Full wwPDB EM Validation Report

Dec 9, 2023 – 06:38 pm GMT

PDB ID	:	8OPN
EMDB ID	:	EMD-17077
Title	:	Human Coronavirus HKU1 spike glycoprotein in complex with an alpha2,8-linked 9-O-acetylated disialoside (1-up state)
Authors	:	Pronker, M.F.; Creutznacher, R.; Hurdiss, D.L.
Deposited on	:	2023-04-07
Resolution	:	4.70 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

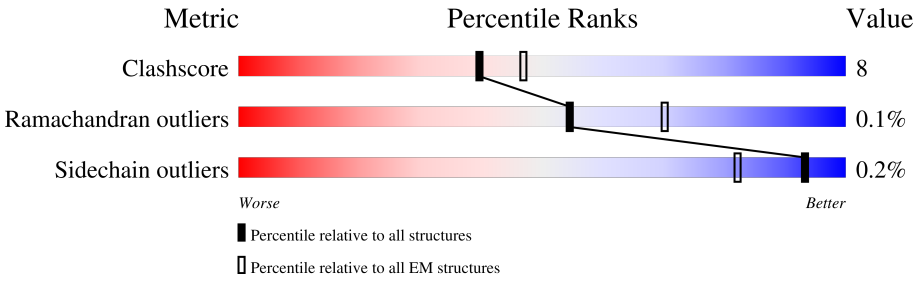
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1326	18% 70% 19% 11%
1	B	1326	14% 70% 19% 11%
1	C	1326	14% 71% 18% 11%
2	D	2	50% 100%
2	E	2	50% 100%
2	F	2	50% 50% 50%
2	G	2	50% 50% 50%
3	H	2	50% 50%

