



## Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 06:29 PM EDT

PDB ID : 10RJ / pdb\_000010rj  
EMDB ID : EMD-75408  
Title : Heparin-induced cis tetrameric complex of VEGF, VEGFR2 and Neuropilin 1  
Authors : Chen, L.; Bai, X.; Zhang, X.  
Deposited on : 2026-02-03  
Resolution : 3.34 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>.

---

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  
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

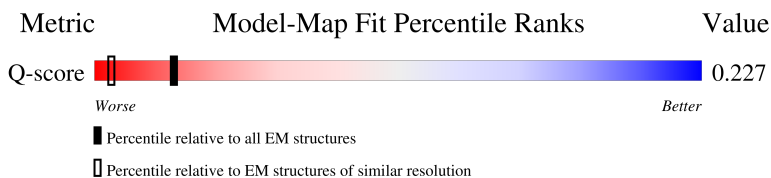
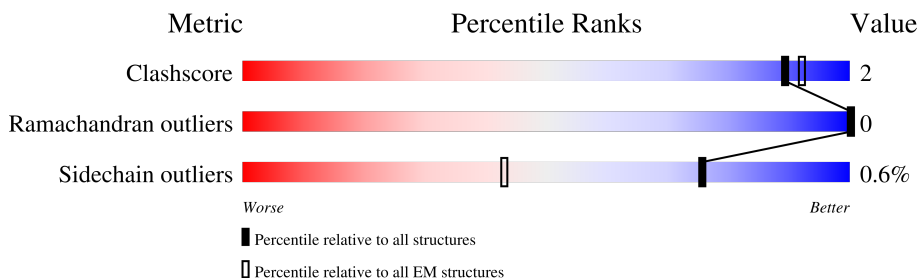
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



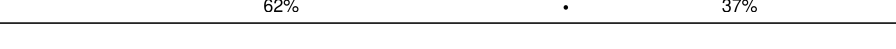

The reported resolution of this entry is 3.34 Å.

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	14446 ( 2.84 - 3.84 )

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	E	847	
1	F	847	
1	K	847	
1	L	847	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	A	175	 11% 79% 5% 17%
2	B	175	 8% 79% 5% 17%
2	G	175	 11% 79% 5% 17%
2	H	175	 8% 79% 5% 17%
3	C	754	 21% 78% 20%
3	D	754	 26% 77% 20%
3	I	754	 21% 78% 20%
3	J	754	 26% 77% 20%
4	M	2	 100%
4	N	2	 100%
5	O	28	 43% 57%
5	P	28	 43% 57%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 83098 atoms, of which 40832 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 Neuropilin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	562	Total	C	H	N	O	S	0	0
			8784	2842	4312	753	852	25		
1	L	562	Total	C	H	N	O	S	0	0
			8784	2842	4312	753	852	25		
1	E	537	Total	C	H	N	O	S	0	0
			8324	2700	4083	716	804	21		
1	K	537	Total	C	H	N	O	S	0	0
			8324	2700	4083	716	804	21		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLU	-	expression tag	UNP P97333
F	20	LEU	-	expression tag	UNP P97333
F	21	GLU	-	expression tag	UNP P97333
F	856	GLY	-	expression tag	UNP P97333
F	857	THR	-	expression tag	UNP P97333
F	858	HIS	-	expression tag	UNP P97333
F	859	HIS	-	expression tag	UNP P97333
F	860	HIS	-	expression tag	UNP P97333
F	861	HIS	-	expression tag	UNP P97333
F	862	HIS	-	expression tag	UNP P97333
F	863	HIS	-	expression tag	UNP P97333
F	864	HIS	-	expression tag	UNP P97333
F	865	HIS	-	expression tag	UNP P97333
L	19	GLU	-	expression tag	UNP P97333
L	20	LEU	-	expression tag	UNP P97333
L	21	GLU	-	expression tag	UNP P97333
L	856	GLY	-	expression tag	UNP P97333
L	857	THR	-	expression tag	UNP P97333
L	858	HIS	-	expression tag	UNP P97333
L	859	HIS	-	expression tag	UNP P97333
L	860	HIS	-	expression tag	UNP P97333
L	861	HIS	-	expression tag	UNP P97333

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	862	HIS	-	expression tag	UNP P97333
L	863	HIS	-	expression tag	UNP P97333
L	864	HIS	-	expression tag	UNP P97333
L	865	HIS	-	expression tag	UNP P97333
E	19	GLU	-	expression tag	UNP P97333
E	20	LEU	-	expression tag	UNP P97333
E	21	GLU	-	expression tag	UNP P97333
E	856	GLY	-	expression tag	UNP P97333
E	857	THR	-	expression tag	UNP P97333
E	858	HIS	-	expression tag	UNP P97333
E	859	HIS	-	expression tag	UNP P97333
E	860	HIS	-	expression tag	UNP P97333
E	861	HIS	-	expression tag	UNP P97333
E	862	HIS	-	expression tag	UNP P97333
E	863	HIS	-	expression tag	UNP P97333
E	864	HIS	-	expression tag	UNP P97333
E	865	HIS	-	expression tag	UNP P97333
K	19	GLU	-	expression tag	UNP P97333
K	20	LEU	-	expression tag	UNP P97333
K	21	GLU	-	expression tag	UNP P97333
K	856	GLY	-	expression tag	UNP P97333
K	857	THR	-	expression tag	UNP P97333
K	858	HIS	-	expression tag	UNP P97333
K	859	HIS	-	expression tag	UNP P97333
K	860	HIS	-	expression tag	UNP P97333
K	861	HIS	-	expression tag	UNP P97333
K	862	HIS	-	expression tag	UNP P97333
K	863	HIS	-	expression tag	UNP P97333
K	864	HIS	-	expression tag	UNP P97333
K	865	HIS	-	expression tag	UNP P97333

- Molecule 2 is a protein called Isoform VEGF-1 of Vascular endothelial growth factor A, long form.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	146	Total	C	H	N	O	S	0	0
			2347	728	1157	221	220	21		
2	B	146	Total	C	H	N	O	S	0	0
			2347	728	1157	221	220	21		
2	G	146	Total	C	H	N	O	S	0	0
			2347	728	1157	221	220	21		
2	H	146	Total	C	H	N	O	S	0	0
			2347	728	1157	221	220	21		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLU	-	expression tag	UNP Q00731
A	17	LEU	-	expression tag	UNP Q00731
A	18	GLU	-	expression tag	UNP Q00731
A	19	HIS	-	expression tag	UNP Q00731
A	20	HIS	-	expression tag	UNP Q00731
A	21	HIS	-	expression tag	UNP Q00731
A	22	HIS	-	expression tag	UNP Q00731
A	23	HIS	-	expression tag	UNP Q00731
A	24	HIS	-	expression tag	UNP Q00731
A	25	HIS	-	expression tag	UNP Q00731
A	26	HIS	-	expression tag	UNP Q00731
B	16	GLU	-	expression tag	UNP Q00731
B	17	LEU	-	expression tag	UNP Q00731
B	18	GLU	-	expression tag	UNP Q00731
B	19	HIS	-	expression tag	UNP Q00731
B	20	HIS	-	expression tag	UNP Q00731
B	21	HIS	-	expression tag	UNP Q00731
B	22	HIS	-	expression tag	UNP Q00731
B	23	HIS	-	expression tag	UNP Q00731
B	24	HIS	-	expression tag	UNP Q00731
B	25	HIS	-	expression tag	UNP Q00731
B	26	HIS	-	expression tag	UNP Q00731
G	16	GLU	-	expression tag	UNP Q00731
G	17	LEU	-	expression tag	UNP Q00731
G	18	GLU	-	expression tag	UNP Q00731
G	19	HIS	-	expression tag	UNP Q00731
G	20	HIS	-	expression tag	UNP Q00731
G	21	HIS	-	expression tag	UNP Q00731
G	22	HIS	-	expression tag	UNP Q00731
G	23	HIS	-	expression tag	UNP Q00731
G	24	HIS	-	expression tag	UNP Q00731
G	25	HIS	-	expression tag	UNP Q00731
G	26	HIS	-	expression tag	UNP Q00731
H	16	GLU	-	expression tag	UNP Q00731
H	17	LEU	-	expression tag	UNP Q00731
H	18	GLU	-	expression tag	UNP Q00731
H	19	HIS	-	expression tag	UNP Q00731
H	20	HIS	-	expression tag	UNP Q00731
H	21	HIS	-	expression tag	UNP Q00731
H	22	HIS	-	expression tag	UNP Q00731
H	23	HIS	-	expression tag	UNP Q00731
H	24	HIS	-	expression tag	UNP Q00731

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	HIS	-	expression tag	UNP Q00731
H	26	HIS	-	expression tag	UNP Q00731

- Molecule 3 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	604	Total	C	H	N	O	S	0	0
			9420	2986	4699	817	892	26		
3	D	604	Total	C	H	N	O	S	0	0
			9397	2981	4685	814	892	25		
3	I	604	Total	C	H	N	O	S	0	0
			9420	2986	4699	817	892	26		
3	J	604	Total	C	H	N	O	S	0	0
			9397	2981	4685	814	892	25		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLU	-	expression tag	UNP P35918
C	18	LEU	-	expression tag	UNP P35918
C	19	GLU	-	expression tag	UNP P35918
C	761	GLY	-	expression tag	UNP P35918
C	762	THR	-	expression tag	UNP P35918
C	763	HIS	-	expression tag	UNP P35918
C	764	HIS	-	expression tag	UNP P35918
C	765	HIS	-	expression tag	UNP P35918
C	766	HIS	-	expression tag	UNP P35918
C	767	HIS	-	expression tag	UNP P35918
C	768	HIS	-	expression tag	UNP P35918
C	769	HIS	-	expression tag	UNP P35918
C	770	HIS	-	expression tag	UNP P35918
D	17	GLU	-	expression tag	UNP P35918
D	18	LEU	-	expression tag	UNP P35918
D	19	GLU	-	expression tag	UNP P35918
D	761	GLY	-	expression tag	UNP P35918
D	762	THR	-	expression tag	UNP P35918
D	763	HIS	-	expression tag	UNP P35918
D	764	HIS	-	expression tag	UNP P35918
D	765	HIS	-	expression tag	UNP P35918
D	766	HIS	-	expression tag	UNP P35918
D	767	HIS	-	expression tag	UNP P35918
D	768	HIS	-	expression tag	UNP P35918

*Continued on next page...*

Continued from previous page...

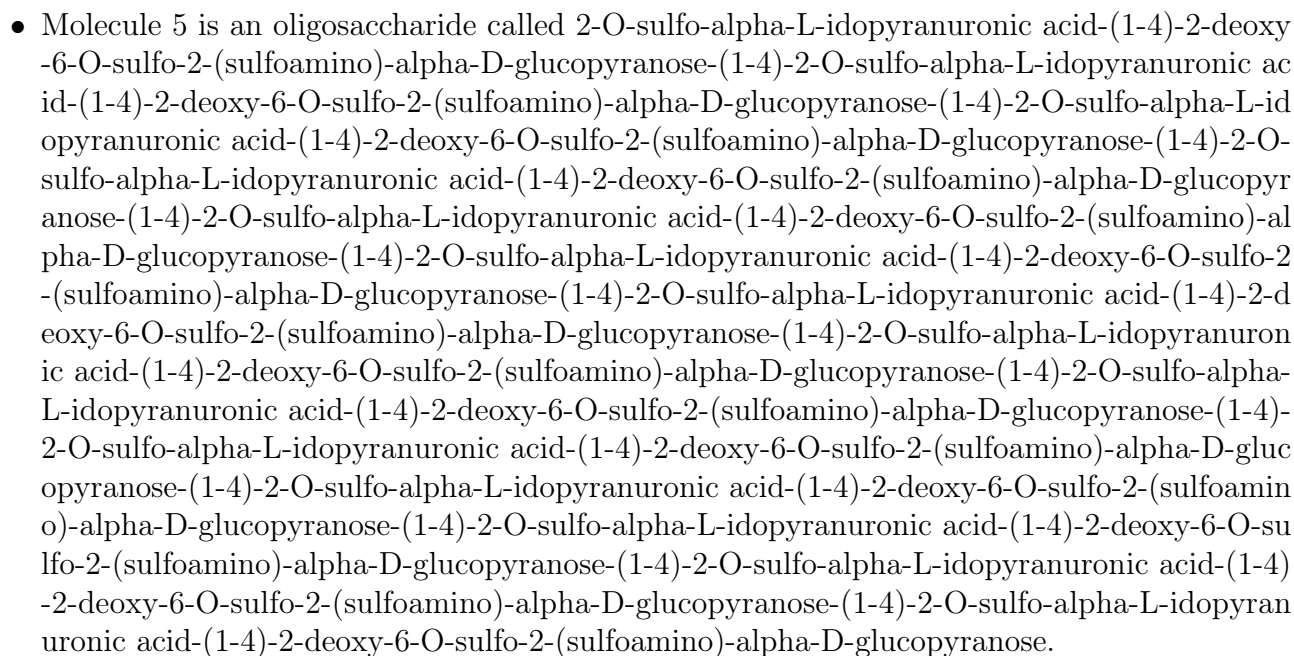
Chain	Residue	Modelled	Actual	Comment	Reference
D	769	HIS	-	expression tag	UNP P35918
D	770	HIS	-	expression tag	UNP P35918
I	17	GLU	-	expression tag	UNP P35918
I	18	LEU	-	expression tag	UNP P35918
I	19	GLU	-	expression tag	UNP P35918
I	761	GLY	-	expression tag	UNP P35918
I	762	THR	-	expression tag	UNP P35918
I	763	HIS	-	expression tag	UNP P35918
I	764	HIS	-	expression tag	UNP P35918
I	765	HIS	-	expression tag	UNP P35918
I	766	HIS	-	expression tag	UNP P35918
I	767	HIS	-	expression tag	UNP P35918
I	768	HIS	-	expression tag	UNP P35918
I	769	HIS	-	expression tag	UNP P35918
I	770	HIS	-	expression tag	UNP P35918
J	17	GLU	-	expression tag	UNP P35918
J	18	LEU	-	expression tag	UNP P35918
J	19	GLU	-	expression tag	UNP P35918
J	761	GLY	-	expression tag	UNP P35918
J	762	THR	-	expression tag	UNP P35918
J	763	HIS	-	expression tag	UNP P35918
J	764	HIS	-	expression tag	UNP P35918
J	765	HIS	-	expression tag	UNP P35918
J	766	HIS	-	expression tag	UNP P35918
J	767	HIS	-	expression tag	UNP P35918
J	768	HIS	-	expression tag	UNP P35918
J	769	HIS	-	expression tag	UNP P35918
J	770	HIS	-	expression tag	UNP P35918

- 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	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	N	2	Total	C	H	N	O	0	0
			55	16	27	2	10		



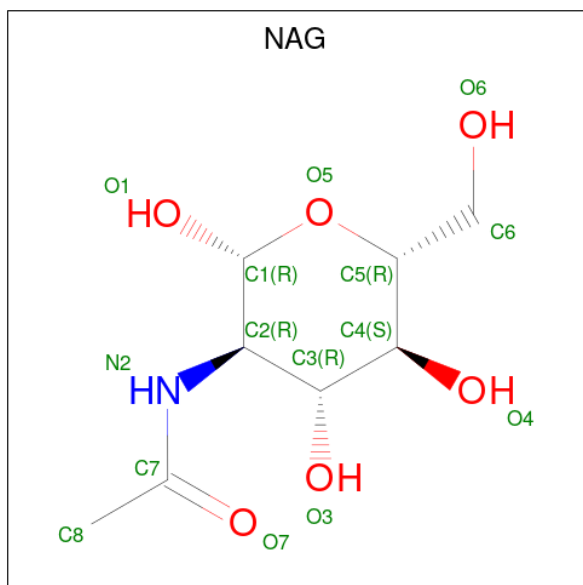


Mol	Chain	Residues	Atoms						AltConf	Trace
5	O	28	Total 703	C 168	H 212	N 14	O 267	S 42	0	0
5	P	28	Total 703	C 168	H 212	N 14	O 267	S 42	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	F	2	Total Ca 2 2	0
6	L	2	Total Ca 2 2	0
6	E	2	Total Ca 2 2	0
6	K	2	Total Ca 2 2	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

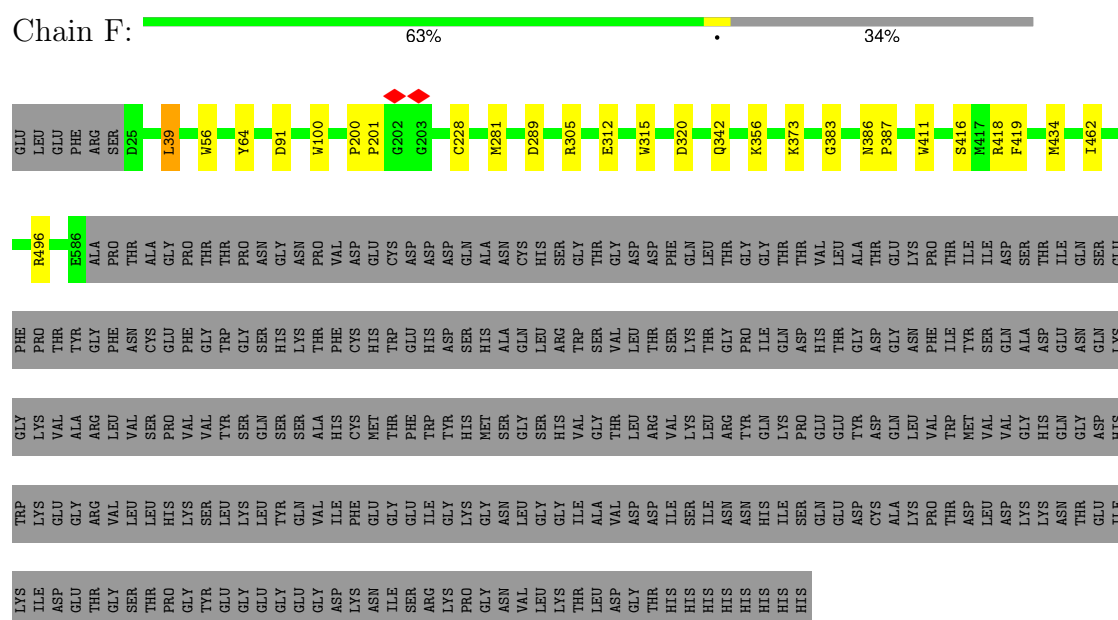


Mol	Chain	Residues	Atoms					AltConf
7	F	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	L	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	E	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	I	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	I	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	K	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	J	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	J	1	Total	C	H	N	O	0
			28	8	14	1	5	

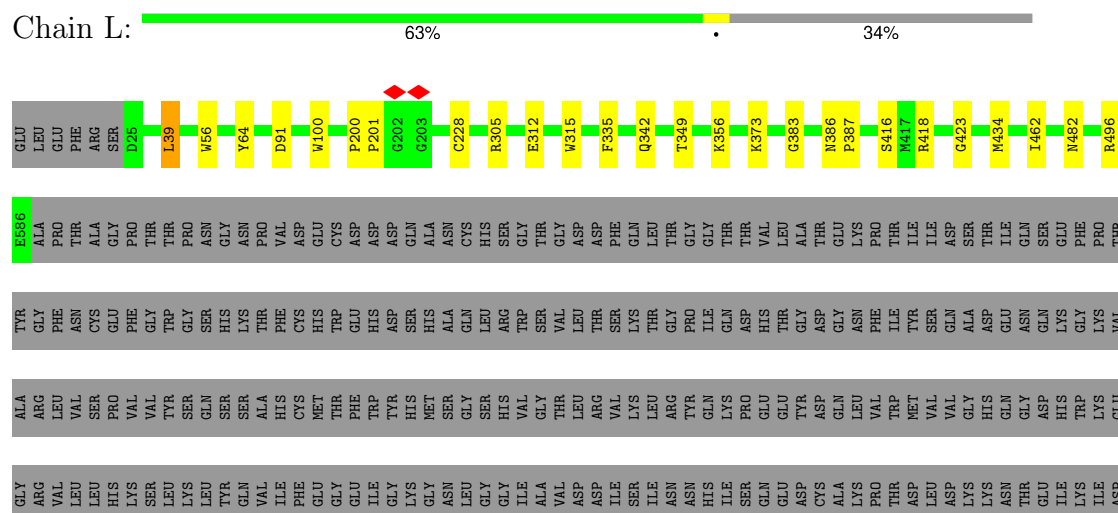
### 3 Residue-property plots

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.

