER	SER	GLY

- Molecule 2: Complement factor B Bb

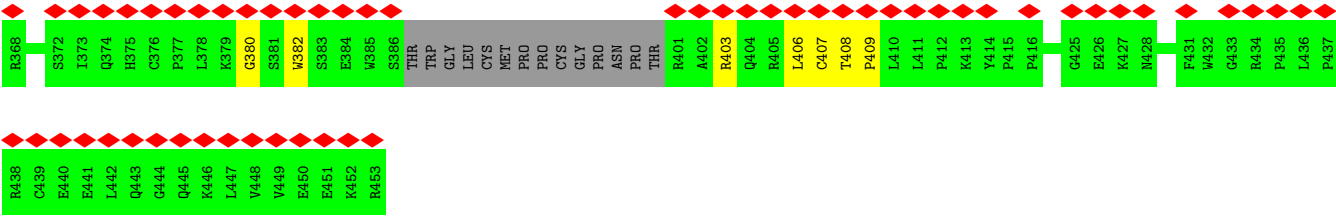
Chain B: 88% 11%



- Molecule 3: Properdin

Chain P: 

THR	THR	LEU	SER	GLU	ALA	MET
ARG	GLU	ALA	GLU	TRP	PHE	ILE
THR	TYR	TYR	ALA	GLN	ALA	THR
ILE	GLU	GLU	CYS	LEU	TYR	GLY
ASN	GLN	ARG	ASP	GLN	GLN	ALA
THR	ARG	ARG	THR	ALA	LYS	GLN
ALA	CYS	ARG	GLN	CYS	ARG	ALA
VAL	CYS	GLY	VAL	GLU	SER	GLN
PRO	GLY	THR	VAL	ASP	GLY	ARG
CYS	PRO	LEU	PRO	GLN	LEU	LEU
P313	PRO	PRO	THR	CYS	CYS	LEU
V314	CYS	CYS	HIS	GLN	GLN	LEU
D315	PRO	PRO	GLY	PRO	PRO	PRO
G316	VAL	VAL	TRP	GLU	CYS	PRO
E317	ALA	ALA	ALA	MET	ARG	LEU
W318	GLY	GLY	THR	GLY	PRO	LEU
D319	TRP	TRP	GLY	TRP	ARG	LEU
S320	GLY	GLY	PRO	GLY	TRP	LEU
W321	TRP	TRP	THR	GLY	TRP	PRO
G322	GLY	GLY	PRO	PRO	SER	ALA
E323	PRO	PRO	CYS	TRP	THR	THR
I328	VAL	VAL	SER	GLU	TRP	GLY
N331	SER	SER	ALA	ALA	ALA	SER
M332	PRO	PRO	SER	CYS	PRO	ASP
K333	CYS	CYS	CYS	SER	CYS	VAL
S334	LEU	LEU	HIS	VAL	SER	LEU
I335	GLY	GLY	GLU	THR	THR	CYS
S336	GLN	GLN	PRO	VAL	VAL	LEU
C337	THR	THR	GLY	THR	THR	CYS
G342	MET	MET	THR	ARG	GLU	GLY
Q343	GLU	GLU	ARG	ARG	LEU	SER
Q344	GLN	ARG	SER	ARG	TYR	GLY
S345	THR	THR	ARG	ALA	ARG	LYS
R346	CYS	CYS	LYS	CYS	ARG	CYS
G347	ASN	THR	CYS	ASN	CYS	LYS
R348	HIS	ASN	SER	HIS	VAL	GLY
T349	PRO	PRO	ALA	PRO	GLY	LEU
C350	VAL	VAL	PRO	ALA	TRP	LEU
R351	PRO	PRO	GLU	ASN	ASN	GLY
G352	GLY	GLY	PRO	LYS	GLY	GLY
R353	PRO	PRO	PRO	HIS	GLY	VAL
K354	PHE	CYS	GLY	CYS	GLY	VAL
F355	CYS	THR	PRO	GLY	VAL	GLY
D356	ALA	ALA	GLY	PRO	LYS	GLU
G357	ASP	ASP	CYS	GLN	VAL	ASP
	ALA	ALA	THR	GLU	ALA	THR
			CYS	THR	LEU	ASN



● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	389342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.785	Depositor
Minimum map value	-1.168	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	342.0, 342.0, 342.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	C	0.27	0/5021	0.48	2/6825 (0.0%)
1	D	0.18	0/7909	0.45	1/10689 (0.0%)
1	E	0.24	2/11912 (0.0%)	0.49	5/16140 (0.0%)
2	B	0.16	0/4100	0.42	1/5548 (0.0%)
3	P	0.19	0/1059	0.48	0/1425
All	All	0.22	2/30001 (0.0%)	0.47	9/40627 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	628	THR	C-N	5.73	1.38	1.33
1	E	633	LYS	CA-C	-5.46	1.45	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	277	ASP	N-CA-C	-8.94	98.48	110.55
1	E	1248	PHE	CA-C-N	7.87	125.20	120.24
1	E	1248	PHE	C-N-CA	7.87	125.20	120.24
1	E	1077	TRP	N-CA-C	7.03	119.84	111.33
1	C	525	PHE	CA-C-N	5.91	125.06	120.33
1	C	525	PHE	C-N-CA	5.91	125.06	120.33
1	D	1337	LYS	CA-CB-CG	5.83	125.77	114.10
1	E	1633	GLU	CA-CB-CG	5.46	125.02	114.10
2	B	316	THR	N-CA-C	5.34	116.79	110.97

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	C	4922	0	4981	37	0
1	D	7760	0	7738	33	0
1	E	11688	0	11676	79	0
2	B	4012	0	3993	29	0
3	P	1032	0	994	6	0
4	A	28	0	25	0	0
5	B	28	0	26	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
6	B	1	0	0	0	0
All	All	29513	0	29472	178	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 3.