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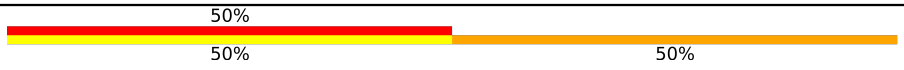
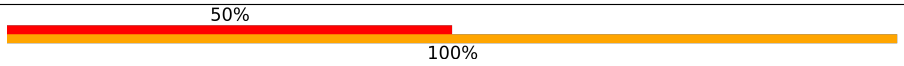
Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28543 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 Spike glycoprotein,General control transcription factor GCN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1183	Total	C	N	O	S	1	0
			9295	5933	1522	1784	56		
1	B	1186	Total	C	N	O	S	1	0
			9321	5953	1524	1787	57		
1	C	1186	Total	C	N	O	S	1	0
			9319	5950	1524	1788	57		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP E0YJ44
A	-9	PRO	-	expression tag	UNP E0YJ44
A	-8	MET	-	expression tag	UNP E0YJ44
A	-7	GLY	-	expression tag	UNP E0YJ44
A	-6	SER	-	expression tag	UNP E0YJ44
A	-5	LEU	-	expression tag	UNP E0YJ44
A	-4	GLN	-	expression tag	UNP E0YJ44
A	-3	PRO	-	expression tag	UNP E0YJ44
A	-2	LEU	-	expression tag	UNP E0YJ44
A	-1	ALA	-	expression tag	UNP E0YJ44
A	0	THR	-	expression tag	UNP E0YJ44
A	1	LEU	-	expression tag	UNP E0YJ44
A	2	TYR	-	expression tag	UNP E0YJ44
A	3	LEU	-	expression tag	UNP E0YJ44
A	4	LEU	-	expression tag	UNP E0YJ44
A	5	GLY	-	expression tag	UNP E0YJ44
A	6	MET	-	expression tag	UNP E0YJ44
A	7	LEU	-	expression tag	UNP E0YJ44
A	8	VAL	-	expression tag	UNP E0YJ44
A	9	ALA	-	expression tag	UNP E0YJ44
A	10	SER	-	expression tag	UNP E0YJ44
A	11	VAL	-	expression tag	UNP E0YJ44
A	756	GLY	ARG	engineered mutation	UNP E0YJ44
A	757	GLY	ARG	engineered mutation	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
A	758	SER	LYS	engineered mutation	UNP E0YJ44
A	759	GLY	ARG	engineered mutation	UNP E0YJ44
A	760	SER	ARG	engineered mutation	UNP E0YJ44
A	1267	LEU	-	linker	UNP E0YJ44
A	1268	ILE	-	linker	UNP E0YJ44
A	1269	LYS	-	linker	UNP E0YJ44
A	1274	ILE	LEU	engineered mutation	UNP P03069
A	1278	ILE	VAL	engineered mutation	UNP P03069
A	1281	ILE	LEU	engineered mutation	UNP P03069
A	1282	GLU	LEU	engineered mutation	UNP P03069
A	1285	GLN	ASN	engineered mutation	UNP P03069
A	1286	LYS	TYR	engineered mutation	UNP P03069
A	1287	LYS	HIS	engineered mutation	UNP P03069
A	1288	ILE	LEU	engineered mutation	UNP P03069
A	1292	ILE	VAL	engineered mutation	UNP P03069
A	1295	ILE	LEU	engineered mutation	UNP P03069
A	1297	LYS	-	insertion	UNP P03069
A	1298	ILE	-	insertion	UNP P03069
A	1302	PRO	-	expression tag	UNP P03069
A	1303	ARG	-	expression tag	UNP P03069
A	1304	GLY	-	expression tag	UNP P03069
A	1305	SER	-	expression tag	UNP P03069
A	1306	LEU	-	expression tag	UNP P03069
A	1307	GLU	-	expression tag	UNP P03069
A	1308	TRP	-	expression tag	UNP P03069
A	1309	SER	-	expression tag	UNP P03069
A	1310	HIS	-	expression tag	UNP P03069
A	1311	PRO	-	expression tag	UNP P03069
A	1312	GLN	-	expression tag	UNP P03069
A	1313	PHE	-	expression tag	UNP P03069
A	1314	GLU	-	expression tag	UNP P03069
A	1315	LYS	-	expression tag	UNP P03069
B	-10	MET	-	initiating methionine	UNP E0YJ44
B	-9	PRO	-	expression tag	UNP E0YJ44
B	-8	MET	-	expression tag	UNP E0YJ44
B	-7	GLY	-	expression tag	UNP E0YJ44
B	-6	SER	-	expression tag	UNP E0YJ44
B	-5	LEU	-	expression tag	UNP E0YJ44
B	-4	GLN	-	expression tag	UNP E0YJ44
B	-3	PRO	-	expression tag	UNP E0YJ44
B	-2	LEU	-	expression tag	UNP E0YJ44
B	-1	ALA	-	expression tag	UNP E0YJ44