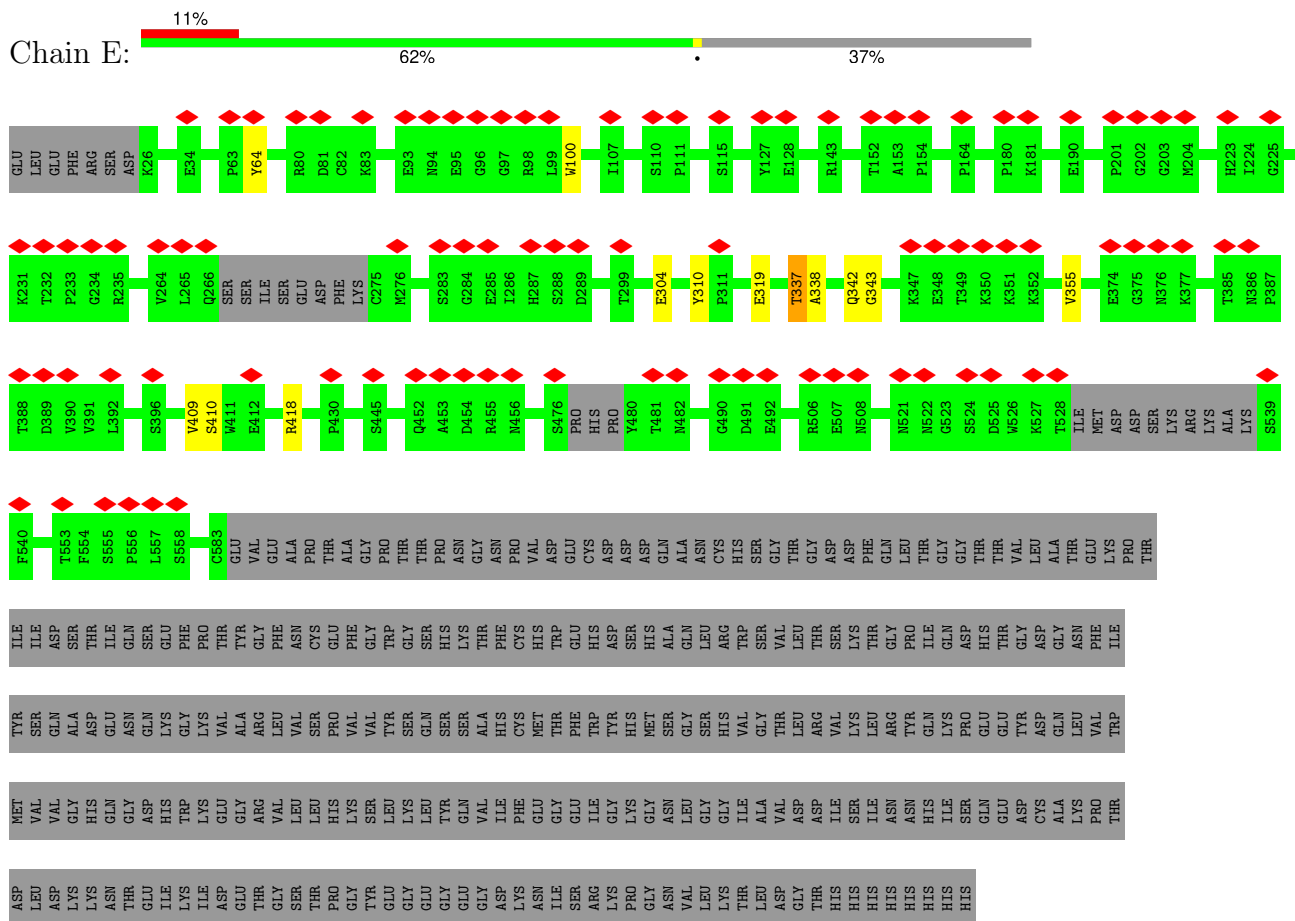
#### • Molecule 1: Neuropilin-1



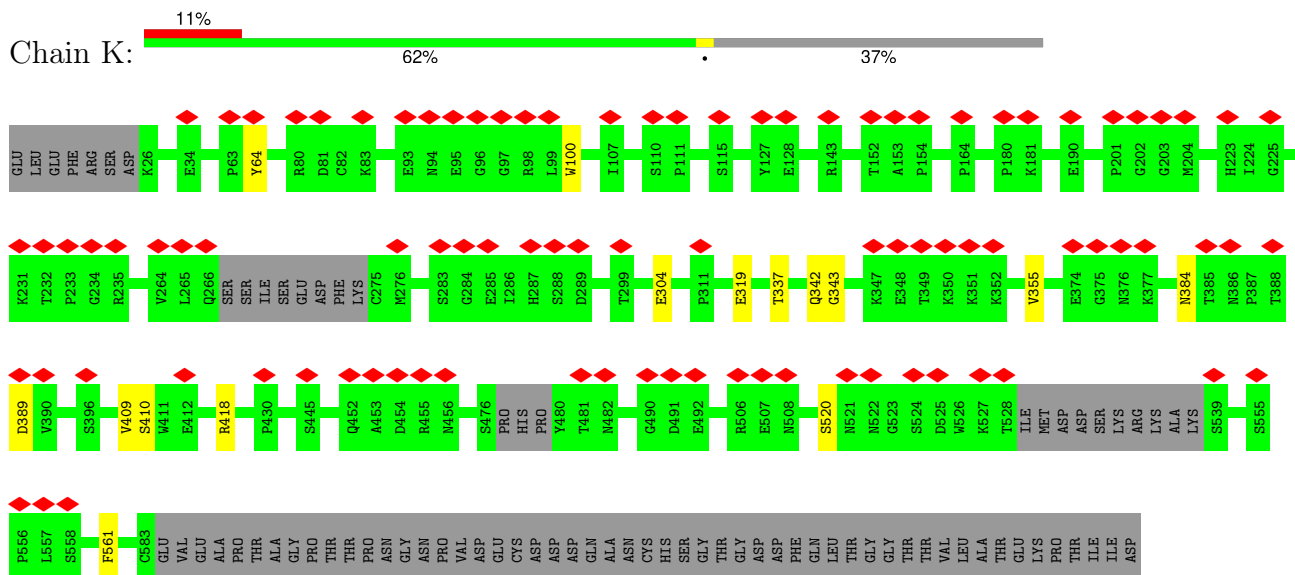
#### • Molecule 1: Neuropilin-1



Chain E:

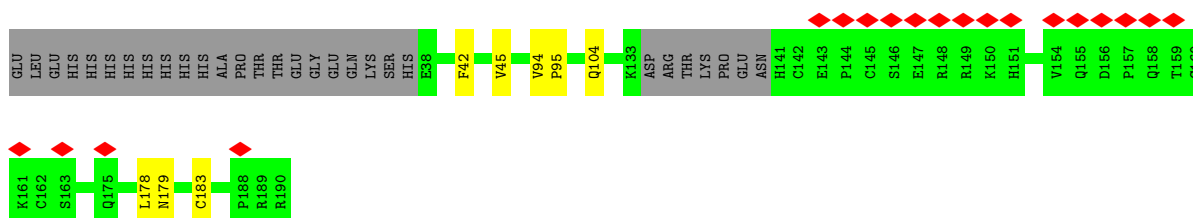


Chain K:

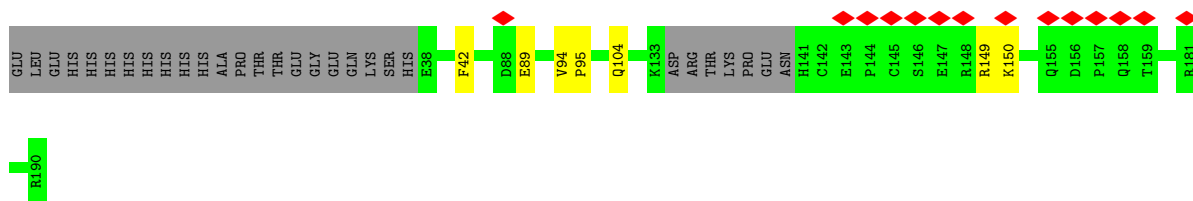
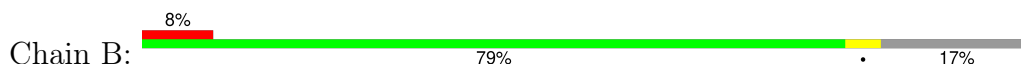


[illegible]

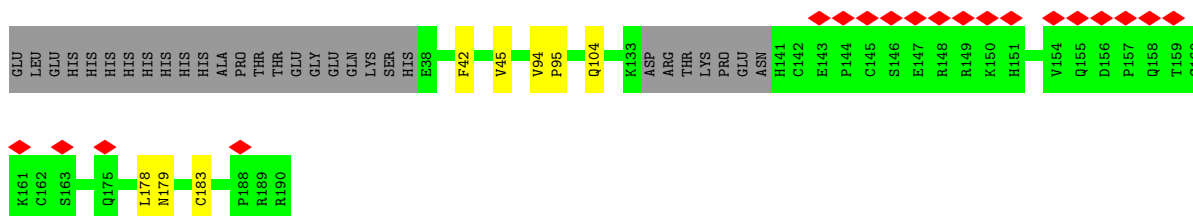
- Molecule 2: Isoform VEGF-1 of Vascular endothelial growth factor A, long form



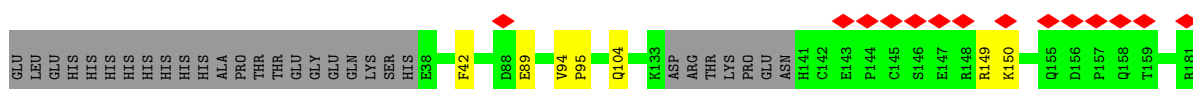
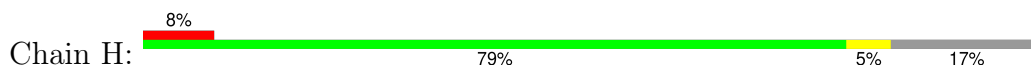
- Molecule 2: Isoform VEGF-1 of Vascular endothelial growth factor A, long form



- Molecule 2: Isoform VEGF-1 of Vascular endothelial growth factor A, long form



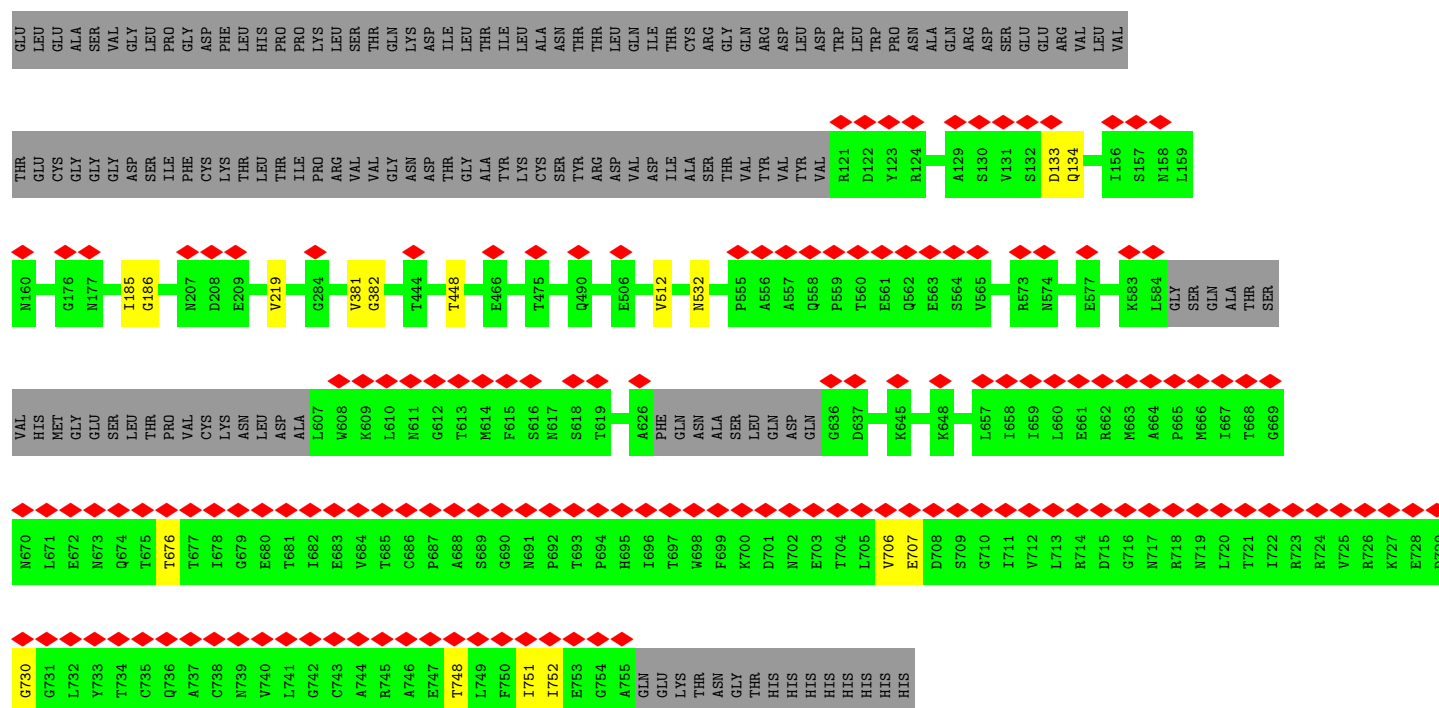
- Molecule 2: Isoform VEGF-1 of Vascular endothelial growth factor A, long form



R190

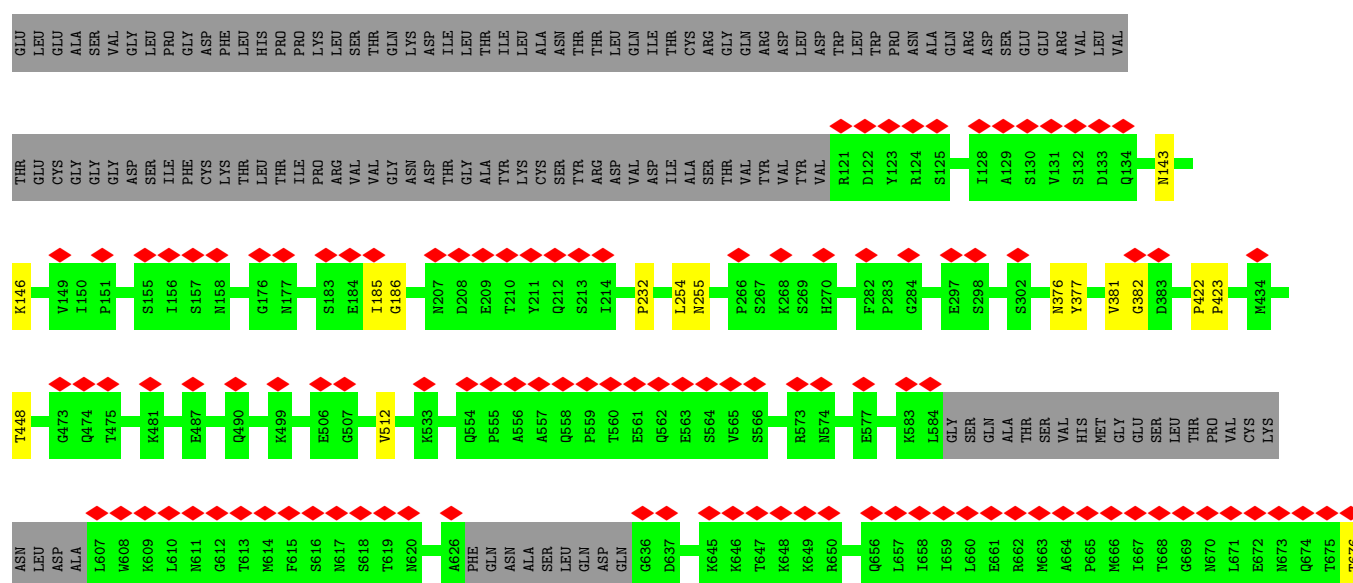
- Molecule 3: Vascular endothelial growth factor receptor 2