All (178) 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:459:SER:HB3	1:C:474:ASN:HB2	1.83	0.61
2:B:514:ALA:HB2	2:B:702:PRO:HG3	1.82	0.60
1:C:366:PRO:O	1:C:478:ARG:NH2	2.35	0.60
2:B:455:VAL:HA	2:B:458:MET:HG2	1.83	0.59
1:E:1007:PRO:HB3	1:E:1017:GLY:HA3	1.84	0.59
1:E:1008:SER:O	1:E:1014:ASN:ND2	2.37	0.58
2:B:263:LEU:HD22	2:B:305:VAL:HG21	1.87	0.57
1:E:1480:TYR:HB3	1:E:1488:SER:HB3	1.85	0.57
2:B:381:ARG:NH1	2:B:421:ASP:OD2	2.38	0.56
2:B:693:ASN:O	2:B:730:ARG:NH1	2.38	0.56
1:E:1536:ALA:O	1:E:1570:LYS:NZ	2.39	0.56
1:C:374:VAL:HG11	1:C:424:VAL:HG11	1.86	0.56
2:B:275:LEU:HB3	2:B:313:THR:HG22	1.88	0.56
1:E:457:HIS:HB3	1:E:476:LEU:HB3	1.88	0.55
1:E:1557:ASP:OD1	1:E:1557:ASP:N	2.39	0.55
2:B:564:LYS:HZ2	2:B:569:ILE:HG13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:VAL:HG12	1:E:775:VAL:HG22	1.88	0.54
1:E:1136:ASN:HA	1:E:1139:LYS:HE3	1.88	0.54
1:E:480:ASP:N	1:E:480:ASP:OD1	2.40	0.54
1:D:1225:LYS:O	1:D:1229:ASN:ND2	2.41	0.54
1:E:1209:LYS:O	1:E:1213:THR:OG1	2.26	0.53
1:E:1079:THR:O	1:E:1082:VAL:HB	2.08	0.53
1:E:1505:LEU:HD21	1:E:1587:PRO:HB3	1.91	0.53
1:D:859:GLU:HG3	1:D:889:PRO:HA	1.91	0.53
1:E:1604:MET:HA	1:E:1627:TRP:O	2.08	0.53
1:D:816:CYS:HA	1:C:613:GLN:HE21	1.74	0.53
1:E:1318:LEU:HD23	1:E:1320:ARG:HH12	1.74	0.52
1:E:57:VAL:HG11	1:E:86:VAL:HG21	1.90	0.52
1:E:454:ASN:HA	1:E:478:ARG:O	2.10	0.52
1:E:945:ARG:NH1	1:E:960:GLU:OE1	2.42	0.52
1:D:1426:ASP:OD1	1:D:1426:ASP:N	2.40	0.51
1:E:59:VAL:HB	1:E:70:SER:HB2	1.93	0.51
1:E:277:ASP:O	1:E:278:GLY:C	2.52	0.51
1:E:319:LEU:HA	1:E:322:LYS:HE2	1.93	0.51
1:E:496:ASN:ND2	1:E:528:SER:O	2.43	0.51
1:E:1138:GLU:HG3	1:E:1185:ARG:HD3	1.93	0.51
1:E:1296:VAL:HA	1:E:1308:THR:HG23	1.93	0.50
2:B:434:VAL:HG11	2:B:454:LYS:HE3	1.93	0.50
1:E:74:THR:OG1	1:E:75:VAL:N	2.45	0.50
1:E:508:ARG:NH1	1:E:512:GLN:O	2.44	0.50
1:D:1557:ASP:OD1	1:D:1557:ASP:N	2.40	0.50
2:B:552:VAL:HG12	2:B:581:LYS:HB3	1.92	0.50
1:E:1421:LEU:HD21	1:E:1459:LEU:HD13	1.94	0.50
1:E:1303:ARG:O	1:E:1306:LYS:NZ	2.45	0.50
1:C:374:VAL:HG21	1:C:389:VAL:HG11	1.93	0.50
1:E:859:GLU:HG3	1:E:889:PRO:HA	1.94	0.49
1:C:81:ASN:O	1:C:505:ARG:NH1	2.45	0.49
1:C:276:GLN:HG2	1:C:281:ARG:HG2	1.93	0.49
1:C:255:ILE:HD12	1:C:291:ILE:HD11	1.95	0.49
2:B:270:ASN:OD1	2:B:308:ARG:NH1	2.46	0.49
1:E:59:VAL:HG22	1:E:108:VAL:HG13	1.95	0.49
1:D:971:VAL:O	1:D:974:THR:OG1	2.29	0.48
1:C:281:ARG:NH1	1:C:342:GLU:OE2	2.46	0.48
1:D:808:SER:HB3	1:C:563:LEU:HD22	1.94	0.48
1:D:940:LYS:NZ	1:D:966:ASP:O	2.39	0.48
1:D:951:ARG:HD2	1:D:1254:ARG:HH21	1.78	0.48
1:C:465:LEU:HD11	1:C:471:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1181:MET:HE3	1:D:1181:MET:HB3	1.79	0.48
2:B:523:THR:OG1	2:B:524:ALA:N	2.47	0.48
1:E:563:LEU:HD22	1:E:808:SER:HB3	1.95	0.47
2:B:273:LEU:HD22	2:B:293:LEU:HD22	1.94	0.47
2:B:458:MET:SD	2:B:458:MET:N	2.86	0.47
1:C:536:THR:HG22	1:C:546:VAL:HG22	1.96	0.47
1:D:775:VAL:HG22	1:C:594:VAL:HG12	1.96	0.47
1:D:1547:THR:HG22	1:D:1565:ILE:HA	1.95	0.47
1:E:1610:ASP:HB3	1:E:1621:ILE:HB	1.96	0.47
1:C:35:ARG:HD2	1:C:126:GLN:HE21	1.79	0.47
1:D:1400:MET:HA	1:D:1448:LEU:O	2.14	0.47
1:E:360:THR:HG21	1:E:372:LEU:HD23	1.96	0.47
1:C:373:MET:HE2	1:C:408:LYS:HE3	1.96	0.47
1:E:1015:MET:HE3	1:E:1081:TYR:HD2	1.80	0.47
2:B:603:THR:HG23	2:B:712:ILE:HG12	1.96	0.47
1:E:1220:TRP:HD1	1:E:1233:THR:HG22	1.80	0.47
2:B:493:GLN:HE21	2:B:642:ARG:HE	1.61	0.47
2:B:624:PRO:HD2	2:B:628:ILE:HG12	1.97	0.47
1:E:1053:TYR:OH	1:E:1095:ILE:O	2.33	0.46
1:E:993:ASP:N	1:E:993:ASP:OD1	2.43	0.46
3:P:315:ASP:OD1	3:P:315:ASP:N	2.47	0.46
2:B:680:PHE:HA	2:B:742:HIS:O	2.16	0.46
1:E:404:ASP:OD1	1:E:404:ASP:N	2.40	0.46
1:E:566:LYS:HE3	1:E:584:LYS:HD2	1.97	0.46
1:C:135:ASP:OD1	1:C:139:TYR:OH	2.31	0.46
1:D:1323:GLU:N	1:D:1323:GLU:OE2	2.49	0.46
2:B:280:SER:OG	1:E:1663:ASN:OXT	2.34	0.46
1:E:1548:ARG:NH1	1:E:1566:GLU:OE2	2.49	0.46
1:D:1499:ASP:O	1:D:1591:ARG:NH1	2.45	0.46
1:E:966:ASP:OD1	1:E:966:ASP:N	2.43	0.46
1:C:495:MET:HE3	1:C:495:MET:HB3	1.81	0.46
1:C:205:LYS:HD2	1:C:207:ARG:HH21	1.81	0.45
2:B:481:VAL:HG13	2:B:492:LYS:HA	1.98	0.45
1:E:55:VAL:HA	1:E:111:THR:O	2.16	0.45
1:D:682:LYS:HB3	1:D:698:MET:HE1	1.99	0.45
1:C:395:ASP:OD1	1:C:395:ASP:N	2.49	0.45
1:D:840:VAL:HG11	1:D:1473:GLN:HG3	1.99	0.45
1:D:1225:LYS:HB3	1:D:1228:TYR:HD2	1.82	0.45
1:C:212:ASN:N	1:C:212:ASN:OD1	2.50	0.45
1:D:970:GLN:HG3	1:D:1348:TYR:HD2	1.82	0.45
2:B:314:TYR:HA	2:B:318:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1542:ASP:HB2	1:E:1608:SER:HB2	1.98	0.44
1:E:475:PHE:HB2	1:E:515:VAL:HG22	2.00	0.44
1:E:971:VAL:O	1:E:974:THR:OG1	2.34	0.44
1:C:373:MET:HG3	1:C:462:ARG:HH22	1.83	0.44
1:D:1363:LEU:HD22	1:D:1479:VAL:HG12	1.99	0.44
1:D:1497:LYS:HD2	1:D:1497:LYS:HA	1.72	0.44
1:E:484:GLU:O	1:E:508:ARG:NH2	2.50	0.44
1:C:355:ILE:HG23	1:C:439:ARG:HB2	1.98	0.44
1:D:1008:SER:O	1:D:1447:TYR:OH	2.34	0.44
1:E:1189:VAL:HG21	1:E:1213:THR:HG21	2.00	0.44
1:E:1577:GLN:N	1:E:1580:GLN:OE1	2.47	0.44
1:C:167:ILE:HB	1:C:176:LYS:HB3	1.99	0.44
2:B:290:LYS:NZ	2:B:342:ILE:O	2.51	0.43
1:E:1597:GLU:N	1:E:1597:GLU:OE2	2.49	0.43
2:B:604:THR:OG1	2:B:618:GLN:OE1	2.35	0.43
1:E:980:ILE:HG22	1:E:1344:VAL:HG22	2.00	0.43
3:P:380:GLY:HA3	3:P:409:PRO:HA	2.00	0.43
2:B:371:ASP:OD1	2:B:371:ASP:N	2.49	0.43
1:C:102:ARG:HG3	1:C:660:LEU:HD12	2.01	0.43
1:D:1296:VAL:HG22	1:D:1309:HIS:HB2	2.00	0.43
1:E:1547:THR:HG22	1:E:1565:ILE:HA	2.01	0.43
1:E:1656:MET:HE3	1:E:1656:MET:HB3	1.84	0.43
1:C:242:PHE:HA	1:C:347:PRO:HD2	1.99	0.43
1:E:1360:LYS:HA	1:E:1360:LYS:HD2	1.83	0.42
1:C:374:VAL:O	1:C:406:VAL:HA	2.18	0.42
1:D:1036:LYS:NZ	1:D:1313:TRP:O	2.43	0.42
2:B:749:LEU:HD23	2:B:749:LEU:HA	1.93	0.42
1:E:487:ILE:HD11	1:E:537:LEU:HB3	2.01	0.42
1:C:367:GLY:HA3	1:C:478:ARG:HH22	1.84	0.42
1:D:1297:SER:HA	1:D:1307:ILE:O	2.20	0.42
3:P:318:TRP:NE1	3:P:361:ALA:O	2.45	0.42
1:E:530:ARG:NH1	1:E:628:THR:O	2.46	0.42
1:C:59:VAL:HG22	1:C:108:VAL:HG22	2.02	0.42
1:E:81:ASN:O	1:E:505:ARG:NH1	2.52	0.42
1:E:1644:LYS:HD3	1:E:1644:LYS:HA	1.77	0.42
2:B:517:SER:OG	2:B:518:GLU:N	2.51	0.42
1:E:1362:ASP:O	1:E:1390:THR:HA	2.20	0.42
1:C:164:MET:HE3	1:C:211:GLU:HG3	2.02	0.42
1:C:205:LYS:HE3	1:C:205:LYS:HB2	1.94	0.42
2:B:279:ASP:HB2	1:E:1663:ASN:HA	2.02	0.42
1:E:463:THR:OG1	1:E:464:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:957:VAL:HG12	1:E:1335:GLU:HB3	2.02	0.42
1:C:311:VAL:HG21	1:C:319:LEU:HD21	2.01	0.42
2:B:755:LYS:HA	2:B:755:LYS:HD3	1.85	0.41
3:P:318:TRP:CE2	3:P:360:CYS:HB3	2.55	0.41
3:P:382:TRP:HA	3:P:407:CYS:HA	2.02	0.41
1:E:1547:THR:HB	1:E:1563:MET:HB3	2.02	0.41
1:E:1134:ARG:HD2	1:E:1134:ARG:HA	1.76	0.41
1:D:1120:GLU:HG3	1:D:1122:ALA:H	1.85	0.41
2:B:281:ILE:O	2:B:344:TYR:OH	2.33	0.41
1:E:1370:ALA:HB3	1:E:1383:THR:HG23	2.03	0.41
1:E:1527:VAL:HG12	1:E:1531:GLU:HB2	2.02	0.41
1:E:1549:LEU:HD11	1:E:1561:TYR:HB3	2.01	0.41
1:D:972:PRO:HG2	1:D:1585:ILE:HD13	2.02	0.41
1:E:244:TYR:HB3	1:E:247:ASN:HB2	2.02	0.41
3:P:406:LEU:HD23	3:P:406:LEU:HA	1.91	0.41
1:E:1171:LYS:O	1:E:1175:PHE:HB2	2.20	0.41
2:B:366:MET:H	2:B:366:MET:HG2	1.62	0.41
1:E:1019:THR:HG23	1:E:1020:PRO:HD3	2.02	0.41
1:C:167:ILE:HG12	1:C:206:ILE:HG12	2.02	0.41
1:D:1007:PRO:O	1:D:1482:TYR:OH	2.33	0.41
1:E:96:PHE:HD1	1:E:104:LYS:HG2	1.85	0.41
1:E:127:SER:OG	1:E:161:ARG:NH1	2.51	0.41
1:E:337:ASP:OD1	1:E:337:ASP:N	2.54	0.41
1:E:764:ARG:HB3	1:E:797:ASP:HB3	2.03	0.41
1:C:633:LYS:HE3	1:C:633:LYS:HB2	1.68	0.41
1:E:1510:LEU:HD12	1:E:1510:LEU:HA	1.96	0.40
1:D:1385:ILE:HG12	1:D:1462:LYS:HG2	2.03	0.40
1:D:1604:MET:HA	1:D:1627:TRP:O	2.21	0.40
1:E:58:THR:HG23	1:E:109:GLN:HG2	2.03	0.40
1:C:120:VAL:O	1:C:656:GLN:NE2	2.54	0.40
1:D:1545:TYR:HE1	1:D:1568:THR:HG23	1.86	0.40
1:E:461:LEU:HD13	1:C:461:LEU:HB2	2.03	0.40
1:E:478:ARG:HD2	1:E:478:ARG:HA	1.85	0.40
1:E:237:GLU:HA	1:E:238:PRO:HD3	1.97	0.40
1:E:1284:LYS:HB3	1:E:1284:LYS:HE3	1.87	0.40
1:C:249:LYS:HE2	1:C:249:LYS:HB3	1.86	0.40
1:D:833:LEU:HD23	1:D:927:LYS:HB2	2.02	0.40
1:D:1293:ASN:HA	1:D:1311:ILE:O	2.21	0.40
1:C:391:VAL:HG23	1:C:409:LEU:HD22	2.03	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	C	628/1663 (38%)	619 (99%)	9 (1%)	0	100	100
1	D	964/1663 (58%)	942 (98%)	22 (2%)	0	100	100
1	E	1450/1663 (87%)	1400 (97%)	50 (3%)	0	100	100
2	B	503/505 (100%)	487 (97%)	16 (3%)	0	100	100
3	P	123/453 (27%)	117 (95%)	6 (5%)	0	100	100
All	All	3668/5947 (62%)	3565 (97%)	103 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	557/1468 (38%)	540 (97%)	17 (3%)	35	65
1	D	859/1468 (58%)	842 (98%)	17 (2%)	48	76
1	E	1307/1468 (89%)	1267 (97%)	40 (3%)	35	65
2	B	445/446 (100%)	433 (97%)	12 (3%)	39	69
3	P	113/378 (30%)	111 (98%)	2 (2%)	51	78
All	All	3281/5228 (63%)	3193 (97%)	88 (3%)	40	69