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP E0YJ44
B	1	LEU	-	expression tag	UNP E0YJ44
B	2	TYR	-	expression tag	UNP E0YJ44
B	3	LEU	-	expression tag	UNP E0YJ44
B	4	LEU	-	expression tag	UNP E0YJ44
B	5	GLY	-	expression tag	UNP E0YJ44
B	6	MET	-	expression tag	UNP E0YJ44
B	7	LEU	-	expression tag	UNP E0YJ44
B	8	VAL	-	expression tag	UNP E0YJ44
B	9	ALA	-	expression tag	UNP E0YJ44
B	10	SER	-	expression tag	UNP E0YJ44
B	11	VAL	-	expression tag	UNP E0YJ44
B	756	GLY	ARG	engineered mutation	UNP E0YJ44
B	757	GLY	ARG	engineered mutation	UNP E0YJ44
B	758	SER	LYS	engineered mutation	UNP E0YJ44
B	759	GLY	ARG	engineered mutation	UNP E0YJ44
B	760	SER	ARG	engineered mutation	UNP E0YJ44
B	1267	LEU	-	linker	UNP E0YJ44
B	1268	ILE	-	linker	UNP E0YJ44
B	1269	LYS	-	linker	UNP E0YJ44
B	1274	ILE	LEU	engineered mutation	UNP P03069
B	1278	ILE	VAL	engineered mutation	UNP P03069
B	1281	ILE	LEU	engineered mutation	UNP P03069
B	1282	GLU	LEU	engineered mutation	UNP P03069
B	1285	GLN	ASN	engineered mutation	UNP P03069
B	1286	LYS	TYR	engineered mutation	UNP P03069
B	1287	LYS	HIS	engineered mutation	UNP P03069
B	1288	ILE	LEU	engineered mutation	UNP P03069
B	1292	ILE	VAL	engineered mutation	UNP P03069
B	1295	ILE	LEU	engineered mutation	UNP P03069
B	1297	LYS	-	insertion	UNP P03069
B	1298	ILE	-	insertion	UNP P03069
B	1302	PRO	-	expression tag	UNP P03069
B	1303	ARG	-	expression tag	UNP P03069
B	1304	GLY	-	expression tag	UNP P03069
B	1305	SER	-	expression tag	UNP P03069
B	1306	LEU	-	expression tag	UNP P03069
B	1307	GLU	-	expression tag	UNP P03069
B	1308	TRP	-	expression tag	UNP P03069
B	1309	SER	-	expression tag	UNP P03069
B	1310	HIS	-	expression tag	UNP P03069
B	1311	PRO	-	expression tag	UNP P03069

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1312	GLN	-	expression tag	UNP P03069
B	1313	PHE	-	expression tag	UNP P03069
B	1314	GLU	-	expression tag	UNP P03069
B	1315	LYS	-	expression tag	UNP P03069
C	-10	MET	-	initiating methionine	UNP E0YJ44
C	-9	PRO	-	expression tag	UNP E0YJ44
C	-8	MET	-	expression tag	UNP E0YJ44
C	-7	GLY	-	expression tag	UNP E0YJ44
C	-6	SER	-	expression tag	UNP E0YJ44
C	-5	LEU	-	expression tag	UNP E0YJ44
C	-4	GLN	-	expression tag	UNP E0YJ44
C	-3	PRO	-	expression tag	UNP E0YJ44
C	-2	LEU	-	expression tag	UNP E0YJ44
C	-1	ALA	-	expression tag	UNP E0YJ44
C	0	THR	-	expression tag	UNP E0YJ44
C	1	LEU	-	expression tag	UNP E0YJ44
C	2	TYR	-	expression tag	UNP E0YJ44
C	3	LEU	-	expression tag	UNP E0YJ44
C	4	LEU	-	expression tag	UNP E0YJ44
C	5	GLY	-	expression tag	UNP E0YJ44
C	6	MET	-	expression tag	UNP E0YJ44
C	7	LEU	-	expression tag	UNP E0YJ44
C	8	VAL	-	expression tag	UNP E0YJ44
C	9	ALA	-	expression tag	UNP E0YJ44
C	10	SER	-	expression tag	UNP E0YJ44
C	11	VAL	-	expression tag	UNP E0YJ44
C	756	GLY	ARG	engineered mutation	UNP E0YJ44
C	757	GLY	ARG	engineered mutation	UNP E0YJ44
C	758	SER	LYS	engineered mutation	UNP E0YJ44
C	759	GLY	ARG	engineered mutation	UNP E0YJ44
C	760	SER	ARG	engineered mutation	UNP E0YJ44
C	1267	LEU	-	linker	UNP E0YJ44
C	1268	ILE	-	linker	UNP E0YJ44
C	1269	LYS	-	linker	UNP E0YJ44
C	1274	ILE	LEU	engineered mutation	UNP P03069
C	1278	ILE	VAL	engineered mutation	UNP P03069
C	1281	ILE	LEU	engineered mutation	UNP P03069
C	1282	GLU	LEU	engineered mutation	UNP P03069
C	1285	GLN	ASN	engineered mutation	UNP P03069
C	1286	LYS	TYR	engineered mutation	UNP P03069
C	1287	LYS	HIS	engineered mutation	UNP P03069
C	1288	ILE	LEU	engineered mutation	UNP P03069