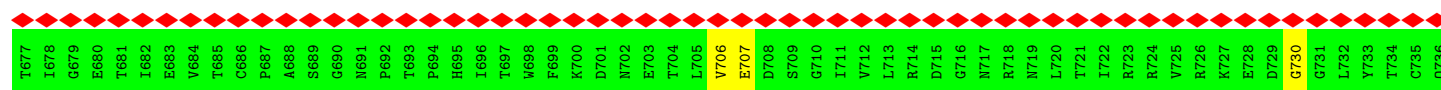
Chain C: 21% 78% 20%



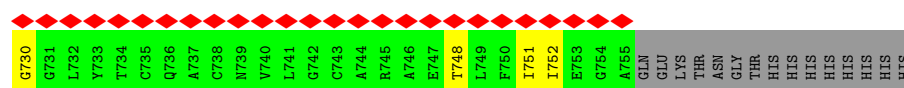
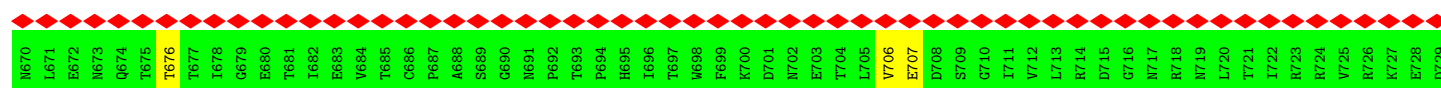
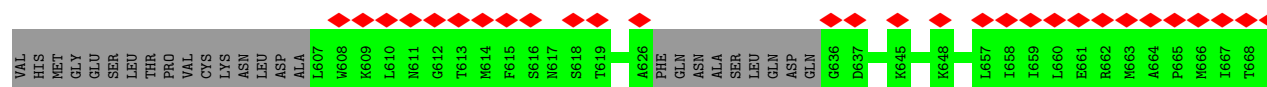
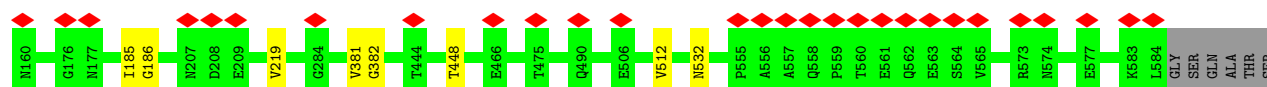
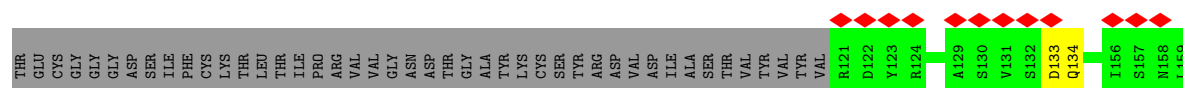
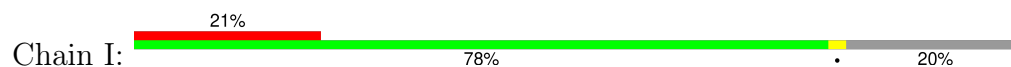
- Molecule 3: Vascular endothelial growth factor receptor 2

Chain D: 26% 77% 20%

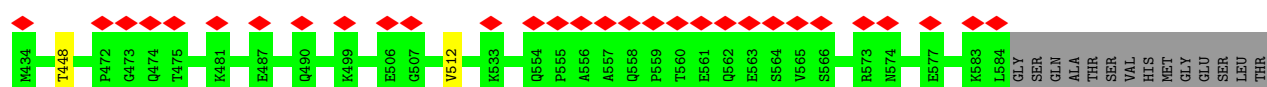
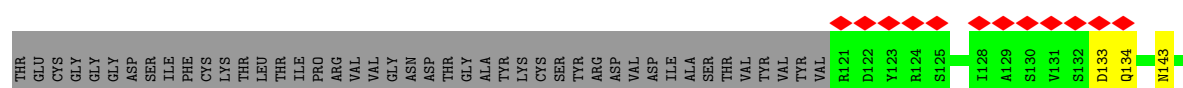
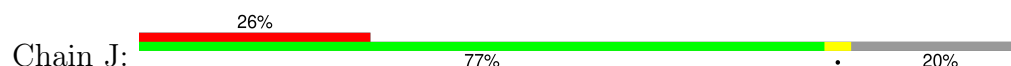


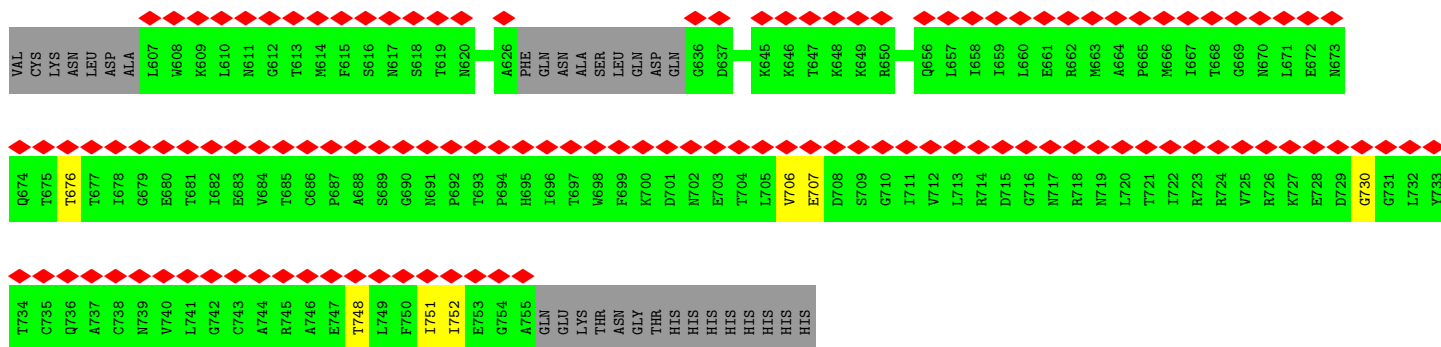


• Molecule 3: Vascular endothelial growth factor receptor 2



• Molecule 3: Vascular endothelial growth factor receptor 2





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

Chain M:  100%



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

Chain N:  100%



- [illegible]

Chain O:  43% 57%





[illegible]

Chain P:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105039	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.936, 0.936, 0.936	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: NAG, CA, IDS, SGN

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	E	0.10	0/4354	0.29	0/5898
1	F	0.11	0/4593	0.34	0/6218
1	K	0.10	0/4354	0.29	0/5898
1	L	0.11	0/4593	0.34	0/6218
2	A	0.11	0/1212	0.30	0/1624
2	B	0.12	0/1212	0.30	0/1624
2	G	0.11	0/1212	0.30	0/1624
2	H	0.12	0/1212	0.30	0/1624
3	C	0.11	0/4821	0.29	0/6554
3	D	0.10	0/4812	0.28	0/6544
3	I	0.11	0/4821	0.29	0/6554
3	J	0.10	0/4812	0.28	0/6544
All	All	0.10	0/42008	0.30	0/56924

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4241	4083	4067	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4472	4312	4310	16	0
1	K	4241	4083	4067	9	0
1	L	4472	4312	4310	15	0
2	A	1190	1157	1152	10	0
2	B	1190	1157	1152	9	0
2	G	1190	1157	1152	10	0
2	H	1190	1157	1152	10	0
3	C	4721	4699	4678	8	0
3	D	4712	4685	4660	13	0
3	I	4721	4699	4678	8	0
3	J	4712	4685	4660	15	0
4	M	28	27	25	0	0
4	N	28	27	25	0	0
5	O	491	212	157	21	0
5	P	491	212	157	20	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
7	C	28	28	26	0	0
7	D	28	28	26	1	0
7	E	14	14	13	0	0
7	F	14	14	13	0	0
7	I	28	28	26	0	0
7	J	28	28	26	1	0
7	K	14	14	13	0	0
7	L	14	14	13	0	0
All	All	42266	40832	40558	152	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 2.

All (152) 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)
2:A:104:GLN:HE21	2:B:42:PHE:H	1.10	0.97
2:G:104:GLN:HE21	2:H:42:PHE:H	1.11	0.96
2:A:42:PHE:H	2:B:104:GLN:HE21	1.19	0.91
2:G:42:PHE:H	2:H:104:GLN:HE21	1.19	0.89
2:G:104:GLN:HE21	2:H:42:PHE:N	1.75	0.84
2:G:42:PHE:N	2:H:104:GLN:HE21	1.76	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:104:GLN:HE21	2:B:42:PHE:N	1.75	0.83
2:A:42:PHE:N	2:B:104:GLN:HE21	1.76	0.82
2:A:104:GLN:NE2	2:B:42:PHE:H	1.85	0.74
2:G:104:GLN:NE2	2:H:42:PHE:H	1.86	0.73
5:P:3:SGN:O2S	5:P:3:SGN:O3	2.07	0.72
5:O:3:SGN:O2S	5:O:3:SGN:O3	2.07	0.69
5:P:4:IDS:O3S	5:P:4:IDS:H3	1.92	0.68
2:G:42:PHE:H	2:H:104:GLN:NE2	1.92	0.67
5:O:4:IDS:H3	5:O:4:IDS:O3S	1.92	0.67
2:A:42:PHE:H	2:B:104:GLN:NE2	1.92	0.64
3:I:751:ILE:C	3:I:752:ILE:HD12	2.24	0.63
3:C:751:ILE:C	3:C:752:ILE:HD12	2.24	0.62
3:D:751:ILE:C	3:D:752:ILE:HD12	2.25	0.62
3:J:751:ILE:C	3:J:752:ILE:HD12	2.25	0.62
5:O:6:IDS:H3	5:O:7:SGN:H3	1.82	0.59
5:P:6:IDS:H3	5:P:7:SGN:H3	1.82	0.59
1:K:342:GLN:N	1:K:418:ARG:O	2.35	0.59
1:E:342:GLN:N	1:E:418:ARG:O	2.35	0.58
5:P:5:SGN:O3	5:P:6:IDS:H2	2.04	0.56
5:O:5:SGN:O3	5:O:6:IDS:H2	2.04	0.56
5:P:8:IDS:O1S	5:P:8:IDS:H3	2.05	0.56
5:O:8:IDS:O1S	5:O:8:IDS:H3	2.06	0.56
5:O:1:SGN:O6S	5:O:1:SGN:O5	2.24	0.55
1:F:305:ARG:NH2	1:F:312:GLU:OE2	2.40	0.54
5:P:1:SGN:O6S	5:P:1:SGN:O5	2.24	0.54
1:L:305:ARG:NH2	1:L:312:GLU:OE2	2.40	0.54
5:P:21:SGN:O6S	5:P:21:SGN:O5	2.26	0.53
1:L:200:PRO:N	1:L:201:PRO:HD2	2.24	0.52
1:F:200:PRO:N	1:F:201:PRO:HD2	2.24	0.52
5:O:21:SGN:O6S	5:O:21:SGN:O5	2.26	0.52
2:H:89:GLU:OE2	3:J:255:ASN:N	2.39	0.51
1:K:342:GLN:O	1:K:418:ARG:N	2.43	0.51
1:K:343:GLY:O	1:K:418:ARG:NE	2.39	0.51
5:O:23:SGN:O6S	5:O:23:SGN:O5	2.29	0.51
1:E:343:GLY:O	1:E:418:ARG:NE	2.39	0.51
1:E:355:VAL:HG13	1:E:410:SER:O	2.11	0.50
3:I:448:THR:HG22	3:I:512:VAL:HG12	1.92	0.50
1:E:342:GLN:O	1:E:418:ARG:N	2.43	0.50
3:C:448:THR:HG22	3:C:512:VAL:HG12	1.92	0.50
5:P:3:SGN:O2S	5:P:3:SGN:C3	2.60	0.50
1:K:355:VAL:HG13	1:K:410:SER:O	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:23:SGN:O6S	5:P:23:SGN:O5	2.29	0.49
1:L:356:LYS:O	1:L:383:GLY:N	2.43	0.49
3:D:232:PRO:HD3	7:D:801:NAG:H81	1.95	0.48
5:O:3:SGN:O2S	5:O:3:SGN:C3	2.60	0.48
5:P:26:IDS:O3S	5:P:26:IDS:H3	2.13	0.48
5:O:26:IDS:O3S	5:O:26:IDS:H3	2.13	0.48
3:J:232:PRO:HD3	7:J:801:NAG:H81	1.95	0.48
5:P:22:IDS:O3S	5:P:22:IDS:H3	2.14	0.48
5:O:17:SGN:O6S	5:O:17:SGN:O5	2.30	0.48
5:O:28:IDS:O3S	5:O:28:IDS:H3	2.14	0.48
5:O:22:IDS:O3S	5:O:22:IDS:H3	2.14	0.47
5:P:17:SGN:O6S	5:P:17:SGN:O5	2.30	0.47
1:F:315:TRP:O	1:F:416:SER:HA	2.15	0.47
1:F:356:LYS:O	1:F:383:GLY:N	2.43	0.47
5:P:13:SGN:O5S	5:P:13:SGN:H5	2.15	0.47
5:P:28:IDS:O3S	5:P:28:IDS:H3	2.15	0.47
2:B:89:GLU:OE2	3:D:255:ASN:N	2.38	0.47
3:C:730:GLY:HA2	3:C:752:ILE:HD13	1.95	0.47
3:I:730:GLY:HA2	3:I:752:ILE:HD13	1.95	0.47
3:I:133:ASP:OD1	3:I:134:GLN:N	2.48	0.47
5:P:5:SGN:H4	5:P:6:IDS:C5	2.45	0.47
1:L:315:TRP:O	1:L:416:SER:HA	2.15	0.47
1:L:91:ASP:HB2	1:L:100:TRP:HE1	1.80	0.46
1:F:91:ASP:HB2	1:F:100:TRP:HE1	1.80	0.46
5:O:13:SGN:O5S	5:O:13:SGN:H5	2.15	0.46
3:C:133:ASP:OD1	3:C:134:GLN:N	2.48	0.46
3:D:730:GLY:HA2	3:D:752:ILE:HD13	1.97	0.46
5:O:5:SGN:H4	5:O:6:IDS:C5	2.45	0.46
3:J:730:GLY:HA2	3:J:752:ILE:HD13	1.97	0.46
3:D:448:THR:HG22	3:D:512:VAL:HG12	1.98	0.45
5:P:16:IDS:H4	5:P:17:SGN:N2	2.32	0.45
5:O:16:IDS:H4	5:O:17:SGN:N2	2.32	0.45
5:O:24:IDS:H3	5:O:24:IDS:O3S	2.17	0.44
1:F:462:ILE:HD12	1:F:462:ILE:N	2.33	0.44
5:P:24:IDS:H3	5:P:24:IDS:O3S	2.17	0.44
5:O:6:IDS:C3	5:O:7:SGN:N2	2.81	0.44
1:L:386:ASN:HB2	1:L:387:PRO:HD2	2.00	0.44
1:F:342:GLN:N	1:F:418:ARG:O	2.51	0.44
3:D:381:VAL:HG12	3:D:382:GLY:N	2.33	0.44
3:J:381:VAL:HG12	3:J:382:GLY:N	2.33	0.43
1:F:386:ASN:HB2	1:F:387:PRO:HD2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:448:THR:HG22	3:J:512:VAL:HG12	1.98	0.43
3:I:381:VAL:HG12	3:I:382:GLY:N	2.34	0.43
1:L:462:ILE:HD12	1:L:462:ILE:N	2.33	0.43
3:J:422:PRO:O	3:J:423:PRO:C	2.62	0.43
1:F:289:ASP:OD1	1:F:289:ASP:N	2.51	0.43
2:B:94:VAL:HG13	2:B:95:PRO:HD2	2.01	0.43
5:P:6:IDS:C3	5:P:7:SGN:N2	2.81	0.43
3:C:381:VAL:HG12	3:C:382:GLY:N	2.34	0.42
3:C:706:VAL:HG12	3:C:707:GLU:N	2.34	0.42
3:D:706:VAL:HG12	3:D:707:GLU:N	2.35	0.42
3:I:706:VAL:HG12	3:I:707:GLU:N	2.34	0.42
3:J:143:ASN:ND2	5:P:28:IDS:O3	2.52	0.42
3:J:706:VAL:HG12	3:J:707:GLU:N	2.35	0.42
3:D:143:ASN:ND2	5:O:28:IDS:O3	2.53	0.42
2:H:94:VAL:HG13	2:H:95:PRO:HD2	2.02	0.42
1:K:64:TYR:C	1:K:64:TYR:CD1	2.97	0.42
1:L:342:GLN:N	1:L:418:ARG:O	2.51	0.42
2:G:179:ASN:ND2	1:K:319:GLU:OE2	2.49	0.42
3:D:143:ASN:HB2	3:D:146:LYS:HG2	2.01	0.42
3:J:143:ASN:HB2	3:J:146:LYS:HG2	2.01	0.42
1:F:496:ARG:HG2	1:F:496:ARG:O	2.20	0.42
2:A:42:PHE:O	2:A:45:VAL:HG22	2.19	0.42
3:J:376:ASN:O	3:J:377:TYR:C	2.63	0.42
1:F:373:LYS:NZ	5:O:17:SGN:O3	2.49	0.42
3:I:185:ILE:HG13	3:I:186:GLY:N	2.35	0.42
1:L:200:PRO:N	1:L:201:PRO:CD	2.83	0.41
1:L:39:LEU:HD11	1:L:56:TRP:CG	2.55	0.41
1:E:64:TYR:C	1:E:64:TYR:CD1	2.97	0.41
3:D:422:PRO:O	3:D:423:PRO:C	2.62	0.41
3:J:185:ILE:HG13	3:J:186:GLY:N	2.35	0.41
3:C:185:ILE:HG13	3:C:186:GLY:N	2.35	0.41
3:C:448:THR:HG22	3:C:512:VAL:CG1	2.50	0.41
2:G:42:PHE:O	2:G:45:VAL:HG22	2.19	0.41
1:K:520:SER:O	1:K:561:PHE:N	2.51	0.41
1:F:39:LEU:HD11	1:F:56:TRP:CG	2.55	0.41
3:J:133:ASP:OD1	3:J:134:GLN:N	2.52	0.41
2:G:94:VAL:HG13	2:G:95:PRO:HD2	2.02	0.41
1:L:335:PHE:O	1:L:423:GLY:HA3	2.21	0.41
1:L:496:ARG:O	1:L:496:ARG:HG2	2.20	0.41
3:D:376:ASN:O	3:D:377:TYR:C	2.63	0.41
2:A:94:VAL:HG13	2:A:95:PRO:HD2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:LEU:HD11	2:A:183:CYS:HA	2.02	0.41
2:B:149:ARG:O	2:B:150:LYS:C	2.64	0.41
1:E:310:TYR:O	1:E:418:ARG:NH1	2.52	0.41
3:J:216:TYR:C	3:J:217:ILE:HD12	2.46	0.41
1:F:200:PRO:N	1:F:201:PRO:CD	2.83	0.41
1:L:373:LYS:NZ	5:P:17:SGN:O3	2.48	0.41
1:E:409:VAL:O	1:E:409:VAL:HG12	2.20	0.41
3:D:185:ILE:HG13	3:D:186:GLY:N	2.35	0.41
1:K:409:VAL:O	1:K:409:VAL:HG12	2.20	0.41
1:F:281:MET:HE3	1:F:419:PHE:CZ	2.56	0.40
5:O:3:SGN:O3	5:O:3:SGN:S1	2.64	0.40
3:D:448:THR:HG22	3:D:512:VAL:CG1	2.51	0.40
2:G:178:LEU:HD11	2:G:183:CYS:HA	2.02	0.40
2:H:149:ARG:O	2:H:150:LYS:C	2.64	0.40
3:I:448:THR:HG22	3:I:512:VAL:CG1	2.50	0.40
1:F:64:TYR:CD1	1:F:64:TYR:C	2.99	0.40
2:A:179:ASN:ND2	1:E:319:GLU:OE2	2.49	0.40
1:F:320:ASP:O	1:F:411:TRP:CZ2	2.75	0.40
1:L:64:TYR:CD1	1:L:64:TYR:C	2.99	0.40
1:L:349:THR:OG1	2:H:190:ARG:O	2.36	0.40
1:E:337:THR:O	1:E:338:ALA:HB2	2.22	0.40
1:K:384:ASN:ND2	1:K:389:ASP:O	2.55	0.40
3:J:448:THR:HG22	3:J:512:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	E	529/847 (62%)	514 (97%)	15 (3%)	0	100	100
1	F	560/847 (66%)	546 (98%)	14 (2%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	529/847 (62%)	515 (97%)	14 (3%)	0	100	100
1	L	560/847 (66%)	546 (98%)	14 (2%)	0	100	100
2	A	142/175 (81%)	138 (97%)	4 (3%)	0	100	100
2	B	142/175 (81%)	140 (99%)	2 (1%)	0	100	100
2	G	142/175 (81%)	138 (97%)	4 (3%)	0	100	100
2	H	142/175 (81%)	140 (99%)	2 (1%)	0	100	100
3	C	598/754 (79%)	585 (98%)	13 (2%)	0	100	100
3	D	598/754 (79%)	571 (96%)	27 (4%)	0	100	100
3	I	598/754 (79%)	585 (98%)	13 (2%)	0	100	100
3	J	598/754 (79%)	571 (96%)	27 (4%)	0	100	100
All	All	5138/7104 (72%)	4989 (97%)	149 (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	E	461/737 (63%)	458 (99%)	3 (1%)	76	79
1	F	492/737 (67%)	488 (99%)	4 (1%)	73	78
1	K	461/737 (63%)	458 (99%)	3 (1%)	76	79
1	L	492/737 (67%)	488 (99%)	4 (1%)	73	78
2	A	140/168 (83%)	140 (100%)	0	100	100
2	B	140/168 (83%)	140 (100%)	0	100	100
2	G	140/168 (83%)	140 (100%)	0	100	100
2	H	140/168 (83%)	140 (100%)	0	100	100
3	C	525/665 (79%)	521 (99%)	4 (1%)	73	78
3	D	523/665 (79%)	520 (99%)	3 (1%)	78	81
3	I	525/665 (79%)	521 (99%)	4 (1%)	73	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	523/665 (79%)	520 (99%)	3 (1%)	78	81
All	All	4562/6280 (73%)	4534 (99%)	28 (1%)	76	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	39	LEU
1	F	228	CYS
1	F	434	MET
1	F	482	ASN
1	L	39	LEU
1	L	228	CYS
1	L	434	MET
1	L	482	ASN
3	C	219	VAL
3	C	532	ASN
3	C	676	THR
3	C	748	THR
1	E	100	TRP
1	E	304	GLU
1	E	337	THR
3	D	254	LEU
3	D	676	THR
3	D	748	THR
3	I	219	VAL
3	I	532	ASN
3	I	676	THR
3	I	748	THR
1	K	100	TRP
1	K	304	GLU
1	K	337	THR
3	J	254	LEU
3	J	676	THR
3	J	748	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	65	GLN
1	F	384	ASN
1	F	452	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	478	HIS
1	L	65	GLN
1	L	384	ASN
1	L	452	GLN
2	A	104	GLN
2	A	111	HIS
2	A	115	HIS
2	A	155	GLN
2	B	104	GLN
2	B	111	HIS
2	B	112	GLN
2	B	115	HIS
3	C	413	HIS
3	C	500	ASN
1	E	261	ASN
1	E	384	ASN
1	E	505	HIS
1	E	543	ASN
3	D	143	ASN
2	G	104	GLN
2	G	115	HIS
2	G	155	GLN
2	H	104	GLN
2	H	111	HIS
2	H	112	GLN
2	H	115	HIS
3	I	413	HIS
3	I	500	ASN
1	K	261	ASN
1	K	384	ASN
1	K	505	HIS
1	K	543	ASN
3	J	143	ASN