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	722	LYS
1	D	762	VAL
1	D	783	LYS
1	D	1097	SER
1	D	1261	TYR
1	D	1294	LEU
1	D	1310	ARG
1	D	1321	SER
1	D	1324	THR
1	D	1455	GLU
1	D	1509	GLU
1	D	1549	LEU
1	D	1552	VAL
1	D	1576	VAL
1	D	1595	LYS
1	D	1604	MET
1	D	1619	SER
2	B	280	SER
2	B	281	ILE
2	B	366	MET
2	B	460	ASN
2	B	500	SER
2	B	530	VAL
2	B	571	GLU
2	B	577	VAL
2	B	587	LYS
2	B	619	LYS
2	B	631	LEU
2	B	705	VAL
3	P	403	ARG
3	P	408	THR
1	E	38	SER
1	E	52	ASP
1	E	58	THR
1	E	74	THR
1	E	116	VAL
1	E	143	SER
1	E	182	SER
1	E	199	VAL
1	E	297	SER
1	E	300	VAL
1	E	376	VAL
1	E	397	VAL

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Mol	Chain	Res	Type
1	E	447	SER
1	E	513	ASP
1	E	520	SER
1	E	537	LEU
1	E	555	VAL
1	E	638	VAL
1	E	755	ILE
1	E	864	VAL
1	E	879	LYS
1	E	928	SER
1	E	973	ASP
1	E	1005	VAL
1	E	1019	THR
1	E	1093	ILE
1	E	1124	VAL
1	E	1151	LEU
1	E	1185	ARG
1	E	1188	THR
1	E	1237	LEU
1	E	1272	THR
1	E	1367	ILE
1	E	1421	LEU
1	E	1444	LEU
1	E	1488	SER
1	E	1528	THR
1	E	1569	ILE
1	E	1609	SER
1	E	1626	THR
1	C	45	GLU
1	C	89	THR
1	C	140	THR
1	C	186	LEU
1	C	199	VAL
1	C	294	GLU
1	C	360	THR
1	C	372	LEU
1	C	382	SER
1	C	406	VAL
1	C	449	VAL
1	C	460	VAL
1	C	500	LEU
1	C	551	VAL

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Mol	Chain	Res	Type
1	C	604	VAL
1	C	633	LYS
1	C	648	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	853	ASN
1	D	1026	HIS
1	D	1198	GLN
1	D	1355	GLN
1	D	1494	HIS
1	D	1553	GLN
2	B	354	ASN
2	B	417	ASN
2	B	440	ASN
2	B	493	GLN
2	B	562	ASN
3	P	364	GLN
3	P	365	GLN
3	P	369	HIS
1	E	103	ASN
1	E	126	GLN
1	E	185	GLN
1	E	276	GLN
1	E	333	HIS
1	E	354	GLN
1	E	436	GLN
1	E	512	GLN
1	E	1014	ASN
1	E	1226	GLN
1	C	126	GLN
1	C	333	HIS
1	C	496	ASN
1	C	613	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
4	NAG	A	1	3,4	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	A	2	4	14,14,15	0.57	0	17,19,21	0.47	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
4	NAG	A	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

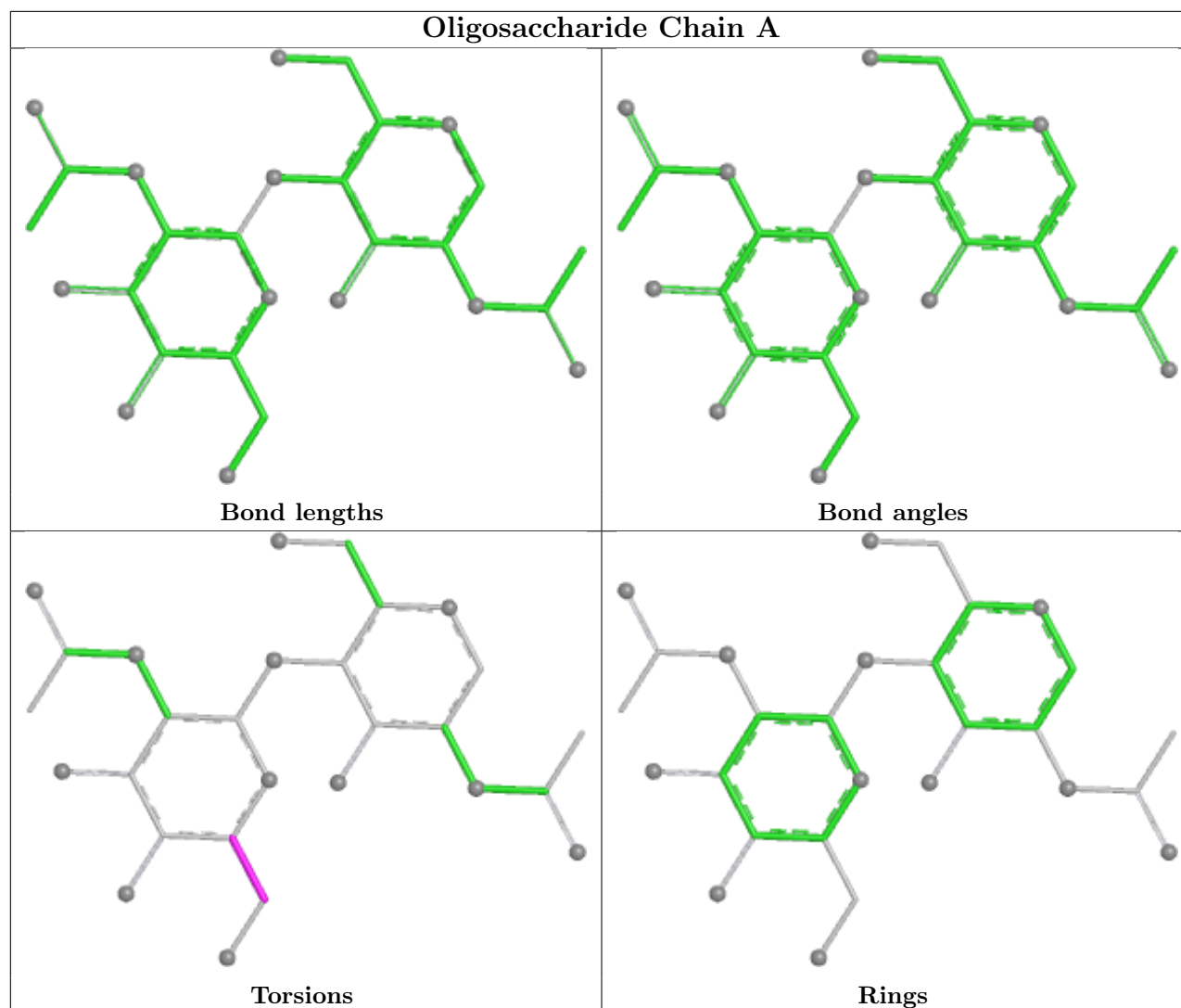
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
5	NAG	B	801	2	14,14,15	0.59	0	17,19,21	0.47	0
5	NAG	C	1701	1	14,14,15	0.28	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	802	2	14,14,15	0.43	0	17,19,21	0.56	0
5	NAG	D	1701	1	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	E	1701	1	14,14,15	0.36	0	17,19,21	0.46	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
5	NAG	B	801	2	-	2/6/23/26	0/1/1/1
5	NAG	C	1701	1	-	4/6/23/26	0/1/1/1
5	NAG	B	802	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1701	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

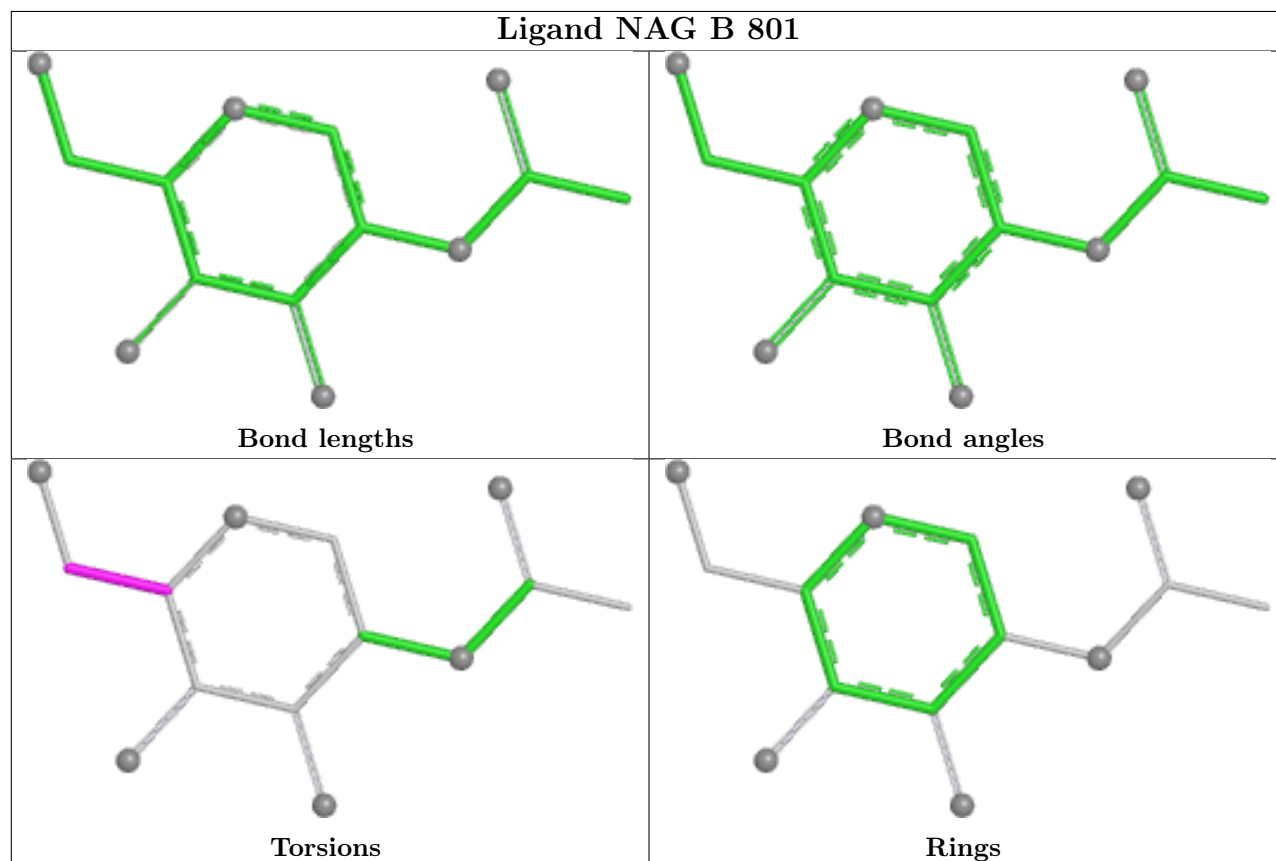
Mol	Chain	Res	Type	Atoms
5	D	1701	NAG	O5-C5-C6-O6
5	D	1701	NAG	C4-C5-C6-O6
5	C	1701	NAG	C8-C7-N2-C2
5	C	1701	NAG	O7-C7-N2-C2
5	B	801	NAG	O5-C5-C6-O6
5	C	1701	NAG	C4-C5-C6-O6
5	B	801	NAG	C4-C5-C6-O6
5	C	1701	NAG	O5-C5-C6-O6

There are no ring outliers.