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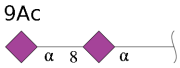
Chain	Residue	Modelled	Actual	Comment	Reference
C	1292	ILE	VAL	engineered mutation	UNP P03069
C	1295	ILE	LEU	engineered mutation	UNP P03069
C	1297	LYS	-	insertion	UNP P03069
C	1298	ILE	-	insertion	UNP P03069
C	1302	PRO	-	expression tag	UNP P03069
C	1303	ARG	-	expression tag	UNP P03069
C	1304	GLY	-	expression tag	UNP P03069
C	1305	SER	-	expression tag	UNP P03069
C	1306	LEU	-	expression tag	UNP P03069
C	1307	GLU	-	expression tag	UNP P03069
C	1308	TRP	-	expression tag	UNP P03069
C	1309	SER	-	expression tag	UNP P03069
C	1310	HIS	-	expression tag	UNP P03069
C	1311	PRO	-	expression tag	UNP P03069
C	1312	GLN	-	expression tag	UNP P03069
C	1313	PHE	-	expression tag	UNP P03069
C	1314	GLU	-	expression tag	UNP P03069
C	1315	LYS	-	expression tag	UNP P03069

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

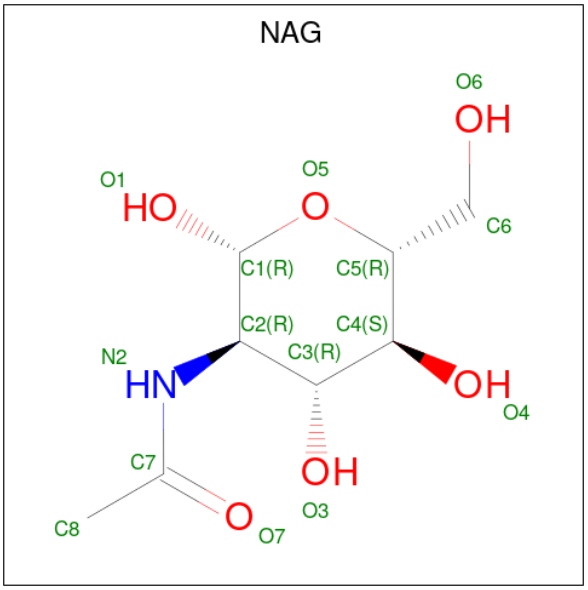
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-N-acetyl-alpha-neuraminic acid.