### 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 ⓘ

60 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	M	1	1,4	14,14,15	0.76	0	17,19,21	1.42	2 (11%)
4	NAG	M	2	4	14,14,15	0.71	0	17,19,21	1.43	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.76	0	17,19,21	1.41	2 (11%)
4	NAG	N	2	4	14,14,15	0.72	0	17,19,21	1.42	1 (5%)
5	SGN	O	1	5	20,20,20	0.72	1 (5%)	25,31,31	1.28	2 (8%)
5	IDS	O	10	5	16,16,17	1.13	2 (12%)	16,24,26	1.12	0
5	SGN	O	11	5	19,19,20	0.82	0	23,29,31	1.48	3 (13%)
5	IDS	O	12	5	16,16,17	1.10	2 (12%)	16,24,26	1.37	1 (6%)
5	SGN	O	13	5	19,19,20	0.91	1 (5%)	23,29,31	1.13	1 (4%)
5	IDS	O	14	5	16,16,17	0.94	1 (6%)	16,24,26	1.02	1 (6%)
5	SGN	O	15	5	19,19,20	0.84	1 (5%)	23,29,31	1.76	4 (17%)
5	IDS	O	16	5	16,16,17	1.01	2 (12%)	16,24,26	0.92	0
5	SGN	O	17	5	19,19,20	0.74	0	23,29,31	1.35	3 (13%)
5	IDS	O	18	5	16,16,17	1.08	2 (12%)	16,24,26	1.03	1 (6%)
5	SGN	O	19	5	19,19,20	0.80	0	23,29,31	1.40	1 (4%)
5	IDS	O	2	5	16,16,17	1.10	2 (12%)	16,24,26	1.50	3 (18%)
5	IDS	O	20	5	16,16,17	1.24	2 (12%)	16,24,26	1.17	1 (6%)
5	SGN	O	21	5	19,19,20	0.87	1 (5%)	23,29,31	1.53	3 (13%)
5	IDS	O	22	5	16,16,17	1.22	2 (12%)	16,24,26	1.47	1 (6%)
5	SGN	O	23	5	19,19,20	0.90	2 (10%)	23,29,31	1.65	3 (13%)
5	IDS	O	24	5	16,16,17	1.22	2 (12%)	16,24,26	1.29	1 (6%)
5	SGN	O	25	5	19,19,20	1.00	2 (10%)	23,29,31	2.54	6 (26%)
5	IDS	O	26	5	16,16,17	1.06	1 (6%)	16,24,26	1.18	1 (6%)
5	SGN	O	27	5	19,19,20	0.83	2 (10%)	23,29,31	1.45	2 (8%)
5	IDS	O	28	5	16,16,17	0.94	1 (6%)	16,24,26	1.00	1 (6%)
5	SGN	O	3	5	19,19,20	0.87	2 (10%)	23,29,31	2.98	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	IDS	O	4	5	16,16,17	1.03	2 (12%)	16,24,26	1.09	1 (6%)
5	SGN	O	5	5	19,19,20	0.78	0	23,29,31	1.80	6 (26%)
5	IDS	O	6	5	16,16,17	1.19	2 (12%)	16,24,26	1.96	2 (12%)
5	SGN	O	7	5	19,19,20	0.77	0	23,29,31	1.55	6 (26%)
5	IDS	O	8	5	16,16,17	1.19	2 (12%)	16,24,26	0.93	0
5	SGN	O	9	5	19,19,20	0.75	0	23,29,31	1.09	1 (4%)
5	SGN	P	1	5	20,20,20	0.73	1 (5%)	25,31,31	1.29	2 (8%)
5	IDS	P	10	5	16,16,17	1.13	2 (12%)	16,24,26	1.12	0
5	SGN	P	11	5	19,19,20	0.82	0	23,29,31	1.48	3 (13%)
5	IDS	P	12	5	16,16,17	1.10	2 (12%)	16,24,26	1.37	1 (6%)
5	SGN	P	13	5	19,19,20	0.90	1 (5%)	23,29,31	1.13	1 (4%)
5	IDS	P	14	5	16,16,17	0.93	1 (6%)	16,24,26	1.02	1 (6%)
5	SGN	P	15	5	19,19,20	0.84	1 (5%)	23,29,31	1.76	4 (17%)
5	IDS	P	16	5	16,16,17	1.01	2 (12%)	16,24,26	0.92	0
5	SGN	P	17	5	19,19,20	0.73	0	23,29,31	1.35	3 (13%)
5	IDS	P	18	5	16,16,17	1.08	2 (12%)	16,24,26	1.03	1 (6%)
5	SGN	P	19	5	19,19,20	0.80	0	23,29,31	1.40	1 (4%)
5	IDS	P	2	5	16,16,17	1.10	2 (12%)	16,24,26	1.51	3 (18%)
5	IDS	P	20	5	16,16,17	1.23	2 (12%)	16,24,26	1.18	1 (6%)
5	SGN	P	21	5	19,19,20	0.87	1 (5%)	23,29,31	1.53	3 (13%)
5	IDS	P	22	5	16,16,17	1.23	2 (12%)	16,24,26	1.47	1 (6%)
5	SGN	P	23	5	19,19,20	0.91	2 (10%)	23,29,31	1.65	3 (13%)
5	IDS	P	24	5	16,16,17	1.22	2 (12%)	16,24,26	1.29	1 (6%)
5	SGN	P	25	5	19,19,20	1.00	1 (5%)	23,29,31	2.54	6 (26%)
5	IDS	P	26	5	16,16,17	1.05	1 (6%)	16,24,26	1.18	1 (6%)
5	SGN	P	27	5	19,19,20	0.84	1 (5%)	23,29,31	1.45	2 (8%)
5	IDS	P	28	5	16,16,17	0.94	1 (6%)	16,24,26	0.99	1 (6%)
5	SGN	P	3	5	19,19,20	0.86	2 (10%)	23,29,31	2.97	9 (39%)
5	IDS	P	4	5	16,16,17	1.03	2 (12%)	16,24,26	1.08	1 (6%)
5	SGN	P	5	5	19,19,20	0.79	0	23,29,31	1.80	6 (26%)
5	IDS	P	6	5	16,16,17	1.20	2 (12%)	16,24,26	1.96	2 (12%)
5	SGN	P	7	5	19,19,20	0.78	1 (5%)	23,29,31	1.54	6 (26%)
5	IDS	P	8	5	16,16,17	1.18	2 (12%)	16,24,26	0.93	0
5	SGN	P	9	5	19,19,20	0.76	0	23,29,31	1.09	1 (4%)

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	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
5	SGN	O	1	5	-	1/11/31/31	0/1/1/1
5	IDS	O	10	5	-	0/9/26/29	0/1/1/1
5	SGN	O	11	5	-	3/11/28/31	0/1/1/1
5	IDS	O	12	5	-	1/9/26/29	0/1/1/1
5	SGN	O	13	5	-	4/11/28/31	0/1/1/1
5	IDS	O	14	5	-	0/9/26/29	0/1/1/1
5	SGN	O	15	5	-	1/11/28/31	0/1/1/1
5	IDS	O	16	5	-	0/9/26/29	0/1/1/1
5	SGN	O	17	5	-	3/11/28/31	0/1/1/1
5	IDS	O	18	5	-	2/9/26/29	0/1/1/1
5	SGN	O	19	5	-	0/11/28/31	0/1/1/1
5	IDS	O	2	5	-	0/9/26/29	0/1/1/1
5	IDS	O	20	5	-	0/9/26/29	0/1/1/1
5	SGN	O	21	5	-	1/11/28/31	0/1/1/1
5	IDS	O	22	5	-	2/9/26/29	0/1/1/1
5	SGN	O	23	5	-	2/11/28/31	0/1/1/1
5	IDS	O	24	5	-	2/9/26/29	0/1/1/1
5	SGN	O	25	5	-	4/11/28/31	0/1/1/1
5	IDS	O	26	5	-	2/9/26/29	0/1/1/1
5	SGN	O	27	5	-	3/11/28/31	0/1/1/1
5	IDS	O	28	5	-	2/9/26/29	0/1/1/1
5	SGN	O	3	5	-	4/11/28/31	0/1/1/1
5	IDS	O	4	5	-	2/9/26/29	0/1/1/1
5	SGN	O	5	5	-	0/11/28/31	0/1/1/1
5	IDS	O	6	5	-	2/9/26/29	0/1/1/1
5	SGN	O	7	5	-	1/11/28/31	0/1/1/1
5	IDS	O	8	5	-	2/9/26/29	0/1/1/1
5	SGN	O	9	5	-	1/11/28/31	0/1/1/1
5	SGN	P	1	5	-	1/11/31/31	0/1/1/1
5	IDS	P	10	5	-	0/9/26/29	0/1/1/1
5	SGN	P	11	5	-	3/11/28/31	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IDS	P	12	5	-	1/9/26/29	0/1/1/1
5	SGN	P	13	5	-	4/11/28/31	0/1/1/1
5	IDS	P	14	5	-	0/9/26/29	0/1/1/1
5	SGN	P	15	5	-	1/11/28/31	0/1/1/1
5	IDS	P	16	5	-	0/9/26/29	0/1/1/1
5	SGN	P	17	5	-	3/11/28/31	0/1/1/1
5	IDS	P	18	5	-	2/9/26/29	0/1/1/1
5	SGN	P	19	5	-	0/11/28/31	0/1/1/1
5	IDS	P	2	5	-	0/9/26/29	0/1/1/1
5	IDS	P	20	5	-	0/9/26/29	0/1/1/1
5	SGN	P	21	5	-	1/11/28/31	0/1/1/1
5	IDS	P	22	5	-	2/9/26/29	0/1/1/1
5	SGN	P	23	5	-	2/11/28/31	0/1/1/1
5	IDS	P	24	5	-	2/9/26/29	0/1/1/1
5	SGN	P	25	5	-	4/11/28/31	0/1/1/1
5	IDS	P	26	5	-	2/9/26/29	0/1/1/1
5	SGN	P	27	5	-	3/11/28/31	0/1/1/1
5	IDS	P	28	5	-	2/9/26/29	0/1/1/1
5	SGN	P	3	5	-	4/11/28/31	0/1/1/1
5	IDS	P	4	5	-	2/9/26/29	0/1/1/1
5	SGN	P	5	5	-	0/11/28/31	0/1/1/1
5	IDS	P	6	5	-	2/9/26/29	0/1/1/1
5	SGN	P	7	5	-	1/11/28/31	0/1/1/1
5	IDS	P	8	5	-	2/9/26/29	0/1/1/1
5	SGN	P	9	5	-	1/11/28/31	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	20	IDS	C1-C2	3.43	1.57	1.51
5	P	20	IDS	C1-C2	3.39	1.57	1.51
5	P	6	IDS	C1-C2	3.27	1.56	1.51
5	O	6	IDS	C1-C2	3.22	1.56	1.51
5	P	22	IDS	C1-C2	3.19	1.56	1.51
5	O	22	IDS	C1-C2	3.17	1.56	1.51
5	O	8	IDS	O6B-C6	-3.09	1.20	1.30
5	P	26	IDS	O6B-C6	-3.08	1.20	1.30
5	P	8	IDS	O6B-C6	-3.07	1.20	1.30
5	O	26	IDS	O6B-C6	-3.06	1.20	1.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	28	IDS	O6B-C6	-3.05	1.20	1.30
5	P	18	IDS	O6B-C6	-3.04	1.21	1.30
5	O	28	IDS	O6B-C6	-3.03	1.21	1.30
5	P	6	IDS	O6B-C6	-3.03	1.21	1.30
5	O	14	IDS	O6B-C6	-3.03	1.21	1.30
5	O	6	IDS	O6B-C6	-3.03	1.21	1.30
5	O	18	IDS	O6B-C6	-3.02	1.21	1.30
5	P	14	IDS	O6B-C6	-3.01	1.21	1.30
5	O	24	IDS	O6B-C6	-3.00	1.21	1.30
5	P	24	IDS	O6B-C6	-2.98	1.21	1.30
5	P	2	IDS	O6B-C6	-2.97	1.21	1.30
5	O	24	IDS	C1-C2	2.96	1.56	1.51
5	O	2	IDS	O6B-C6	-2.95	1.21	1.30
5	O	20	IDS	O6B-C6	-2.94	1.21	1.30
5	P	10	IDS	C1-C2	2.94	1.56	1.51
5	P	22	IDS	O6B-C6	-2.93	1.21	1.30
5	O	22	IDS	O6B-C6	-2.93	1.21	1.30
5	P	24	IDS	C1-C2	2.92	1.56	1.51
5	P	10	IDS	O6B-C6	-2.92	1.21	1.30
5	P	20	IDS	O6B-C6	-2.91	1.21	1.30
5	O	10	IDS	C1-C2	2.91	1.56	1.51
5	O	10	IDS	O6B-C6	-2.91	1.21	1.30
5	O	4	IDS	O6B-C6	-2.89	1.21	1.30
5	P	16	IDS	O6B-C6	-2.88	1.21	1.30
5	O	16	IDS	O6B-C6	-2.88	1.21	1.30
5	O	12	IDS	O6B-C6	-2.87	1.21	1.30
5	O	8	IDS	C1-C2	2.87	1.56	1.51
5	P	4	IDS	O6B-C6	-2.87	1.21	1.30
5	P	12	IDS	O6B-C6	-2.86	1.21	1.30
5	P	8	IDS	C1-C2	2.85	1.56	1.51
5	P	2	IDS	C1-C2	2.74	1.56	1.51
5	O	2	IDS	C1-C2	2.73	1.56	1.51
5	O	18	IDS	C1-C2	2.66	1.55	1.51
5	P	18	IDS	C1-C2	2.66	1.55	1.51
5	P	12	IDS	C1-C2	2.53	1.55	1.51
5	P	25	SGN	O6-S2	2.51	1.63	1.56
5	O	12	IDS	C1-C2	2.50	1.55	1.51
5	O	25	SGN	O6-S2	2.48	1.63	1.56
5	P	16	IDS	C1-C2	2.34	1.55	1.51
5	P	27	SGN	C1-C2	2.33	1.55	1.52
5	O	16	IDS	C1-C2	2.32	1.55	1.51
5	O	23	SGN	C1-C2	2.31	1.55	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	27	SGN	C1-C2	2.29	1.55	1.52
5	P	23	SGN	C1-C2	2.29	1.55	1.52
5	O	15	SGN	C1-C2	2.27	1.55	1.52
5	P	4	IDS	C1-C2	2.23	1.55	1.51
5	O	4	IDS	C1-C2	2.22	1.55	1.51
5	P	15	SGN	C1-C2	2.22	1.55	1.52
5	P	3	SGN	O3S-S1	2.15	1.58	1.47
5	O	3	SGN	O3S-S1	2.14	1.57	1.47
5	O	3	SGN	C1-C2	2.13	1.55	1.52
5	P	21	SGN	C1-C2	2.13	1.55	1.52
5	O	21	SGN	C1-C2	2.13	1.55	1.52
5	P	23	SGN	O3S-S1	2.09	1.57	1.47
5	O	23	SGN	O3S-S1	2.08	1.57	1.47
5	O	1	SGN	O3S-S1	2.06	1.57	1.47
5	P	3	SGN	C1-C2	2.06	1.55	1.52
5	P	1	SGN	O3S-S1	2.05	1.57	1.47
5	O	13	SGN	C1-C2	2.04	1.55	1.52
5	P	13	SGN	C1-C2	2.03	1.55	1.52
5	O	25	SGN	C1-C2	2.02	1.55	1.52
5	P	7	SGN	O3S-S1	2.00	1.57	1.47
5	O	27	SGN	O3S-S1	2.00	1.57	1.47