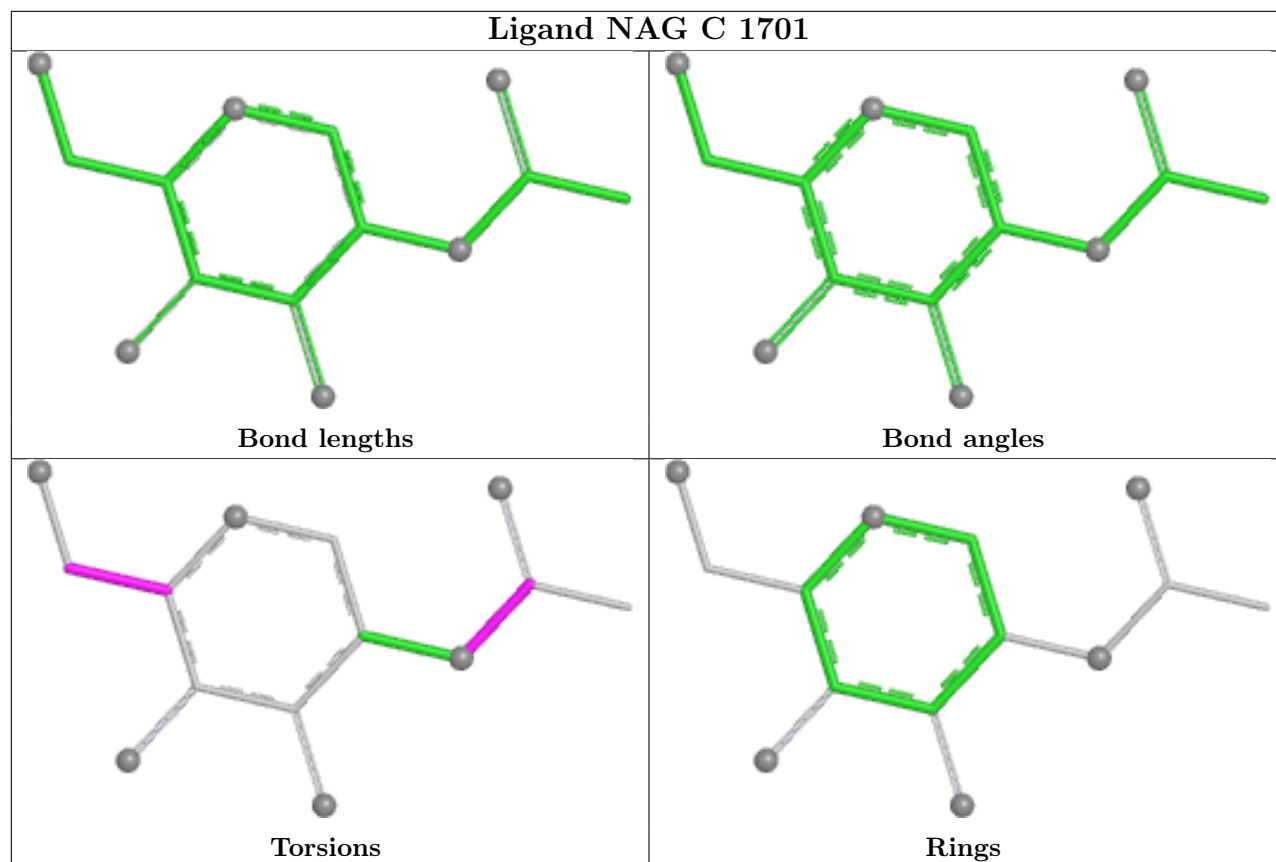
No monomer is involved in short contacts.

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

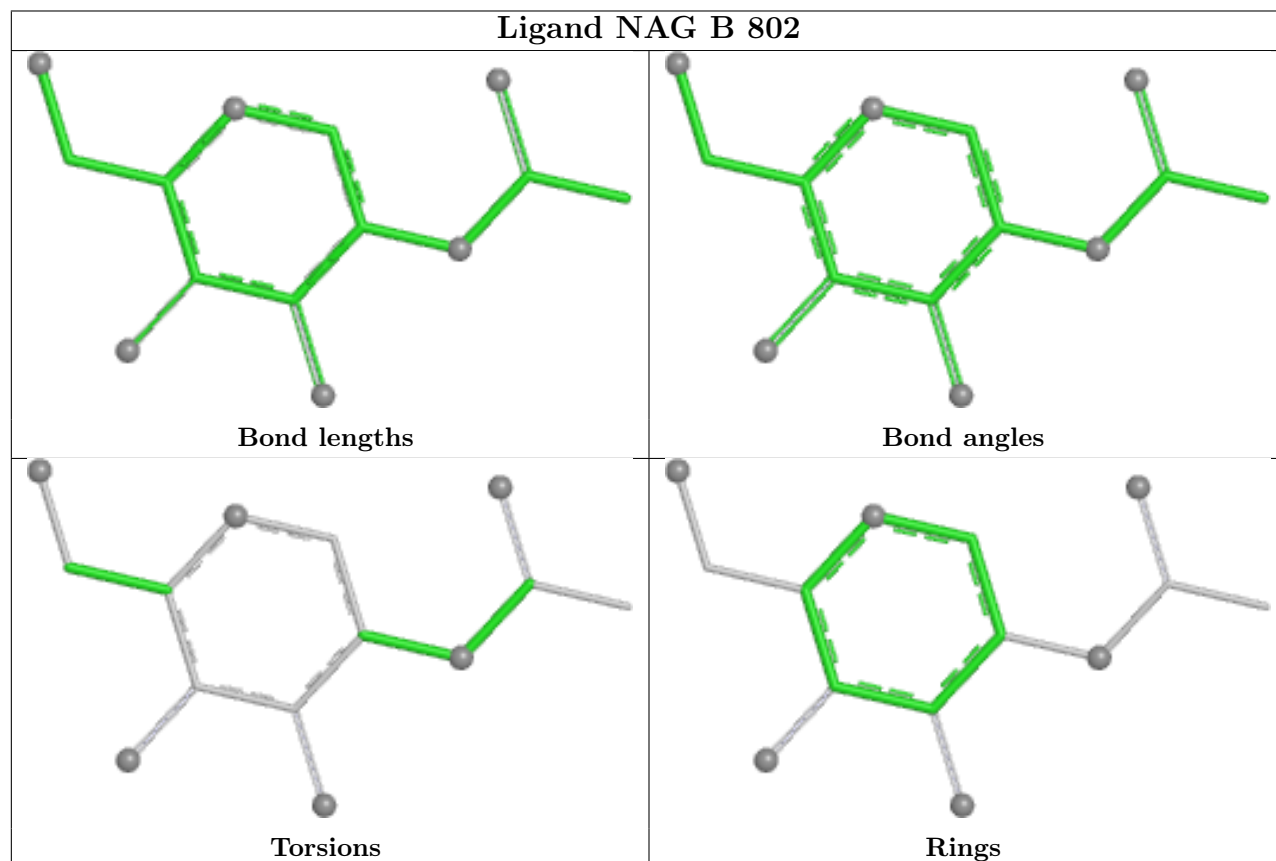
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