Mol	Chain	Residues	Atoms	AltConf	Trace
3	H	2	Total C N O 44 24 2 18	0	0
3	I	2	Total C N O 44 24 2 18	0	0
3	J	2	Total C N O 44 24 2 18	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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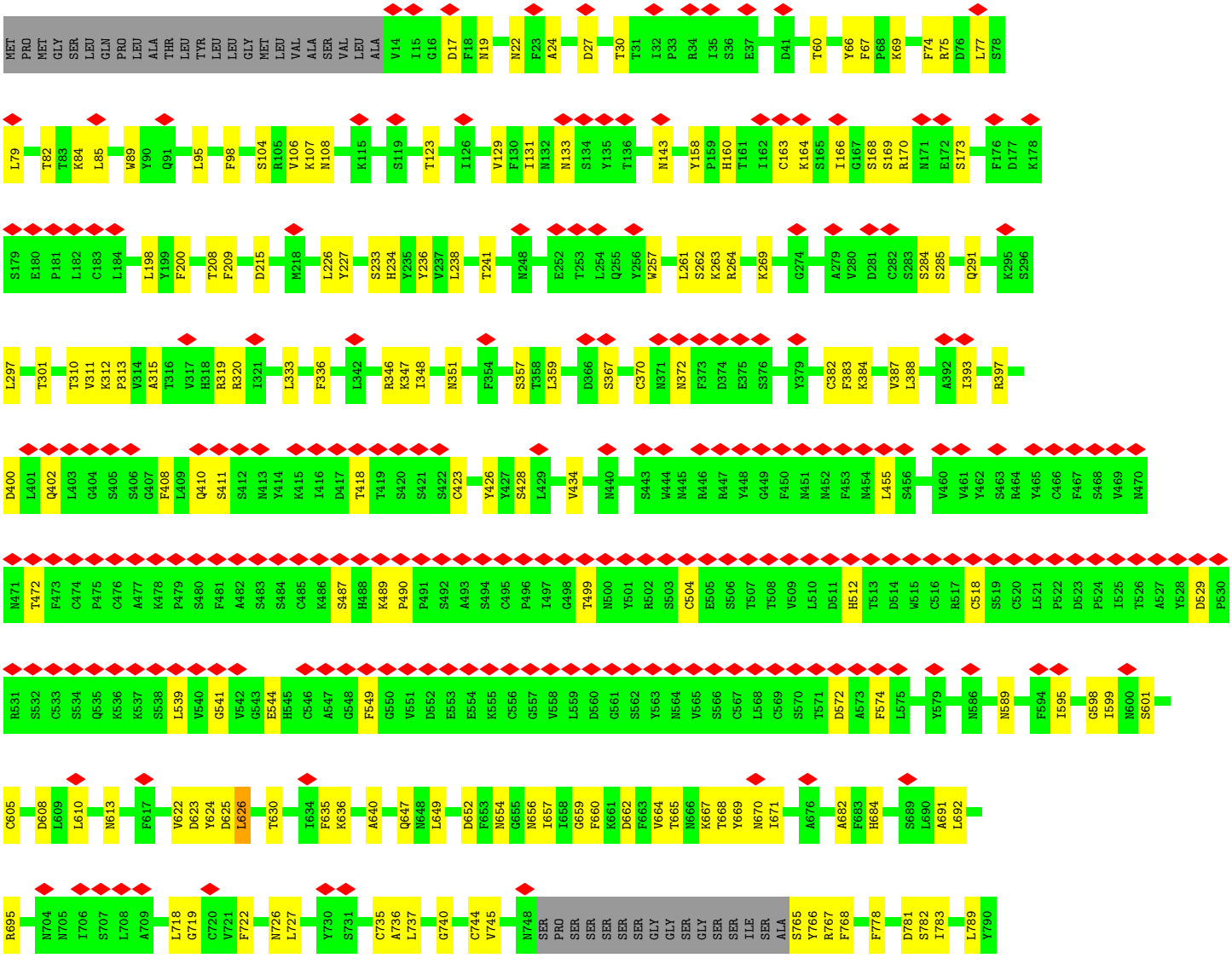
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total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