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	25	SGN	C1-O5-C5	7.01	121.58	112.19
5	P	25	SGN	C1-O5-C5	6.99	121.56	112.19
5	O	3	SGN	O6-C6-C5	6.84	119.75	107.57
5	P	3	SGN	O6-C6-C5	6.83	119.73	107.57
5	P	25	SGN	O6-C6-C5	5.92	118.11	107.57
5	O	25	SGN	O6-C6-C5	5.91	118.11	107.57
5	P	6	IDS	O2-C2-C3	-5.88	98.73	106.95
5	O	6	IDS	O2-C2-C3	-5.86	98.76	106.95
5	O	3	SGN	O4-C4-C5	5.75	123.48	109.32
5	O	3	SGN	O1S-S1-N2	-5.72	99.32	108.88
5	P	3	SGN	O4-C4-C5	5.71	123.38	109.32
5	P	3	SGN	O1S-S1-N2	-5.70	99.35	108.88
5	P	23	SGN	C1-O5-C5	5.38	119.40	112.19
5	O	23	SGN	C1-O5-C5	5.38	119.40	112.19
5	O	21	SGN	C1-O5-C5	5.14	119.07	112.19
5	P	21	SGN	C1-O5-C5	5.08	118.99	112.19
5	O	15	SGN	C1-O5-C5	5.05	118.96	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	2	NAG	C1-O5-C5	5.04	118.94	112.19
5	P	15	SGN	C1-O5-C5	5.03	118.93	112.19
4	N	2	NAG	C1-O5-C5	5.00	118.88	112.19
5	O	25	SGN	C3-C2-N2	4.83	116.67	110.32
5	P	25	SGN	C3-C2-N2	4.81	116.65	110.32
5	O	3	SGN	C3-C4-C5	-4.56	101.96	110.23
5	P	3	SGN	C3-C4-C5	-4.54	101.99	110.23
5	O	3	SGN	C1-O5-C5	4.45	118.15	112.19
5	P	5	SGN	C1-O5-C5	4.43	118.12	112.19
5	P	11	SGN	C1-O5-C5	4.42	118.10	112.19
5	O	19	SGN	C1-O5-C5	4.41	118.10	112.19
5	P	3	SGN	C1-O5-C5	4.40	118.09	112.19
5	O	11	SGN	C1-O5-C5	4.40	118.08	112.19
5	P	19	SGN	C1-O5-C5	4.40	118.08	112.19
5	O	5	SGN	C1-O5-C5	4.39	118.06	112.19
5	O	5	SGN	C1-C2-N2	4.24	116.93	110.22
5	P	5	SGN	C1-C2-N2	4.20	116.87	110.22
5	P	27	SGN	C1-O5-C5	4.15	117.75	112.19
5	O	27	SGN	C1-O5-C5	4.12	117.71	112.19
4	M	1	NAG	O5-C1-C2	-4.06	105.01	111.29
4	N	1	NAG	O5-C1-C2	-4.03	105.05	111.29
5	P	15	SGN	C1-C2-N2	3.97	116.50	110.22
5	O	15	SGN	C1-C2-N2	3.97	116.49	110.22
5	O	22	IDS	C4-C3-C2	3.96	117.42	110.23
5	P	22	IDS	C4-C3-C2	3.95	117.40	110.23
5	P	1	SGN	O5-C1-C2	3.91	113.45	109.52
5	O	1	SGN	O5-C1-C2	3.89	113.43	109.52
5	O	6	IDS	C4-C3-C2	3.83	117.17	110.23
5	P	6	IDS	C4-C3-C2	3.82	117.16	110.23
5	P	17	SGN	C1-C2-N2	3.73	116.11	110.22
5	O	17	SGN	C1-C2-N2	3.71	116.09	110.22
5	O	9	SGN	C1-O5-C5	3.62	117.04	112.19
5	O	27	SGN	C1-C2-N2	3.62	115.94	110.22
5	P	27	SGN	C1-C2-N2	3.61	115.93	110.22
5	P	9	SGN	C1-O5-C5	3.59	117.00	112.19
5	P	1	SGN	O6-C6-C5	3.51	113.82	107.57
5	O	1	SGN	O6-C6-C5	3.51	113.82	107.57
5	P	3	SGN	O6S-S2-O6	3.43	114.25	106.37
5	O	3	SGN	O6S-S2-O6	3.42	114.23	106.37
5	O	24	IDS	C4-C3-C2	3.31	116.23	110.23
5	P	24	IDS	C4-C3-C2	3.30	116.22	110.23
5	O	12	IDS	C4-C3-C2	3.30	116.21	110.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	12	IDS	C4-C3-C2	3.29	116.19	110.23
5	O	15	SGN	C3-C2-N2	-3.16	106.17	110.32
5	P	15	SGN	C3-C2-N2	-3.15	106.18	110.32
5	O	2	IDS	C3-C4-C5	-3.13	103.91	109.30
5	P	2	IDS	C3-C4-C5	-3.13	103.92	109.30
5	P	3	SGN	O6-S2-O5S	-3.13	97.37	106.92
5	O	3	SGN	O6-S2-O5S	-3.13	97.37	106.92
4	N	1	NAG	C1-O5-C5	3.03	116.25	112.19
4	M	1	NAG	C1-O5-C5	3.02	116.24	112.19
5	P	20	IDS	C4-C3-C2	2.97	115.61	110.23
5	O	25	SGN	O4-C4-C3	-2.95	103.43	110.38
5	O	20	IDS	C4-C3-C2	2.94	115.56	110.23
5	P	25	SGN	O4-C4-C3	-2.94	103.45	110.38
5	P	7	SGN	C1-O5-C5	2.90	116.08	112.19
5	O	7	SGN	O4-C4-C3	-2.89	103.56	110.38
5	O	7	SGN	C1-O5-C5	2.89	116.06	112.19
5	P	17	SGN	O6-C6-C5	2.89	112.72	107.57
5	P	3	SGN	C6-C5-C4	2.89	118.13	112.07
5	P	7	SGN	O4-C4-C3	-2.87	103.61	110.38
5	O	3	SGN	C6-C5-C4	2.87	118.09	112.07
5	O	23	SGN	O6-C6-C5	2.86	112.67	107.57
5	O	17	SGN	O6-C6-C5	2.85	112.65	107.57
5	P	23	SGN	O6-C6-C5	2.84	112.63	107.57
5	O	13	SGN	C1-O5-C5	2.84	115.99	112.19
5	P	13	SGN	C1-O5-C5	2.84	115.99	112.19
5	O	11	SGN	O4-C4-C3	2.79	116.94	110.38
5	P	11	SGN	O4-C4-C3	2.78	116.94	110.38
5	O	5	SGN	O4-C4-C5	2.68	115.92	109.32
5	P	21	SGN	O6-C6-C5	2.67	112.33	107.57
5	P	5	SGN	O4-C4-C5	2.67	115.90	109.32
5	O	7	SGN	O6-C6-C5	2.67	112.33	107.57
5	O	21	SGN	O6-C6-C5	2.65	112.28	107.57
5	P	7	SGN	O6-C6-C5	2.65	112.28	107.57
5	O	15	SGN	O2S-S1-N2	-2.63	104.48	108.88
5	O	25	SGN	O5-C5-C6	-2.63	101.91	107.59
5	P	25	SGN	O5-C5-C6	-2.61	101.94	107.59
5	O	28	IDS	O2-C2-C3	2.61	110.59	106.95
5	P	15	SGN	O2S-S1-N2	-2.61	104.53	108.88
5	P	28	IDS	O2-C2-C3	2.59	110.56	106.95
5	O	7	SGN	C1-C2-N2	2.54	114.23	110.22
5	O	5	SGN	O6-C6-C5	2.53	112.08	107.57
5	P	7	SGN	C1-C2-N2	2.52	114.21	110.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	5	SGN	O6-C6-C5	2.51	112.03	107.57
5	P	26	IDS	O2-C2-C3	2.46	110.39	106.95
5	O	11	SGN	O6-C6-C5	2.46	111.95	107.57
5	O	26	IDS	O2-C2-C3	2.45	110.38	106.95
5	O	23	SGN	O4-C4-C5	2.44	115.34	109.32
5	P	23	SGN	O4-C4-C5	2.44	115.33	109.32
5	P	11	SGN	O6-C6-C5	2.44	111.91	107.57
5	P	4	IDS	O3S-S-O2	2.37	111.81	106.37
5	O	4	IDS	O3S-S-O2	2.36	111.81	106.37
5	P	2	IDS	C4-C3-C2	2.36	114.52	110.23
5	O	2	IDS	C4-C3-C2	2.35	114.49	110.23
5	O	3	SGN	O2S-S1-N2	-2.32	105.00	108.88
5	P	3	SGN	O2S-S1-N2	-2.32	105.00	108.88
5	O	25	SGN	O5-C1-C2	-2.30	107.74	111.29
5	P	25	SGN	O5-C1-C2	-2.26	107.80	111.29
5	P	21	SGN	C3-C4-C5	-2.24	106.16	110.23
5	O	21	SGN	C3-C4-C5	-2.23	106.18	110.23
5	O	5	SGN	C4-C3-C2	-2.23	107.75	111.02
5	O	17	SGN	C1-O5-C5	2.22	115.17	112.19
5	P	5	SGN	C4-C3-C2	-2.22	107.76	111.02
5	P	17	SGN	C1-O5-C5	2.18	115.10	112.19
5	O	14	IDS	C4-C3-C2	2.15	114.13	110.23
5	P	14	IDS	C4-C3-C2	2.13	114.09	110.23
5	P	7	SGN	O5-C5-C6	-2.11	103.04	107.59
5	O	7	SGN	O5-C5-C6	-2.10	103.06	107.59
5	P	5	SGN	C3-C4-C5	-2.08	106.47	110.23
5	P	2	IDS	O4-C4-C3	2.07	115.26	110.38
5	O	2	IDS	O4-C4-C3	2.06	115.24	110.38
5	O	5	SGN	C3-C4-C5	-2.06	106.49	110.23
5	P	18	IDS	O2-C2-C3	2.05	109.81	106.95
5	P	7	SGN	O4-C4-C5	-2.04	104.29	109.32
5	O	7	SGN	O4-C4-C5	-2.03	104.31	109.32
5	O	18	IDS	O2-C2-C3	2.03	109.78	106.95

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	3	SGN	C3-C2-N2-S1
5	O	3	SGN	C4-C5-C6-O6
5	O	4	IDS	C1-C2-O2-S
5	O	4	IDS	C3-C2-O2-S

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	O	6	IDS	C4-C5-C6-O6A
5	O	6	IDS	C4-C5-C6-O6B
5	O	8	IDS	C1-C2-O2-S
5	O	8	IDS	C3-C2-O2-S
5	O	13	SGN	C3-C2-N2-S1
5	O	22	IDS	C1-C2-O2-S
5	O	22	IDS	C3-C2-O2-S
5	O	24	IDS	C1-C2-O2-S
5	O	26	IDS	C1-C2-O2-S
5	O	26	IDS	C3-C2-O2-S
5	O	28	IDS	C1-C2-O2-S
5	O	28	IDS	C3-C2-O2-S
5	P	3	SGN	C3-C2-N2-S1
5	P	3	SGN	C4-C5-C6-O6
5	P	4	IDS	C1-C2-O2-S
5	P	4	IDS	C3-C2-O2-S
5	P	6	IDS	C4-C5-C6-O6A
5	P	6	IDS	C4-C5-C6-O6B
5	P	8	IDS	C1-C2-O2-S
5	P	8	IDS	C3-C2-O2-S
5	P	13	SGN	C3-C2-N2-S1
5	P	22	IDS	C1-C2-O2-S
5	P	22	IDS	C3-C2-O2-S
5	P	24	IDS	C1-C2-O2-S
5	P	26	IDS	C1-C2-O2-S
5	P	26	IDS	C3-C2-O2-S
5	P	28	IDS	C1-C2-O2-S
5	P	28	IDS	C3-C2-O2-S
5	O	25	SGN	C6-O6-S2-O6S
5	P	25	SGN	C6-O6-S2-O6S
5	O	17	SGN	C5-C6-O6-S2
5	O	21	SGN	C5-C6-O6-S2
5	P	17	SGN	C5-C6-O6-S2
5	P	21	SGN	C5-C6-O6-S2
5	O	25	SGN	C6-O6-S2-O5S
5	O	27	SGN	C6-O6-S2-O5S
5	P	25	SGN	C6-O6-S2-O5S
5	P	27	SGN	C6-O6-S2-O5S
4	M	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
5	O	25	SGN	C6-O6-S2-O4S
5	P	25	SGN	C6-O6-S2-O4S

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	O	1	SGN	C5-C6-O6-S2
5	O	13	SGN	C5-C6-O6-S2
5	O	23	SGN	C5-C6-O6-S2
5	P	1	SGN	C5-C6-O6-S2
5	P	13	SGN	C5-C6-O6-S2
5	P	23	SGN	C5-C6-O6-S2
5	O	27	SGN	C6-O6-S2-O4S
5	P	27	SGN	C6-O6-S2-O4S
5	O	18	IDS	C3-C2-O2-S
5	O	24	IDS	C3-C2-O2-S
5	P	18	IDS	C3-C2-O2-S
5	P	24	IDS	C3-C2-O2-S
5	O	12	IDS	C1-C2-O2-S
5	P	12	IDS	C1-C2-O2-S
5	P	18	IDS	C1-C2-O2-S
5	O	3	SGN	O5-C5-C6-O6
5	O	7	SGN	O5-C5-C6-O6
5	O	11	SGN	O5-C5-C6-O6
5	O	25	SGN	O5-C5-C6-O6
5	P	3	SGN	O5-C5-C6-O6
5	P	7	SGN	O5-C5-C6-O6
5	P	11	SGN	O5-C5-C6-O6
5	P	25	SGN	O5-C5-C6-O6
5	O	27	SGN	C6-O6-S2-O6S
5	P	27	SGN	C6-O6-S2-O6S
5	O	3	SGN	C1-C2-N2-S1
5	P	3	SGN	C1-C2-N2-S1
5	O	9	SGN	C2-N2-S1-O1S
5	O	13	SGN	C2-N2-S1-O1S
5	O	23	SGN	C2-N2-S1-O1S
5	P	9	SGN	C2-N2-S1-O1S
5	P	13	SGN	C2-N2-S1-O1S
5	P	23	SGN	C2-N2-S1-O1S
5	O	15	SGN	C5-C6-O6-S2
5	P	15	SGN	C5-C6-O6-S2
5	O	18	IDS	C1-C2-O2-S
5	O	11	SGN	C2-N2-S1-O1S
5	O	11	SGN	C2-N2-S1-O2S
5	O	13	SGN	C2-N2-S1-O2S
5	O	17	SGN	C2-N2-S1-O1S
5	O	17	SGN	C2-N2-S1-O2S
5	P	11	SGN	C2-N2-S1-O1S