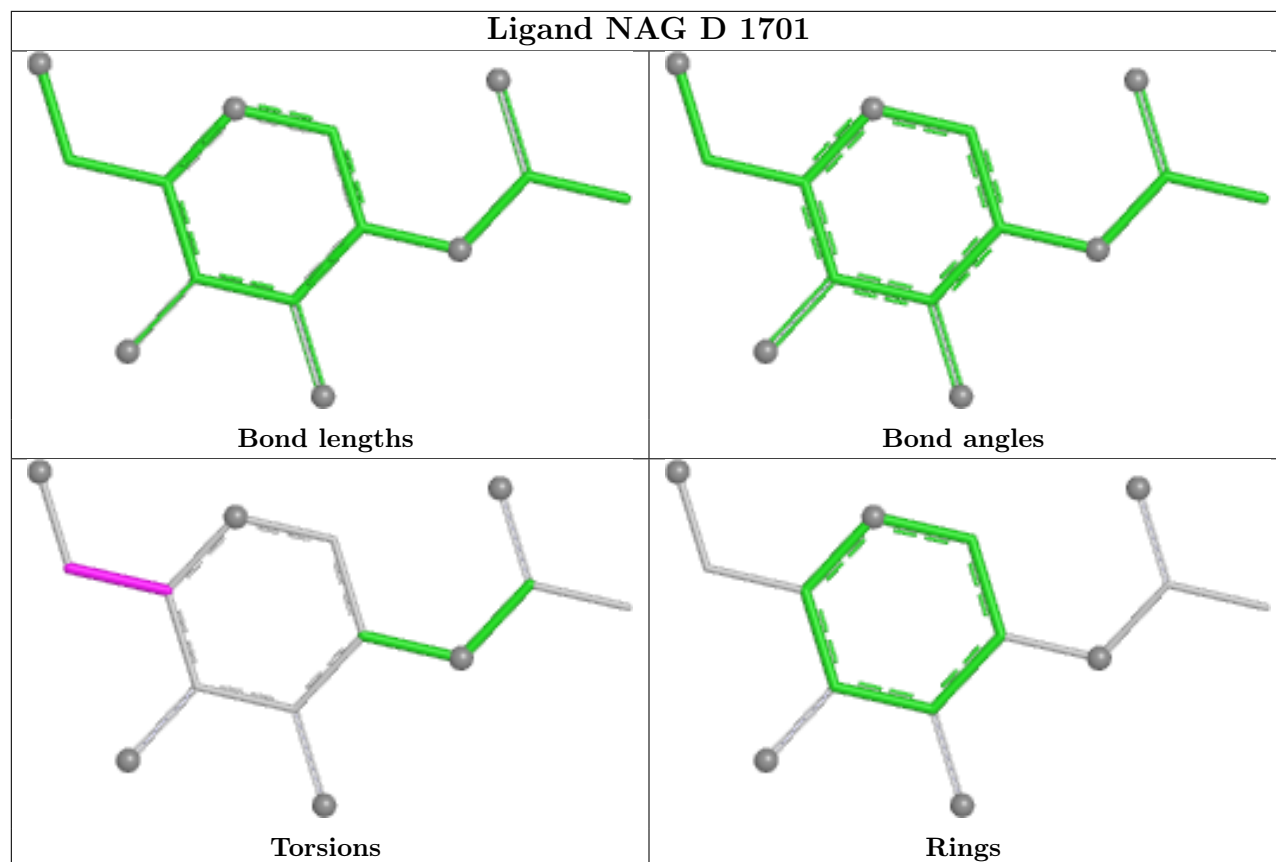
Ligand NAG C 1701



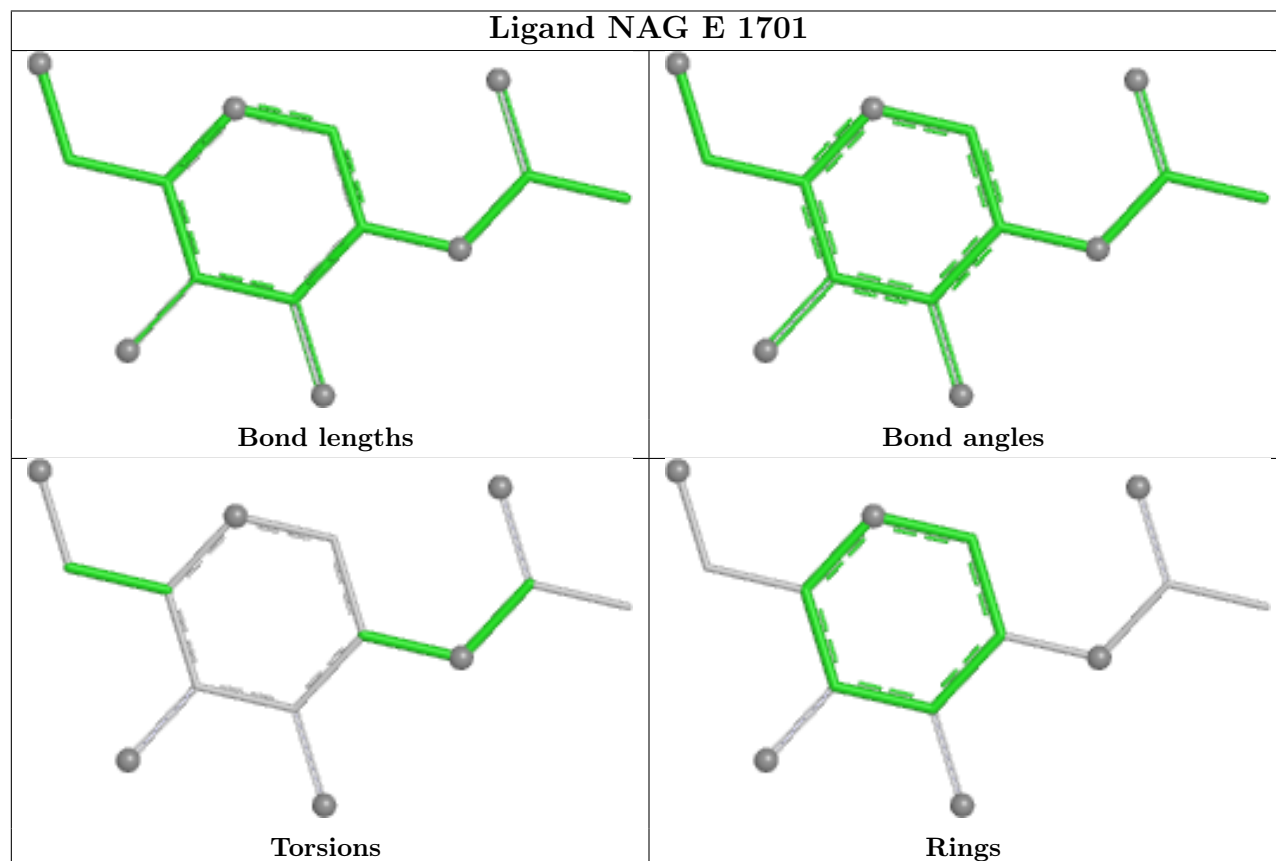
Ligand NAG B 802



Ligand NAG D 1701



Ligand NAG E 1701



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.

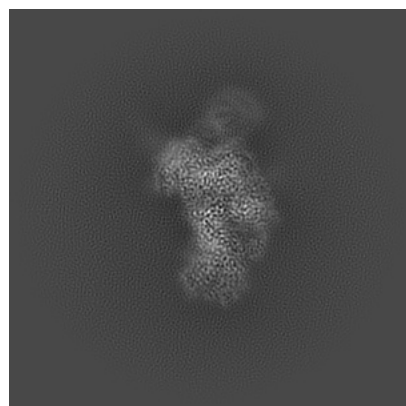
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63895. These allow visual inspection of the internal detail of the map and identification of artifacts.

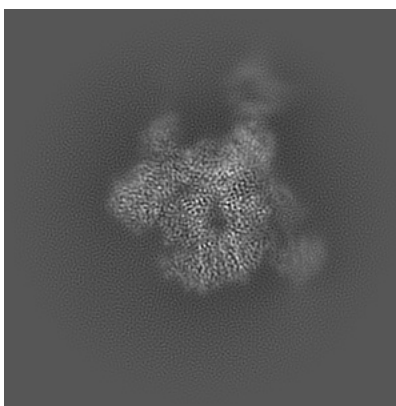
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

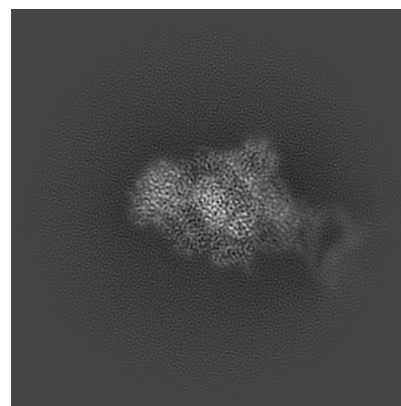
6.1.1 Primary map



X

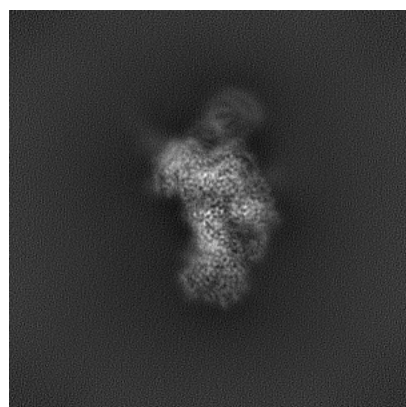


Y

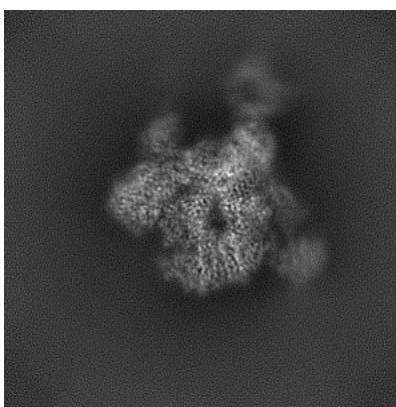


Z

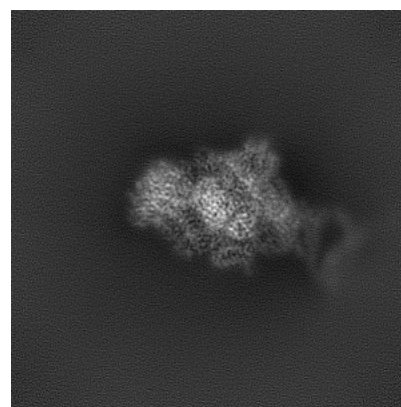
6.1.2 Raw map



X



Y

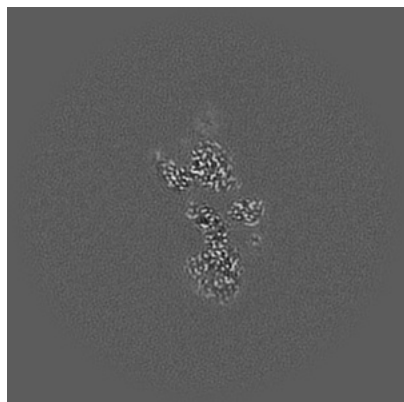


Z

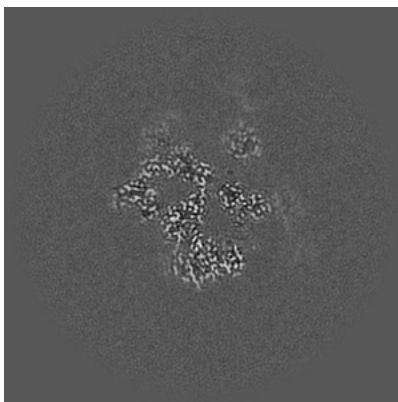
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

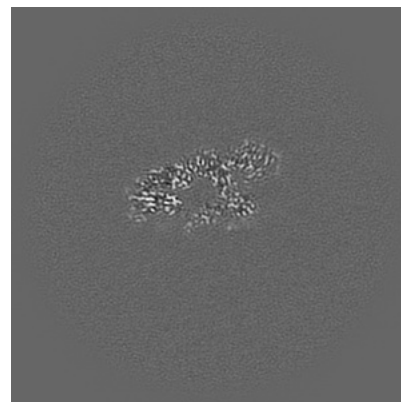
6.2.1 Primary map



X Index: 180

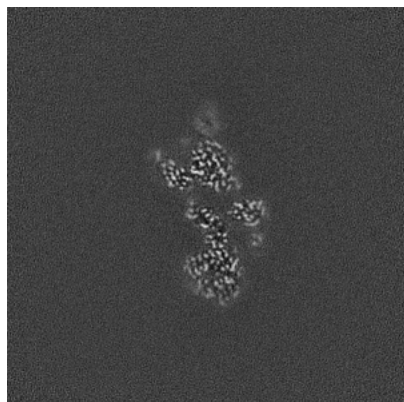


Y Index: 180

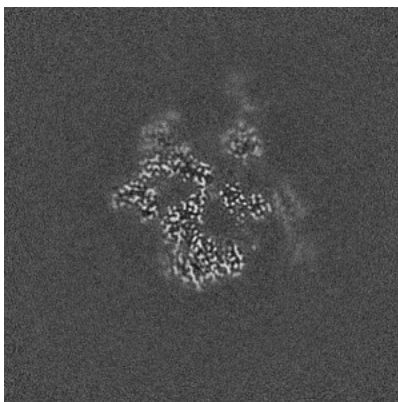


Z Index: 180

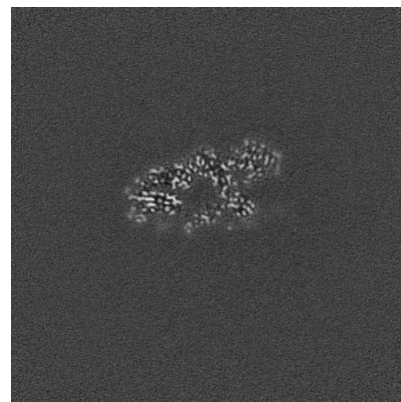
6.2.2 Raw map



X Index: 180



Y Index: 180

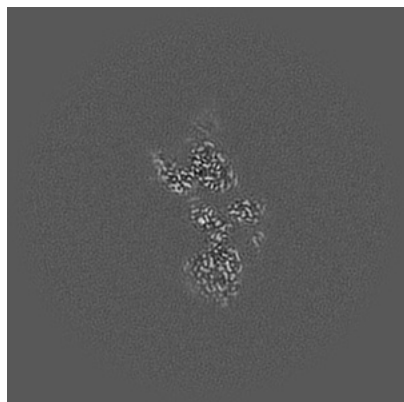


Z Index: 180

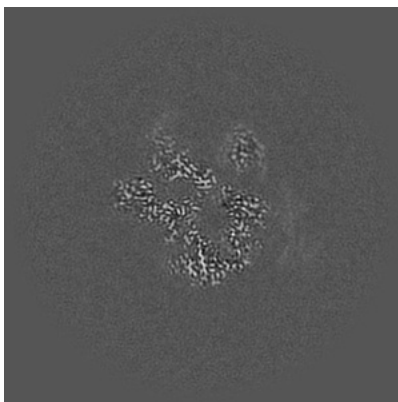
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