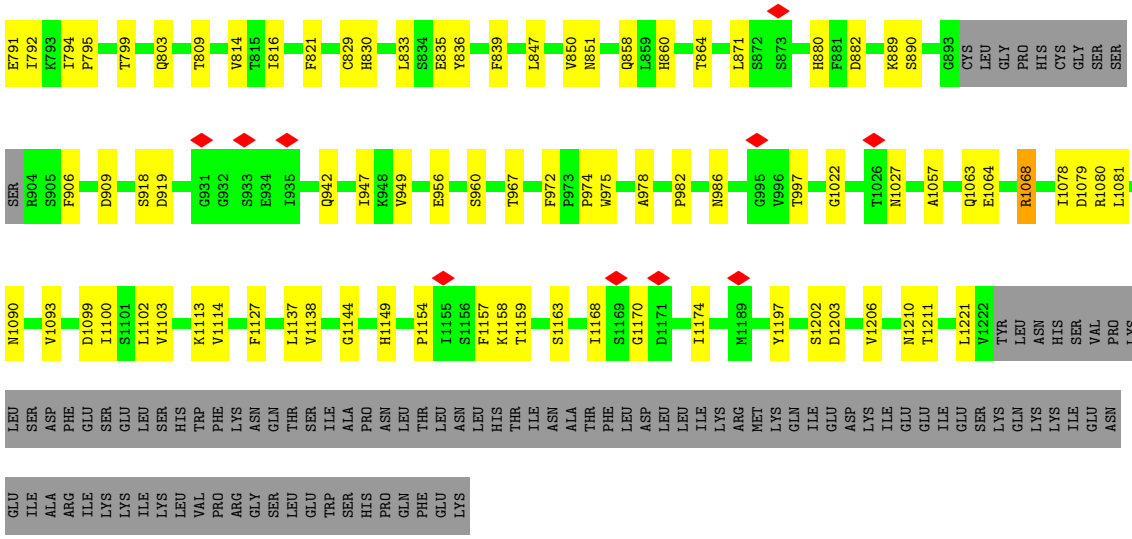
3 Residue-property plots (i)

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: Spike glycoprotein,General control transcription factor GCN4

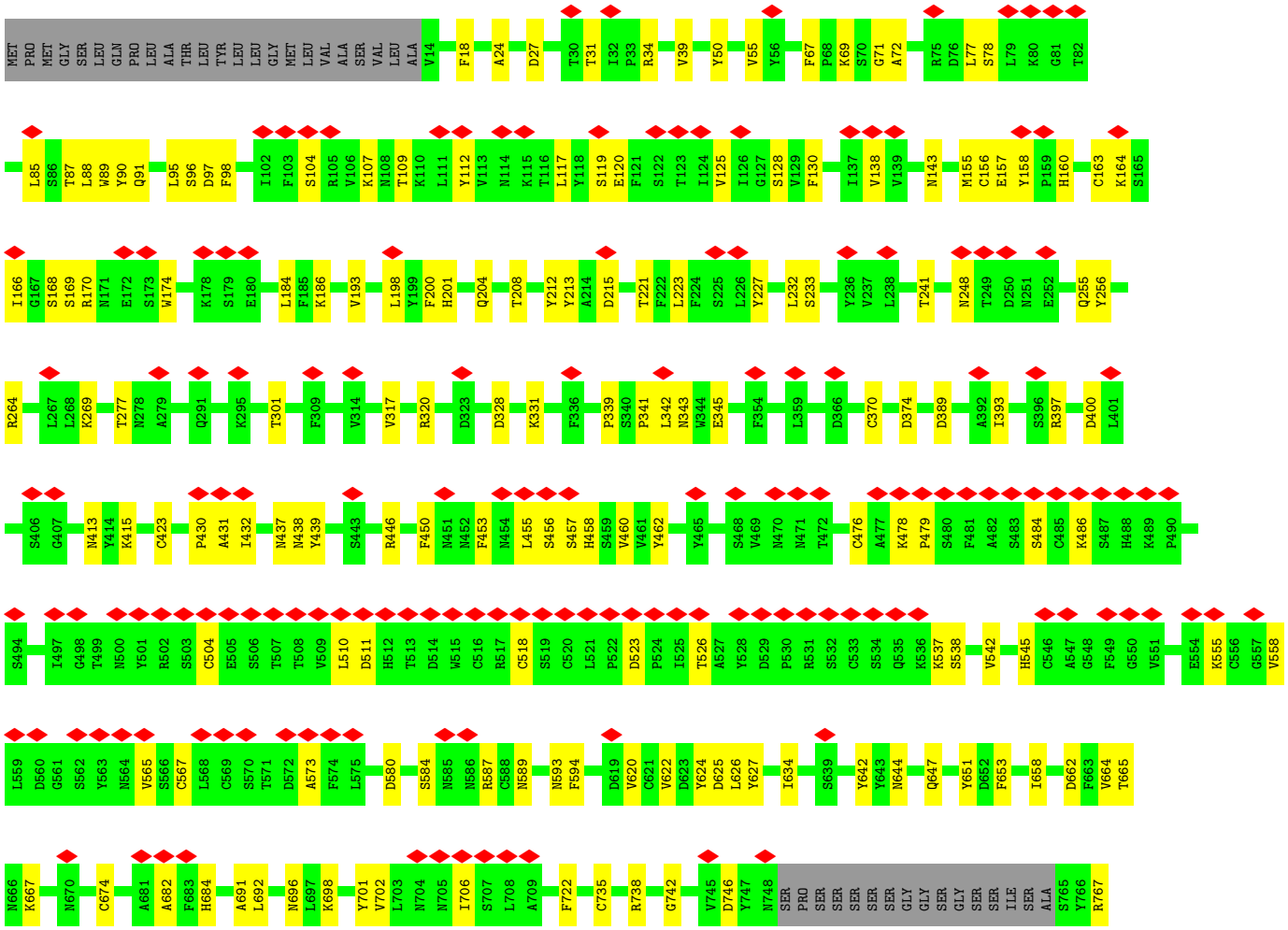
Chain A:

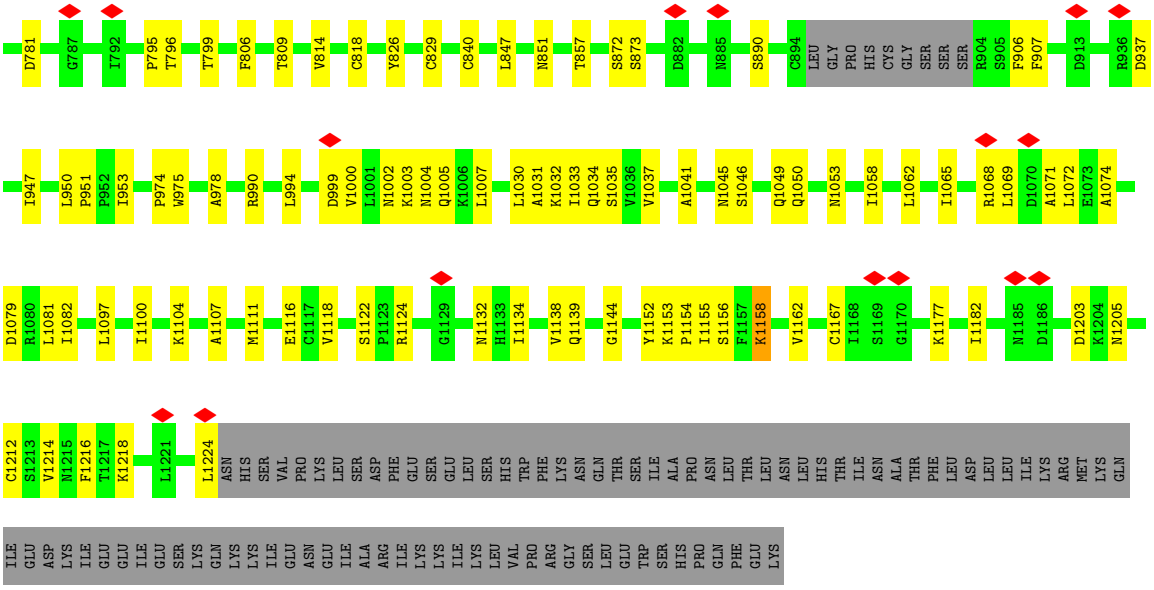




• Molecule 1: Spike glycoprotein,General