*Continued on next page...*

*Continued from previous page...*

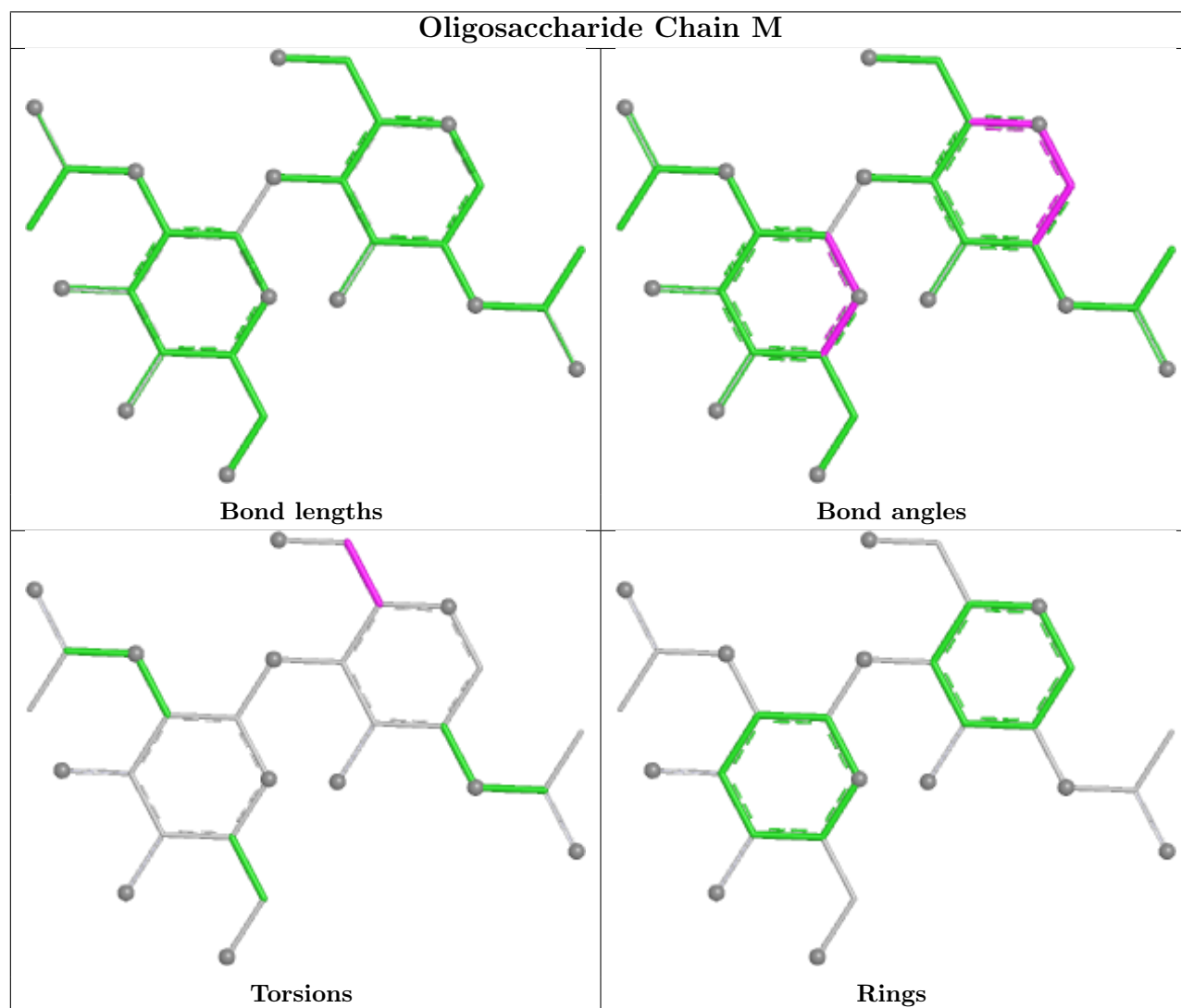
Mol	Chain	Res	Type	Atoms
5	P	11	SGN	C2-N2-S1-O2S
5	P	13	SGN	C2-N2-S1-O2S
5	P	17	SGN	C2-N2-S1-O1S
5	P	17	SGN	C2-N2-S1-O2S

There are no ring outliers.

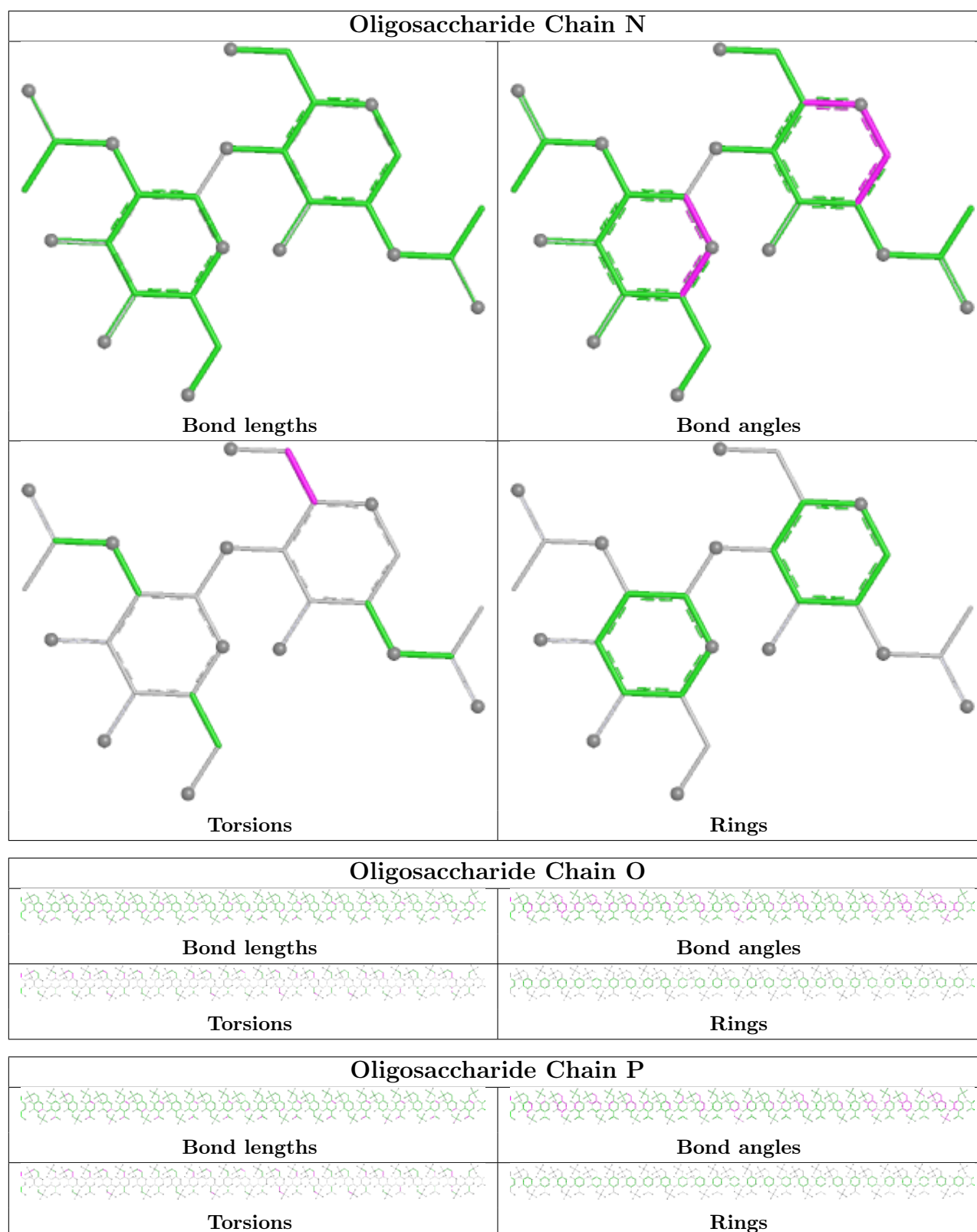
32 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	5	SGN	2	0
5	P	28	IDS	2	0
5	O	4	IDS	1	0
5	O	1	SGN	1	0
5	P	17	SGN	3	0
5	P	16	IDS	1	0
5	O	26	IDS	1	0
5	P	22	IDS	1	0
5	O	6	IDS	4	0
5	O	3	SGN	3	0
5	O	22	IDS	1	0
5	O	17	SGN	3	0
5	O	7	SGN	2	0
5	O	24	IDS	1	0
5	P	23	SGN	1	0
5	P	24	IDS	1	0
5	P	26	IDS	1	0
5	O	28	IDS	2	0
5	P	8	IDS	1	0
5	O	23	SGN	1	0
5	P	4	IDS	1	0
5	P	7	SGN	2	0
5	O	13	SGN	1	0
5	O	8	IDS	1	0
5	P	3	SGN	2	0
5	P	21	SGN	1	0
5	P	1	SGN	1	0
5	P	6	IDS	4	0
5	O	16	IDS	1	0
5	O	5	SGN	2	0
5	P	13	SGN	1	0
5	O	21	SGN	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 oligosaccharide.







## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z  > 2$
7	NAG	L	2002	1	14,14,15	0.75	0	17,19,21	1.18	1 (5%)
7	NAG	D	802	3	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
7	NAG	K	901	1	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
7	NAG	C	801	3	14,14,15	0.65	0	17,19,21	1.09	1 (5%)
7	NAG	D	801	3	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
7	NAG	I	802	3	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
7	NAG	J	802	3	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
7	NAG	F	2002	1	14,14,15	0.75	0	17,19,21	1.18	1 (5%)
7	NAG	C	802	3	14,14,15	0.68	0	17,19,21	0.90	1 (5%)
7	NAG	J	801	3	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
7	NAG	I	801	3	14,14,15	0.66	0	17,19,21	1.10	1 (5%)
7	NAG	E	901	1	14,14,15	0.68	0	17,19,21	1.23	1 (5%)

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
7	NAG	L	2002	1	-	0/6/23/26	0/1/1/1
7	NAG	D	802	3	-	0/6/23/26	0/1/1/1
7	NAG	K	901	1	-	1/6/23/26	0/1/1/1
7	NAG	C	801	3	-	0/6/23/26	0/1/1/1
7	NAG	D	801	3	-	0/6/23/26	0/1/1/1
7	NAG	I	802	3	-	0/6/23/26	0/1/1/1
7	NAG	J	802	3	-	0/6/23/26	0/1/1/1
7	NAG	F	2002	1	-	0/6/23/26	0/1/1/1
7	NAG	C	802	3	-	0/6/23/26	0/1/1/1
7	NAG	J	801	3	-	0/6/23/26	0/1/1/1
7	NAG	I	801	3	-	0/6/23/26	0/1/1/1
7	NAG	E	901	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	901	NAG	C1-O5-C5	3.91	117.42	112.19
7	K	901	NAG	C1-O5-C5	3.90	117.41	112.19
7	L	2002	NAG	C1-O5-C5	3.80	117.28	112.19
7	F	2002	NAG	C1-O5-C5	3.77	117.24	112.19
7	D	801	NAG	C1-O5-C5	3.58	116.98	112.19
7	J	801	NAG	C1-O5-C5	3.51	116.89	112.19
7	I	801	NAG	C1-O5-C5	2.90	116.07	112.19
7	C	801	NAG	C1-O5-C5	2.83	115.98	112.19
7	J	802	NAG	C1-O5-C5	2.13	115.04	112.19
7	D	802	NAG	C1-O5-C5	2.10	115.00	112.19
7	C	802	NAG	C1-O5-C5	2.07	114.96	112.19
7	I	802	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	901	NAG	O5-C5-C6-O6
7	E	901	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	801	NAG	1	0
7	J	801	NAG	1	0

## 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.

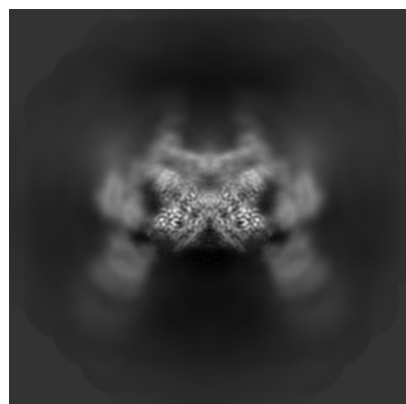
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75408. These allow visual inspection of the internal detail of the map and identification of artifacts.

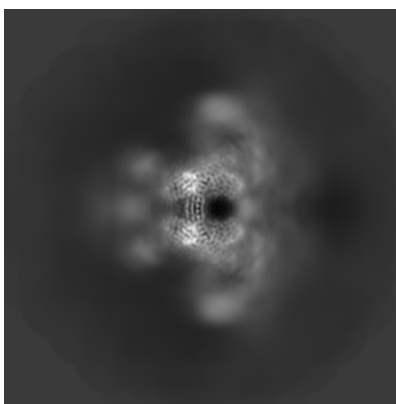
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

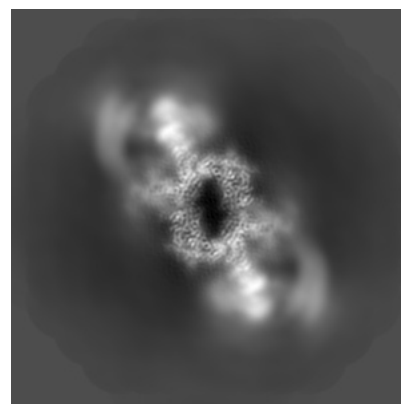
#### 6.1.1 Primary map



X

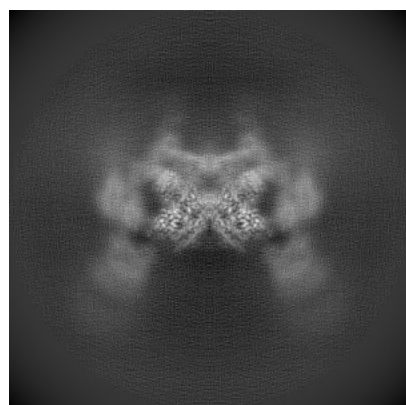


Y

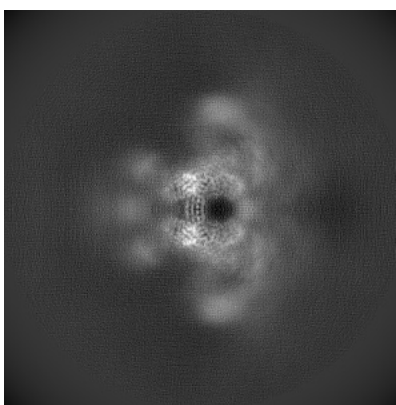


Z

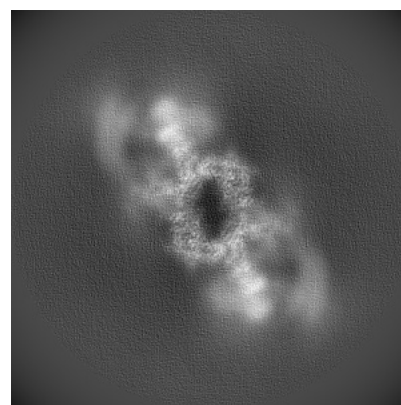
#### 6.1.2 Raw map



X



Y

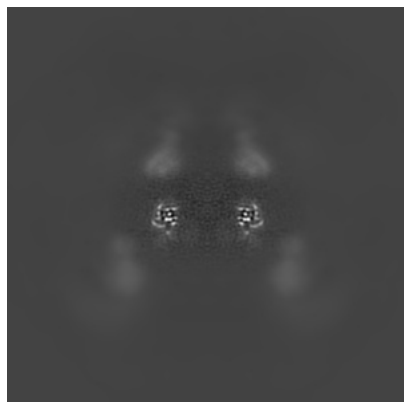


Z

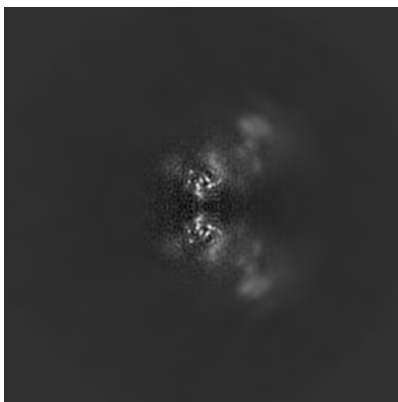
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

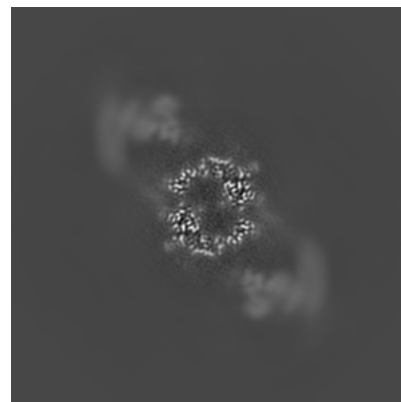
### 6.2.1 Primary map



X Index: 200

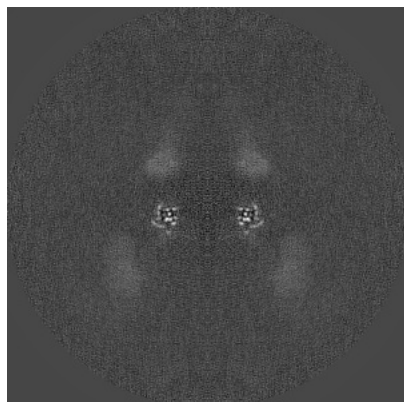


Y Index: 200

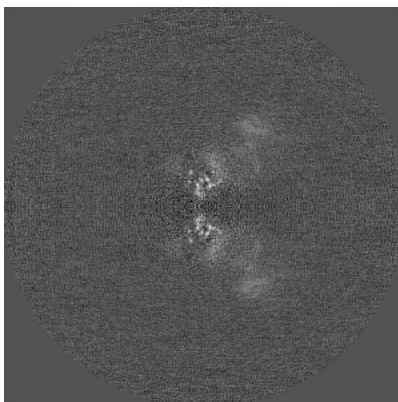


Z Index: 200

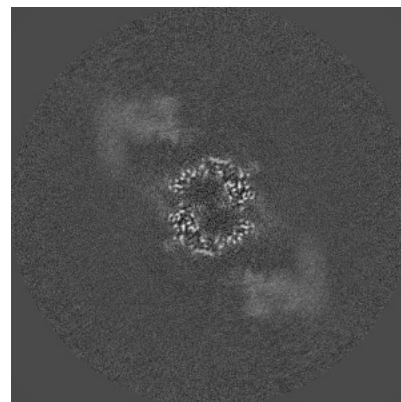
### 6.2.2 Raw map



X Index: 200



Y Index: 200

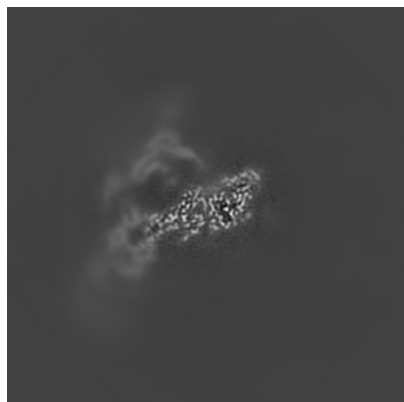


Z Index: 200

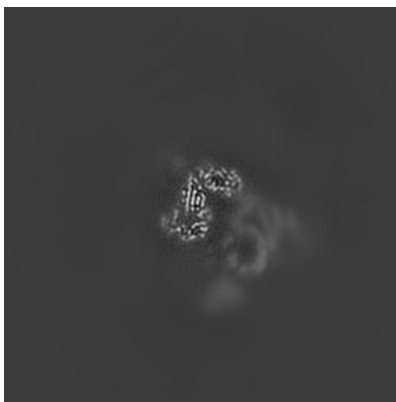
The images above show central slices of the map in three orthogonal directions.