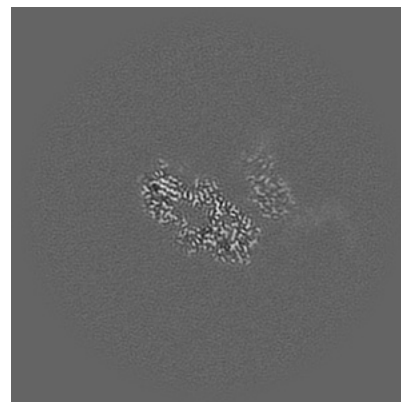
6.3.1 Primary map



X Index: 182

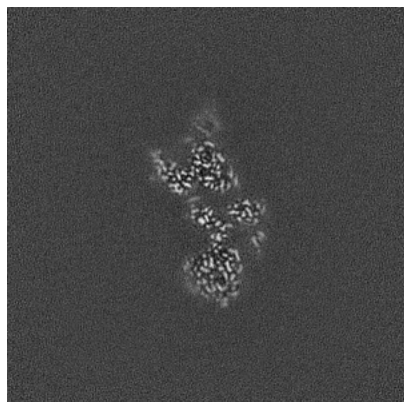


Y Index: 186

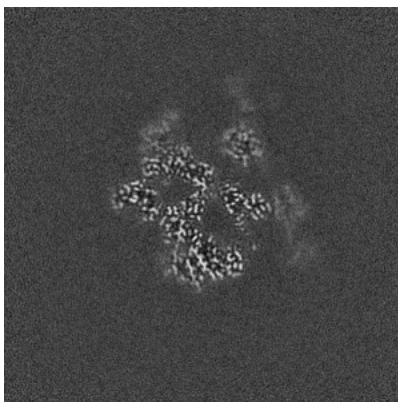


Z Index: 209

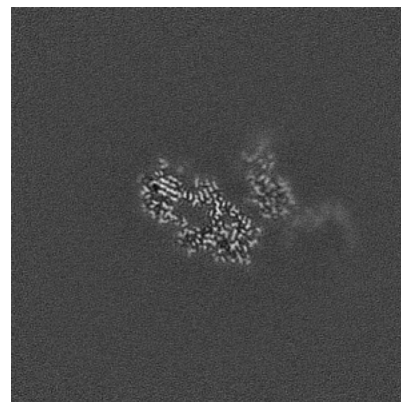
6.3.2 Raw map



X Index: 182



Y Index: 181

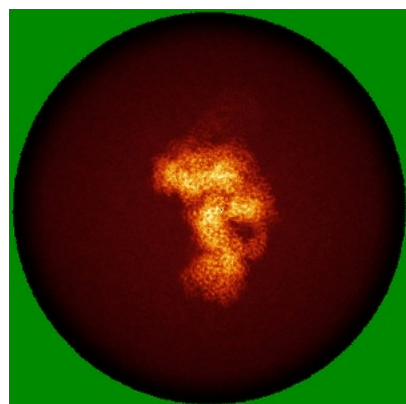


Z Index: 209

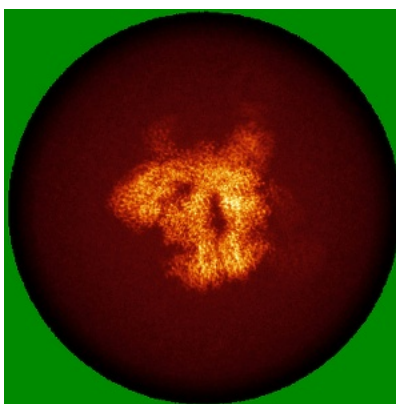
The images above show the largest variance slices of the map in three orthogonal directions.

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

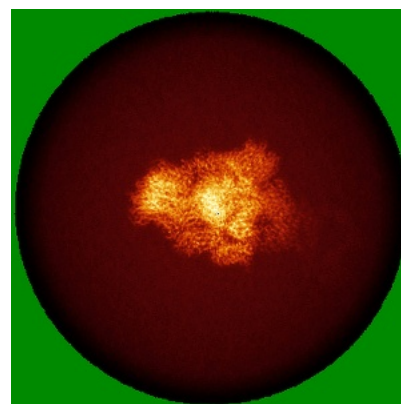
6.4.1 Primary map



X

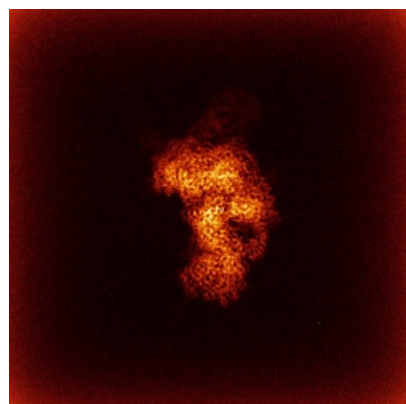


Y

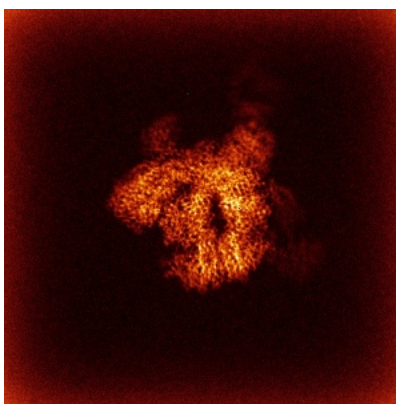


Z

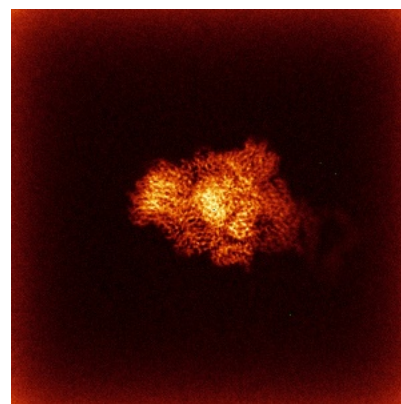
6.4.2 Raw map



X



Y

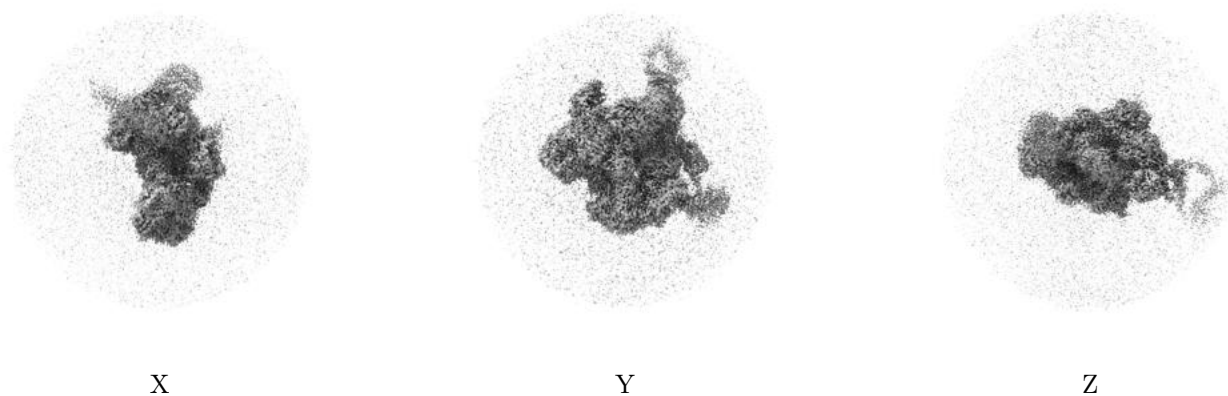


Z

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.

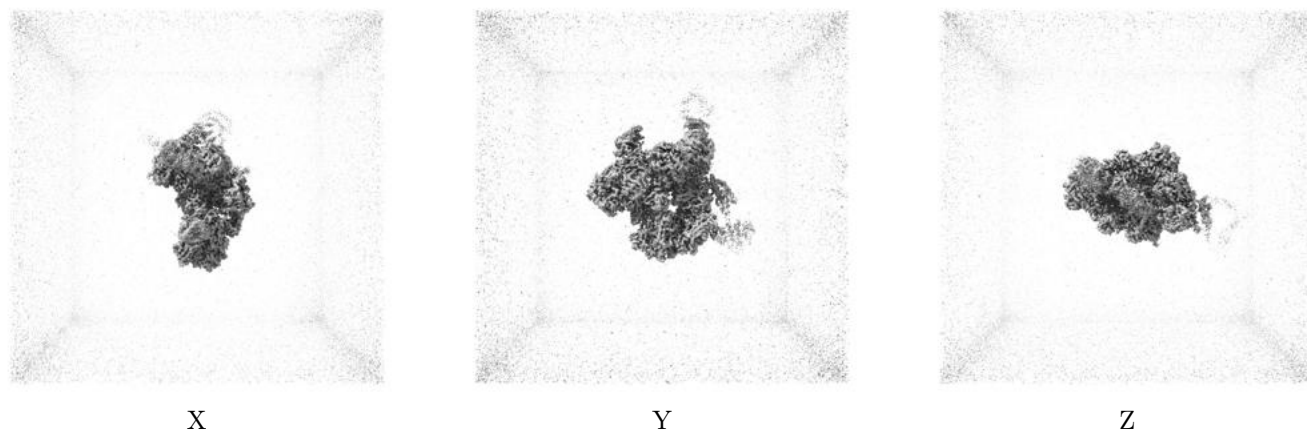
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

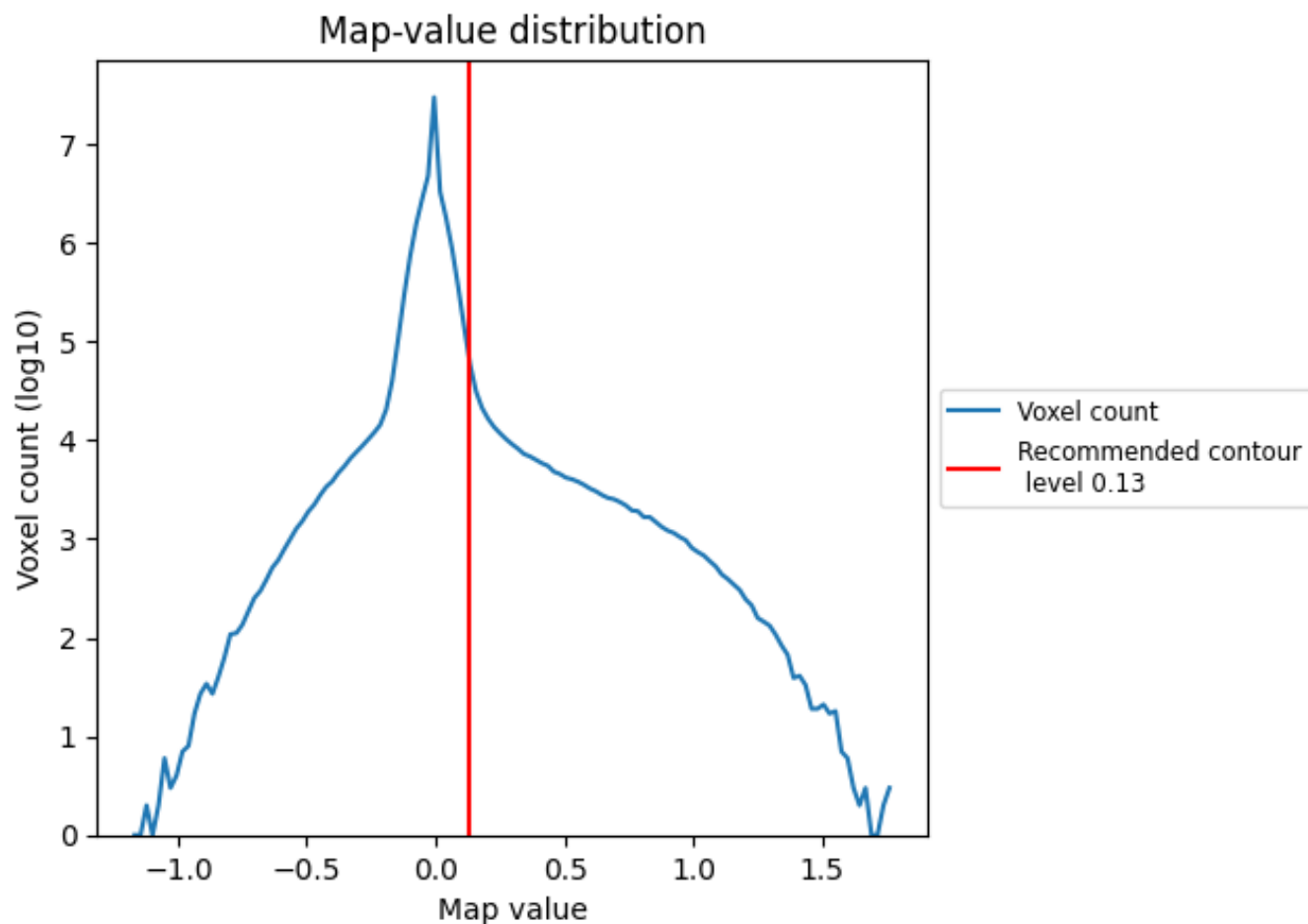
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

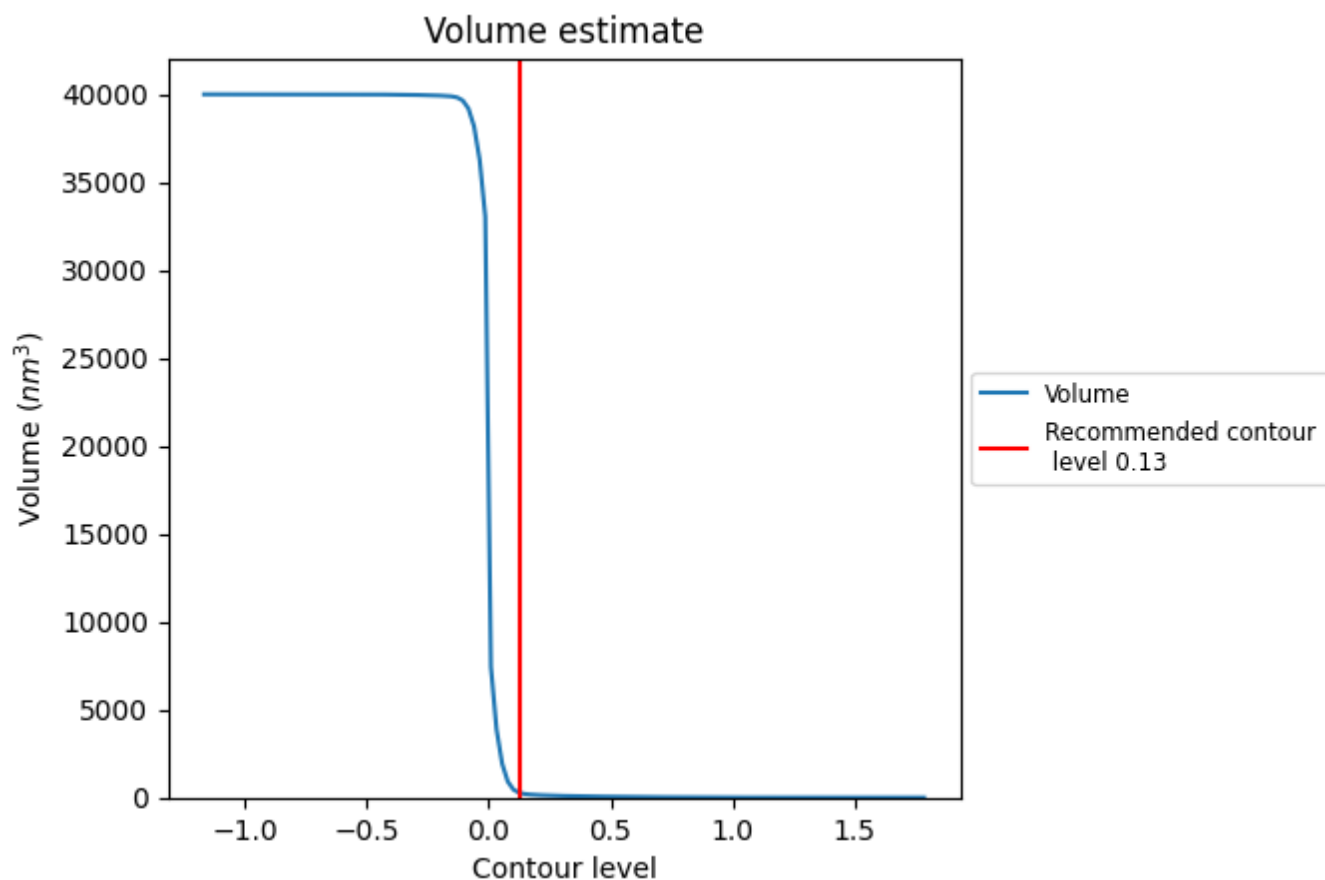
This section contains the results of statistical analysis of the map.

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.

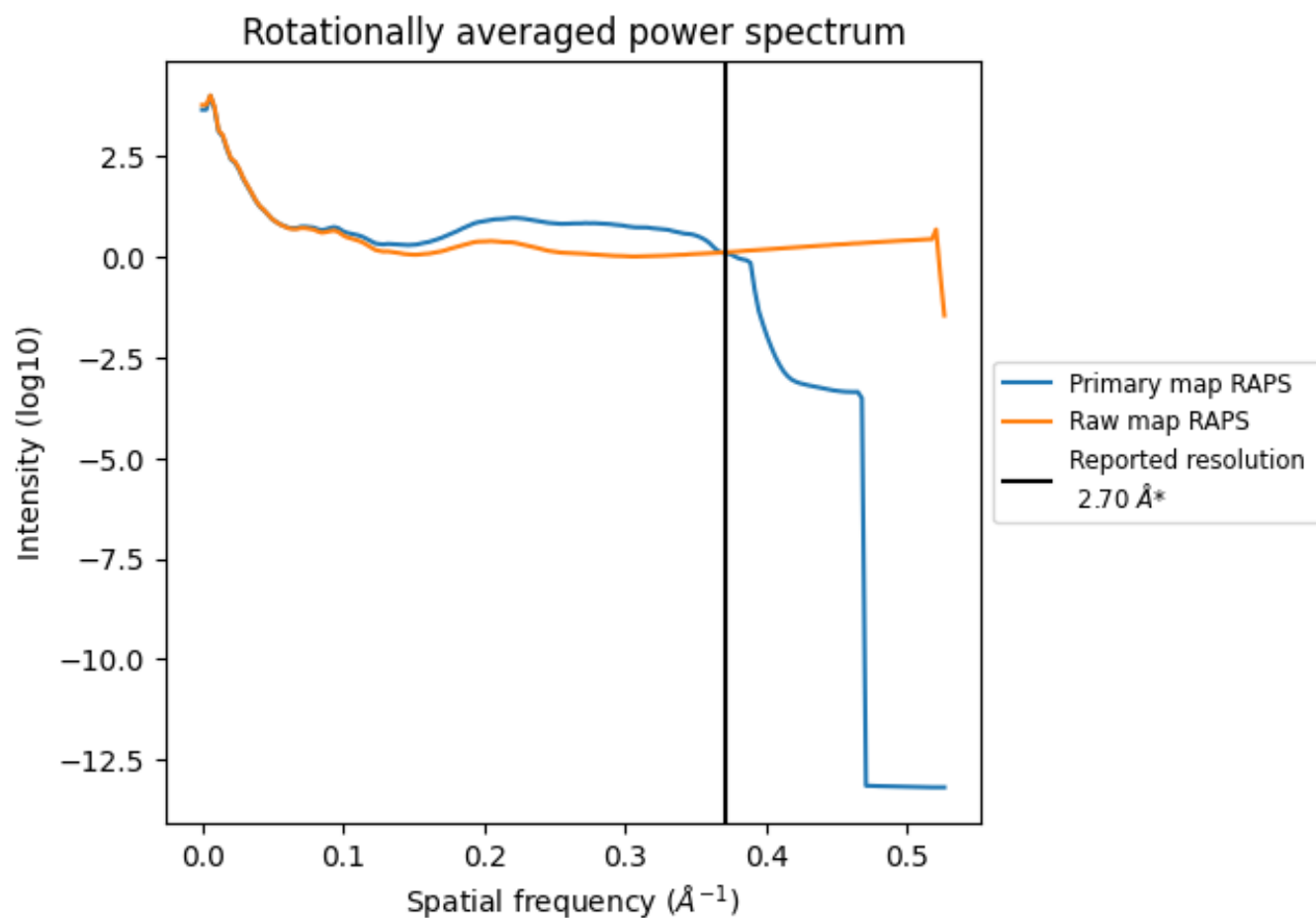
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm^3 ; this corresponds to an approximate mass of 232 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 ⓘ