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

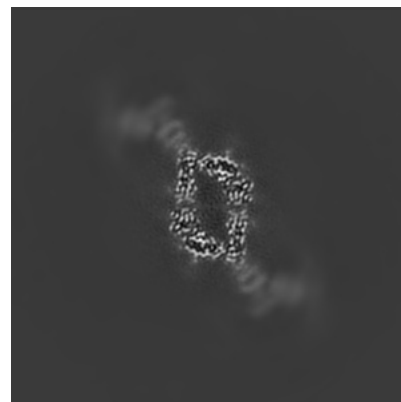
### 6.3.1 Primary map



X Index: 231

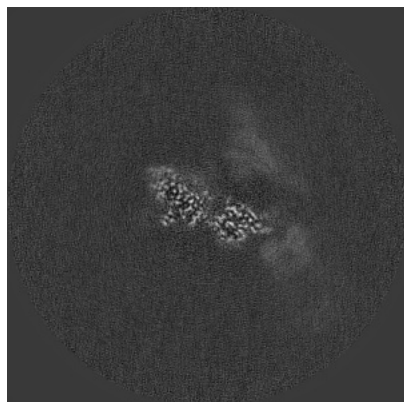


Y Index: 235

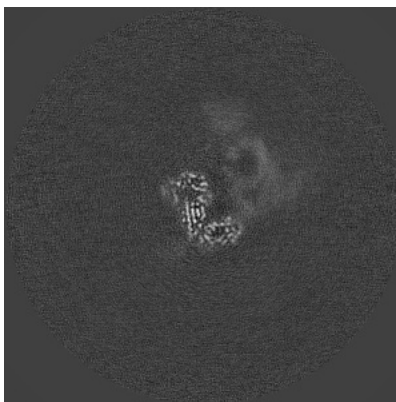


Z Index: 189

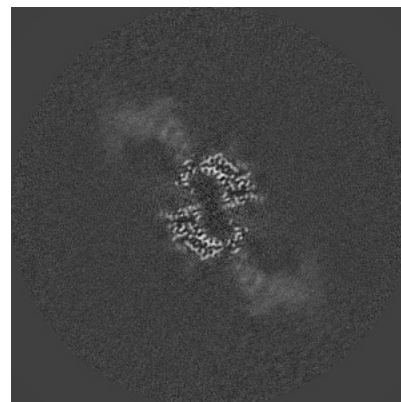
### 6.3.2 Raw map



X Index: 176



Y Index: 165



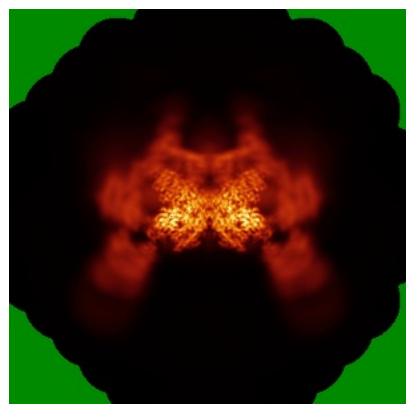
Z Index: 193

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

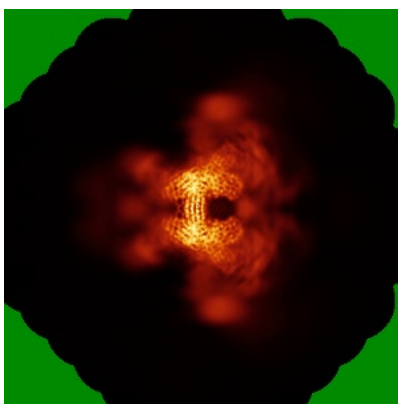


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

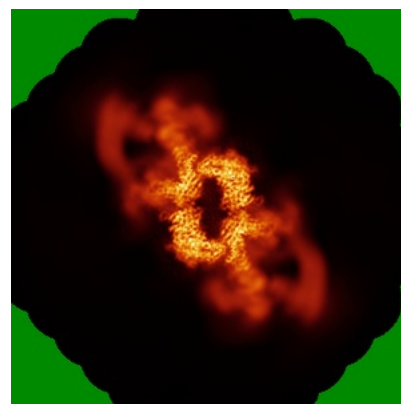
### 6.4.1 Primary map



X

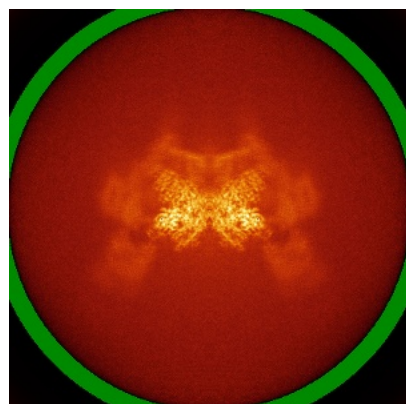


Y

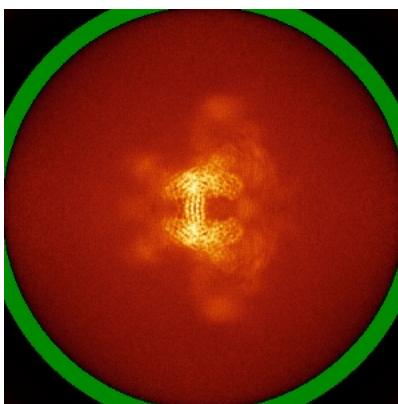


Z

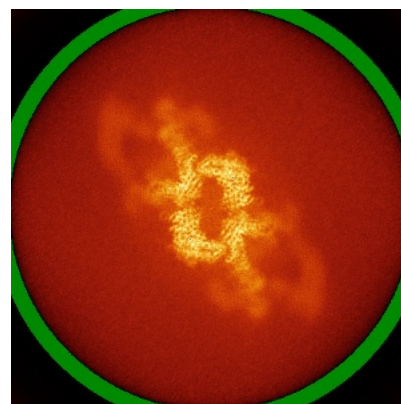
### 6.4.2 Raw map



X



Y

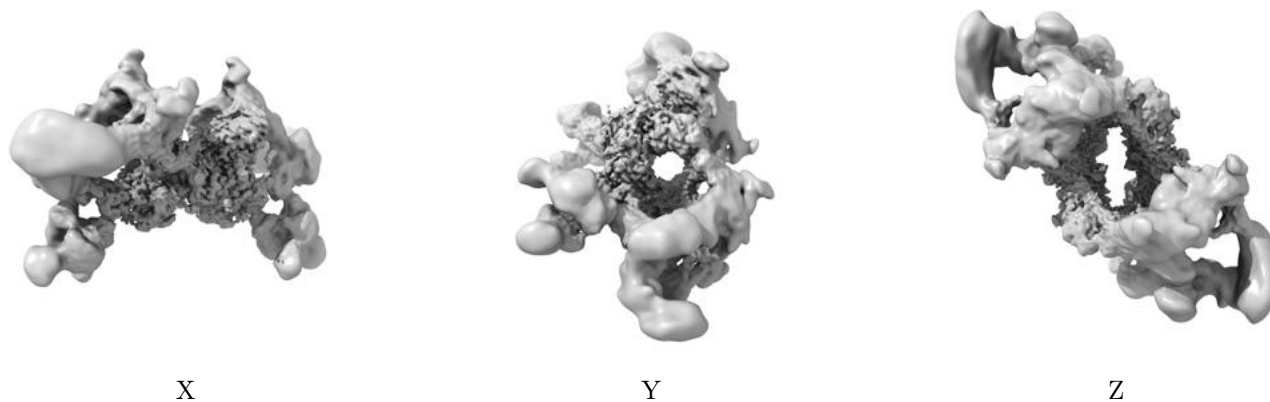


Z

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.

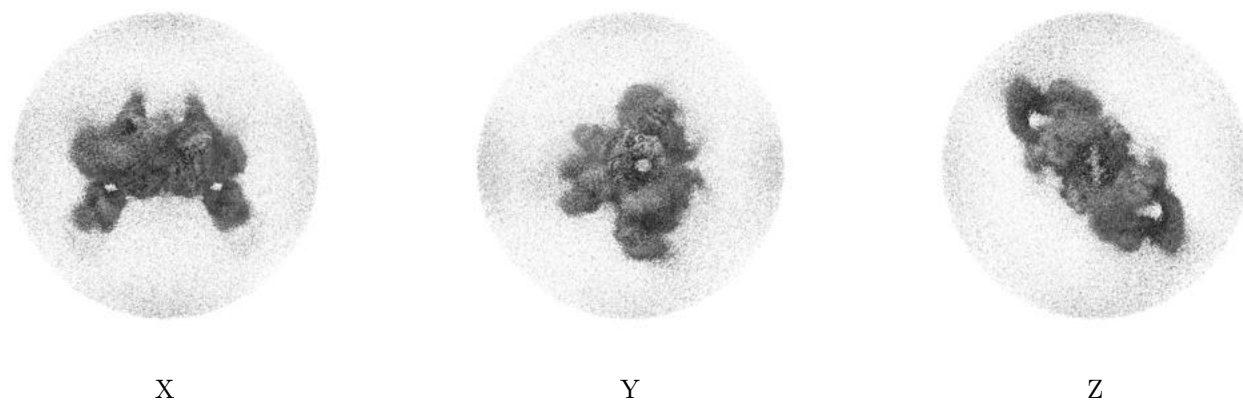
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. 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](#)

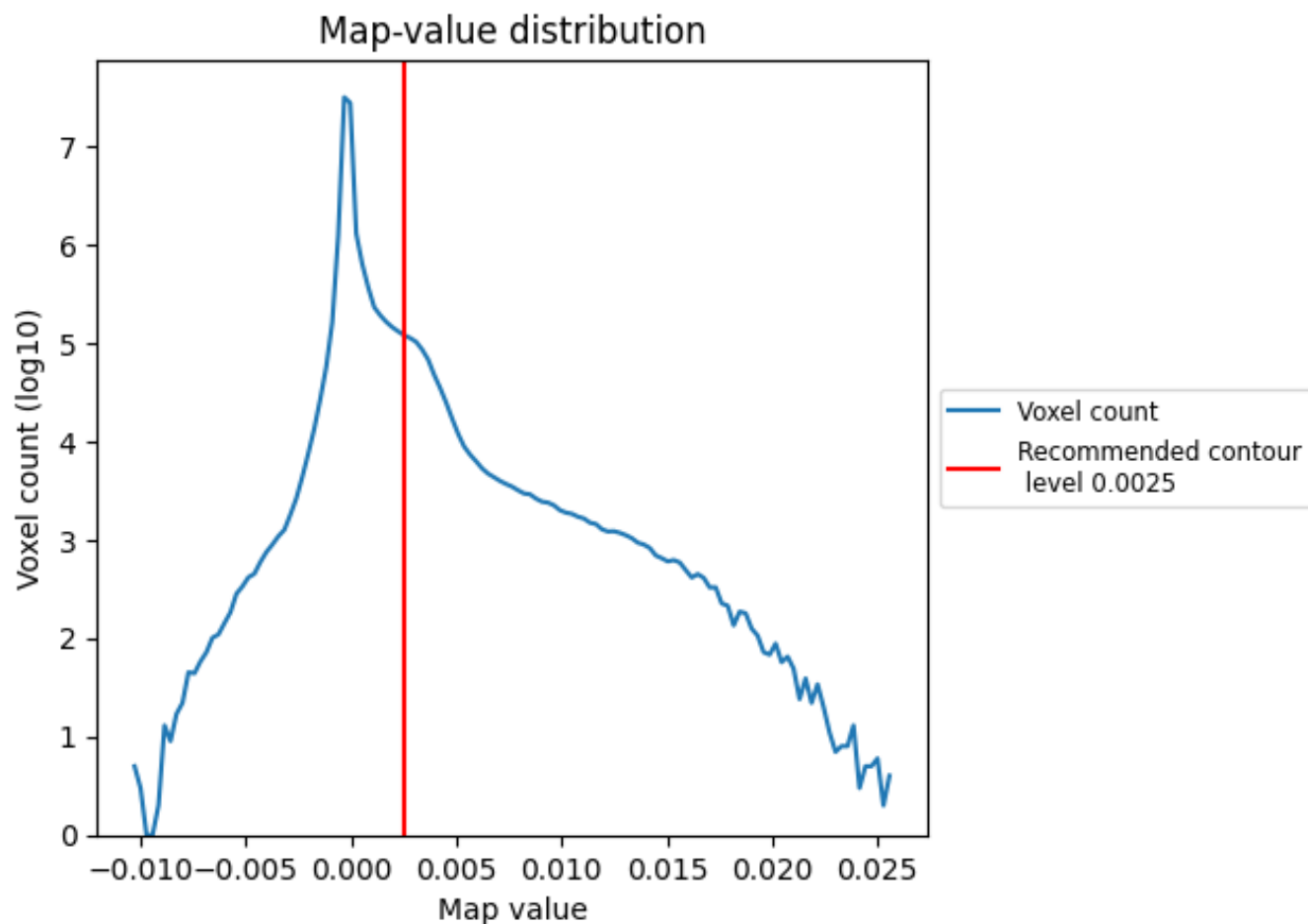
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

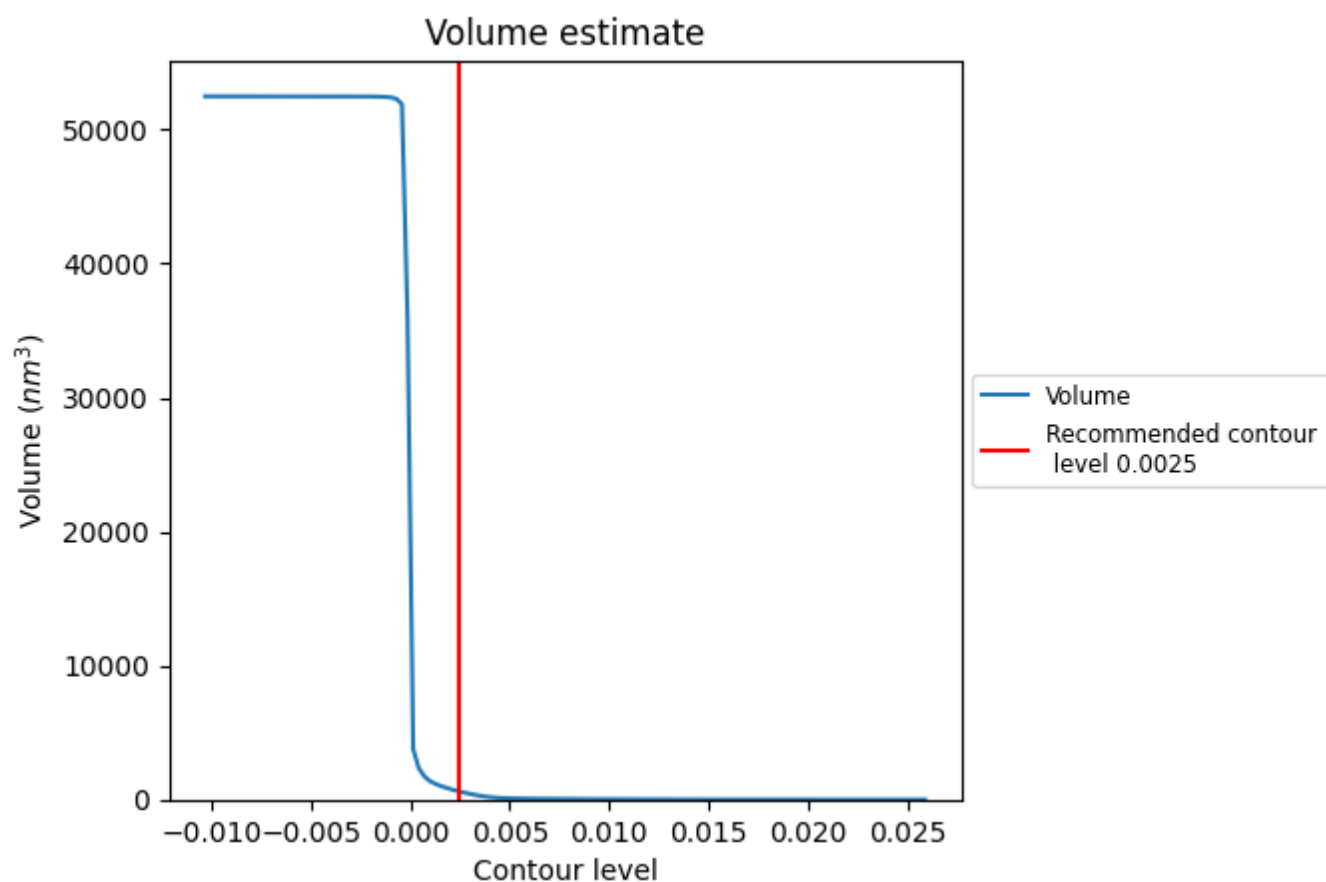
This section contains the results of statistical analysis of the map.