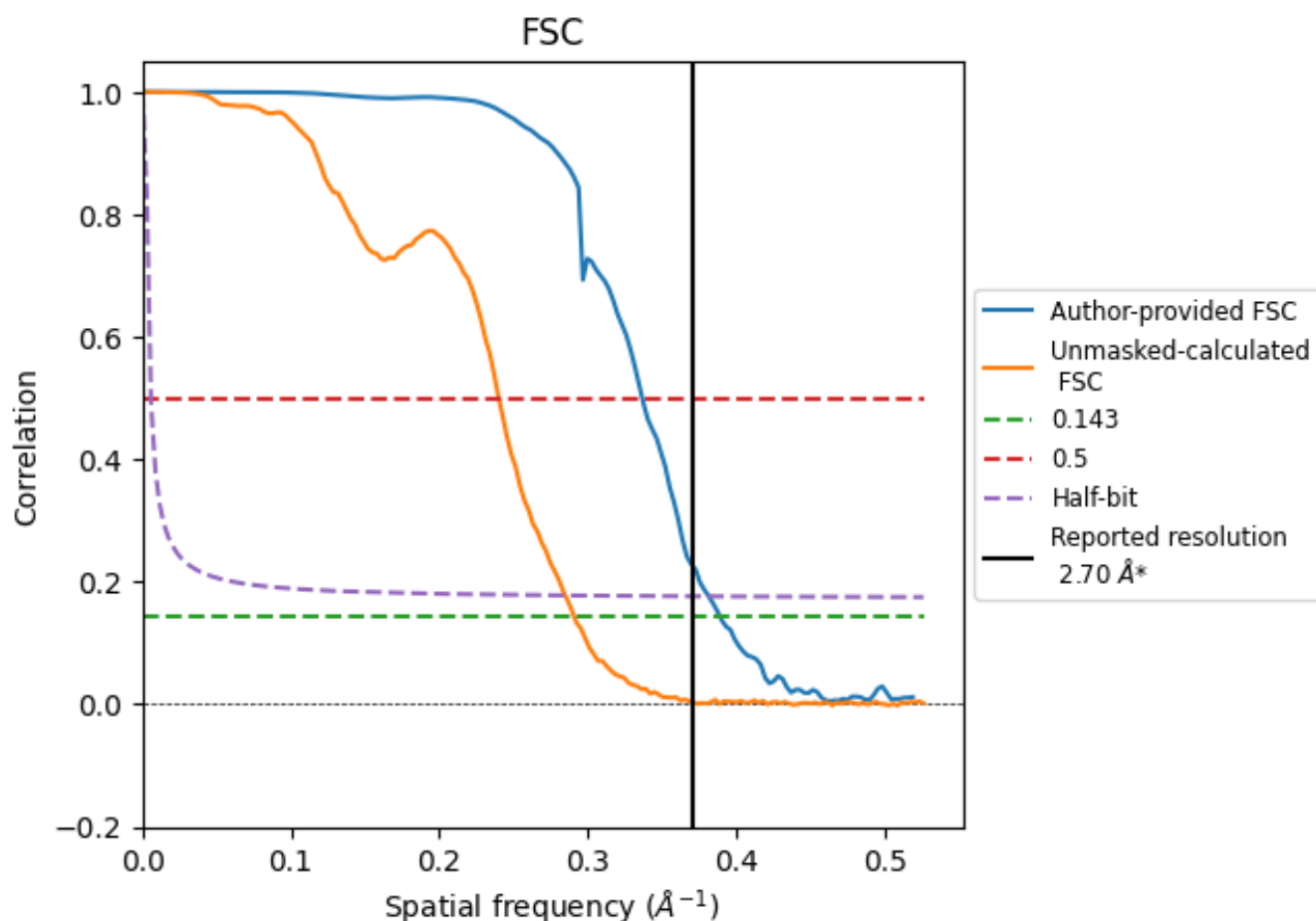


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

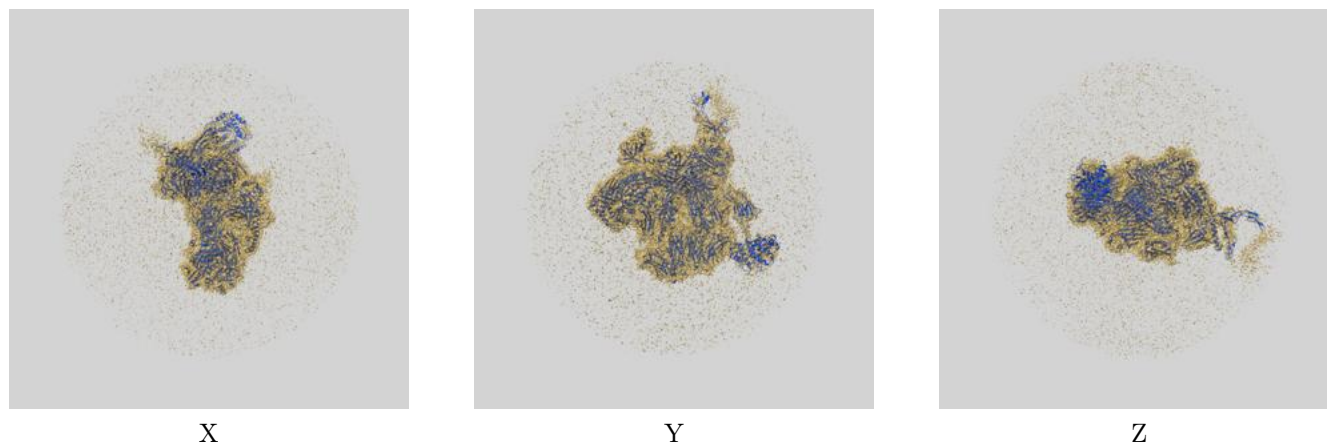
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.57	2.97	2.62
Unmasked-calculated*	3.44	4.17	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

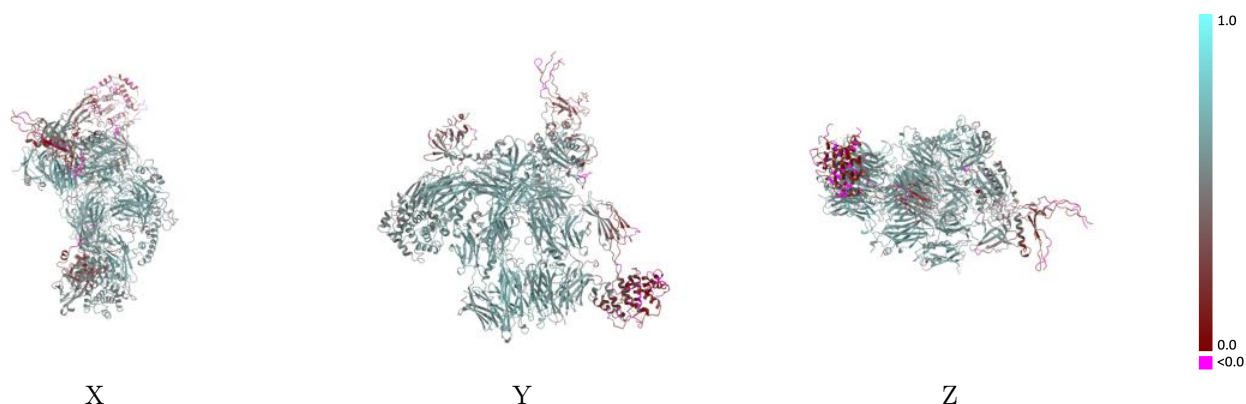
This section contains information regarding the fit between EMDB map EMD-63895 and PDB model 9U62. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



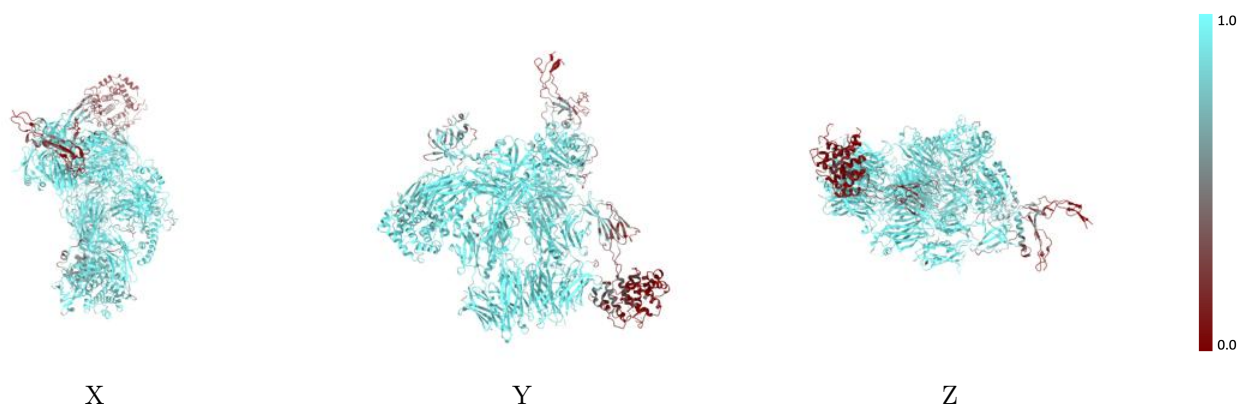
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



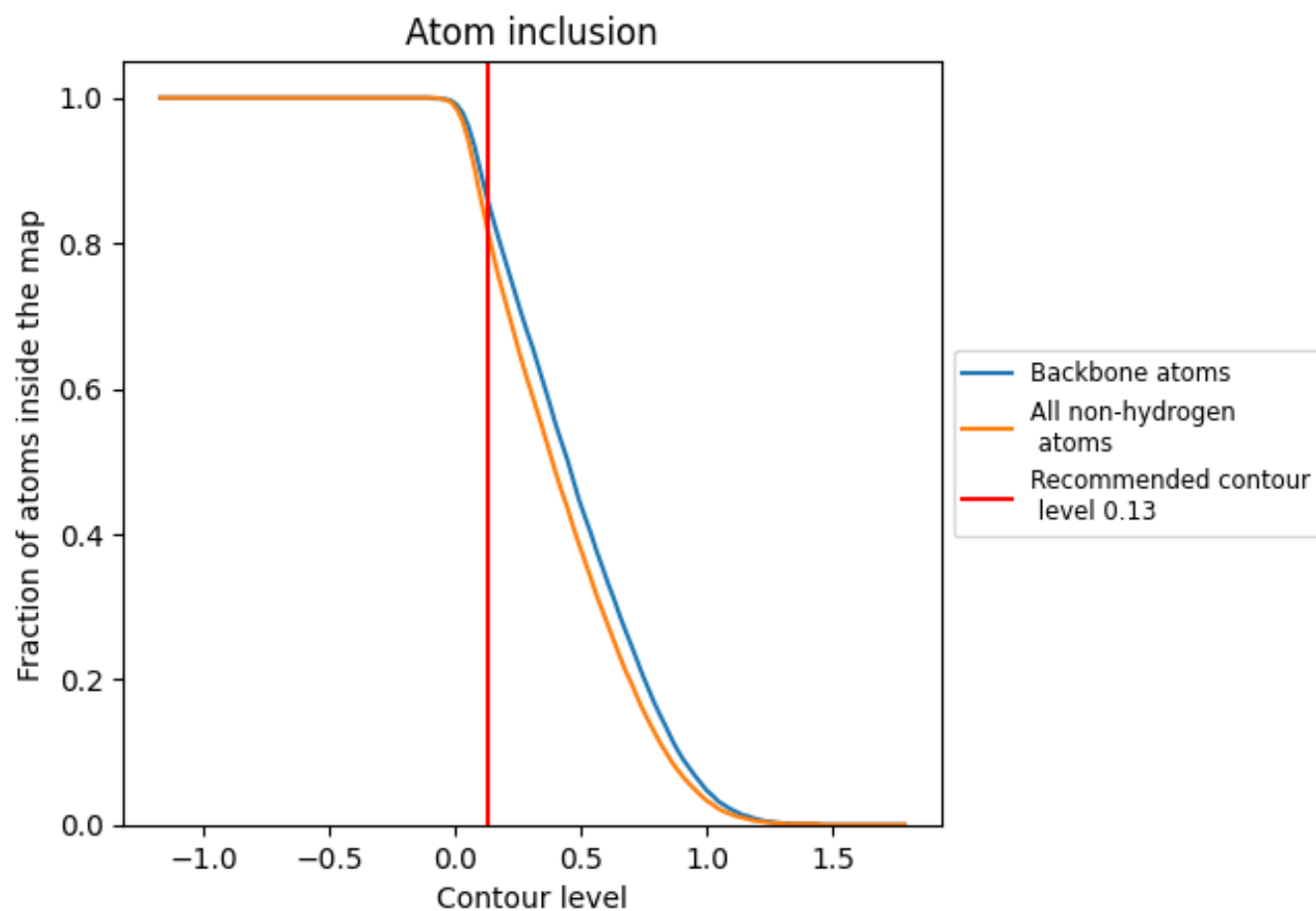
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.5250
A	0.0710	0.2770
B	0.8810	0.5570
C	0.9510	0.6140
D	0.8780	0.5400
E	0.7530	0.4960
P	0.2380	0.1890