### 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.

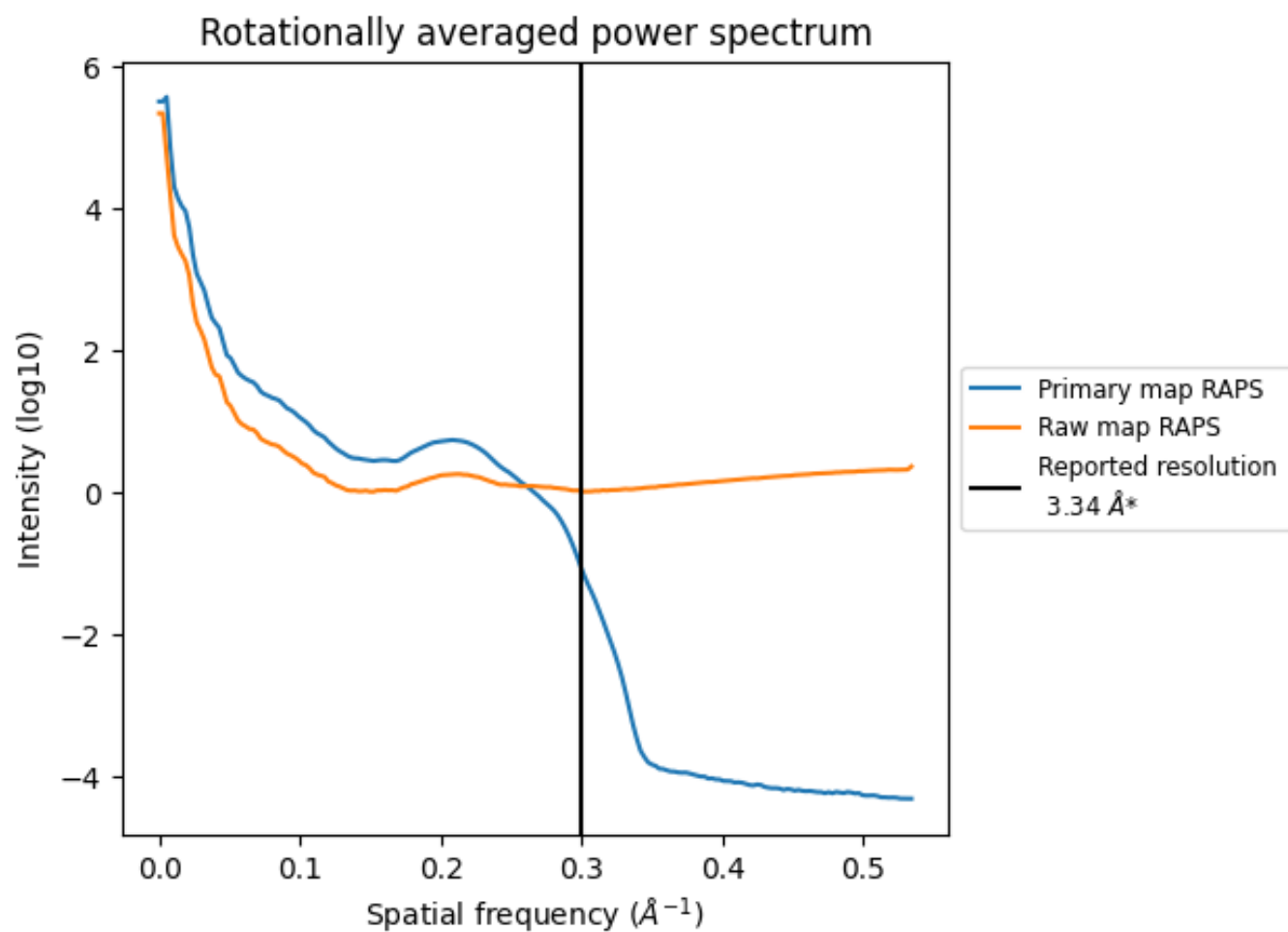
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 595  $\text{nm}^3$ ; this corresponds to an approximate mass of 537 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 ⓘ

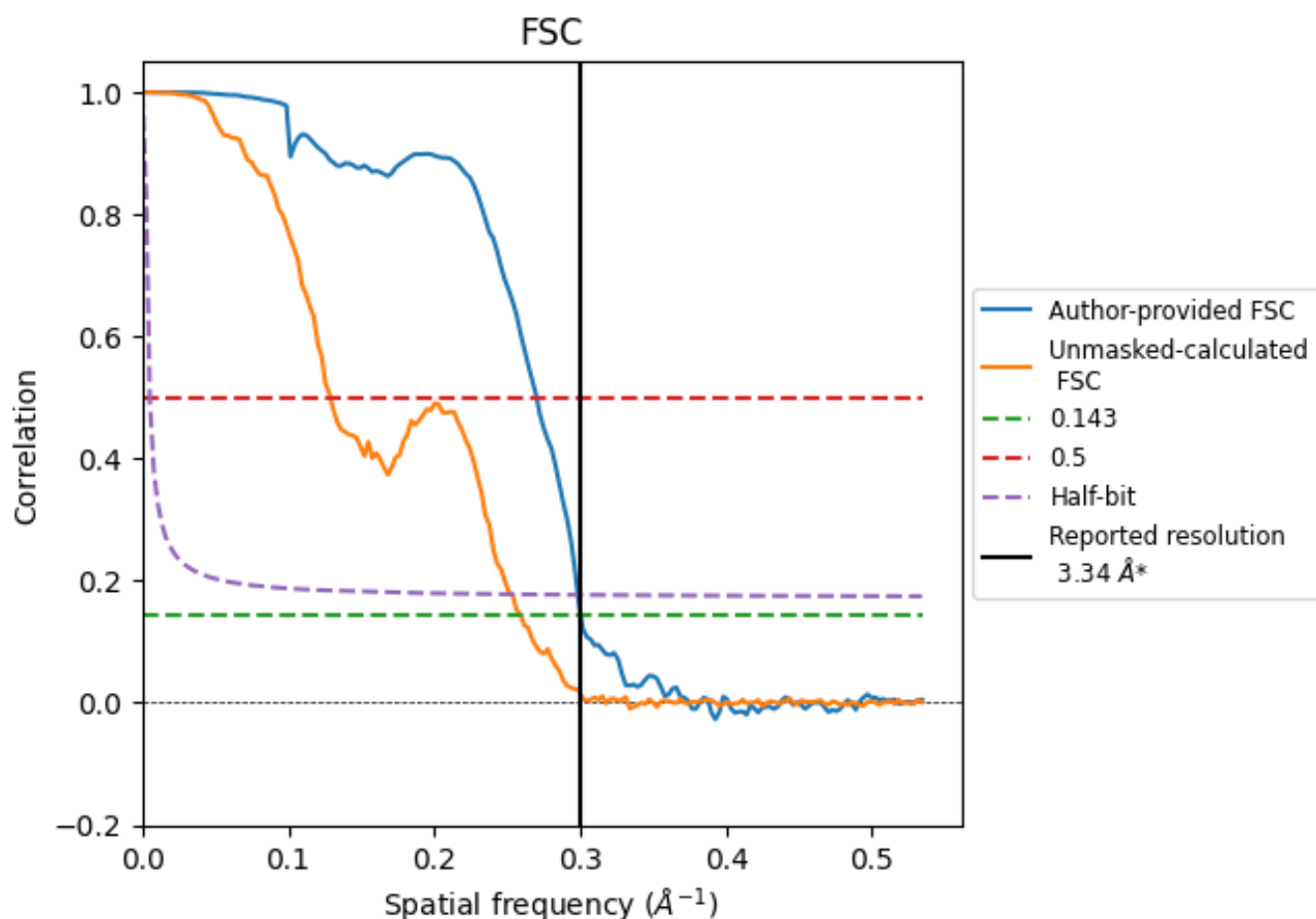


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

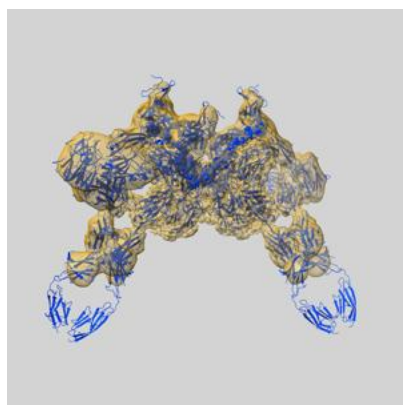
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.33	3.70	3.35
Unmasked-calculated*	3.86	7.76	3.95

\*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 3.86 differs from the reported value 3.34 by more than 10 %

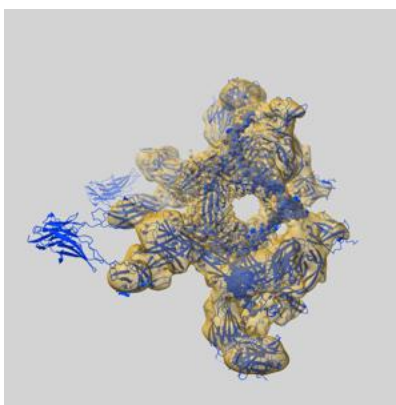
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75408 and PDB model 10RJ. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

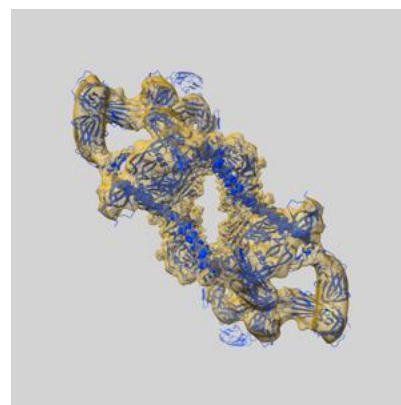
### 9.1 Map-model overlay [i](#)



X



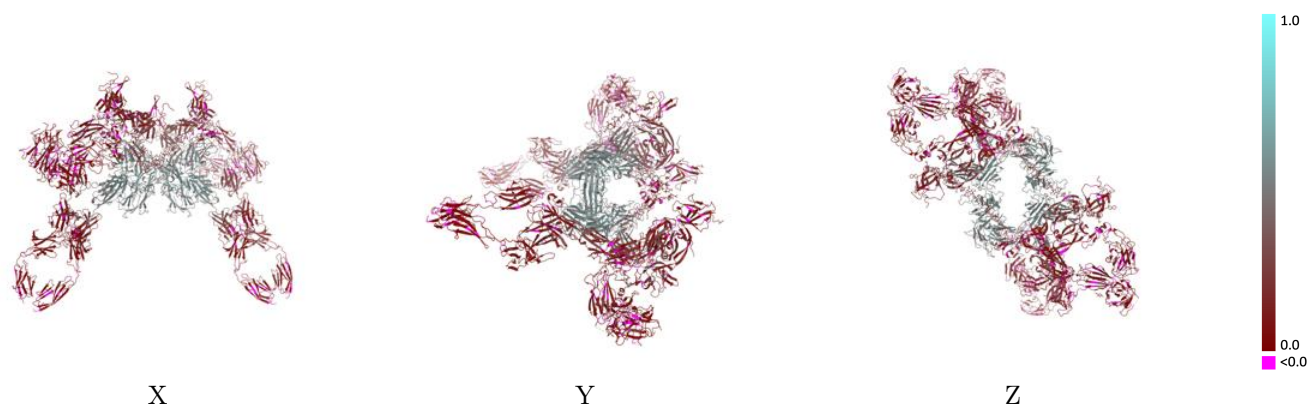
Y



Z

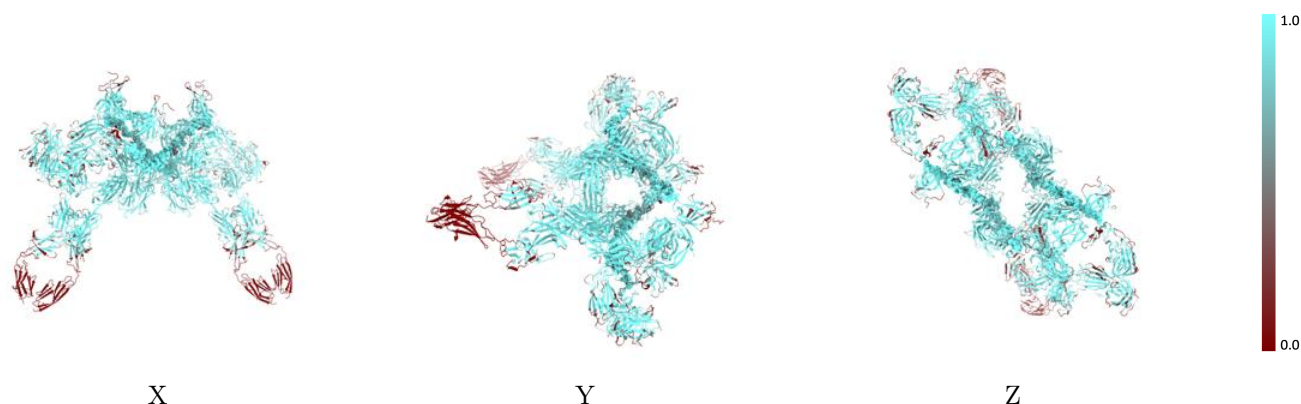
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



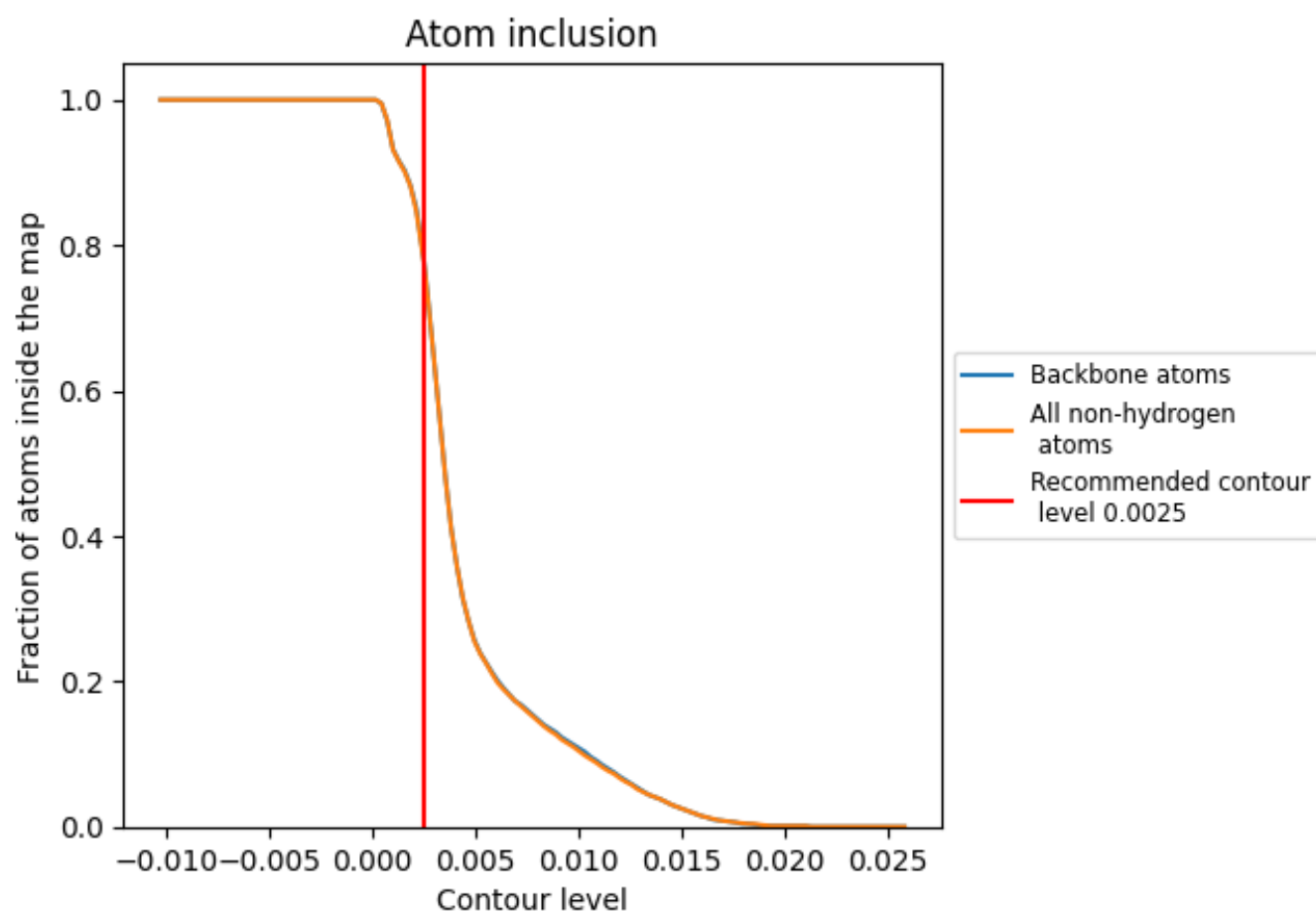
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

## 9.4 Atom inclusion ⓘ





































At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.2270
A	 0.8190	 0.1380
B	 0.8440	 0.1730
C	 0.7170	 0.2370
D	 0.6380	 0.1140
E	 0.7790	 0.0900
F	 0.9580	 0.5000
G	 0.8170	 0.1380
H	 0.8460	 0.1780
I	 0.7180	 0.2390
J	 0.6400	 0.1130
K	 0.7790	 0.0910
L	 0.9590	 0.5010
M	 1.0000	 0.4960
N	 1.0000	 0.5150
O	 0.9180	 0.2160
P	 0.9230	 0.2130