control transcription factor GCN4

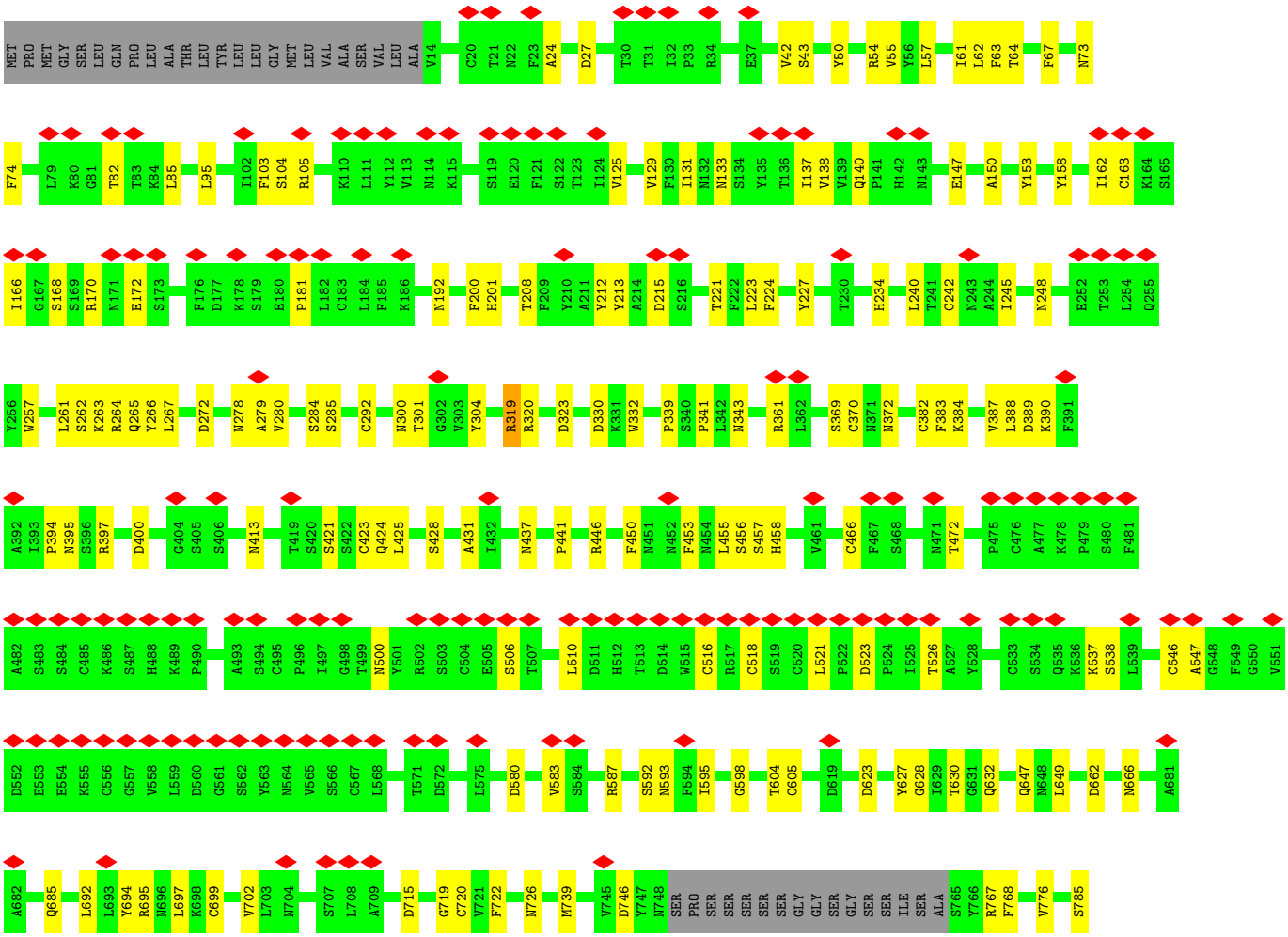
Chain B:

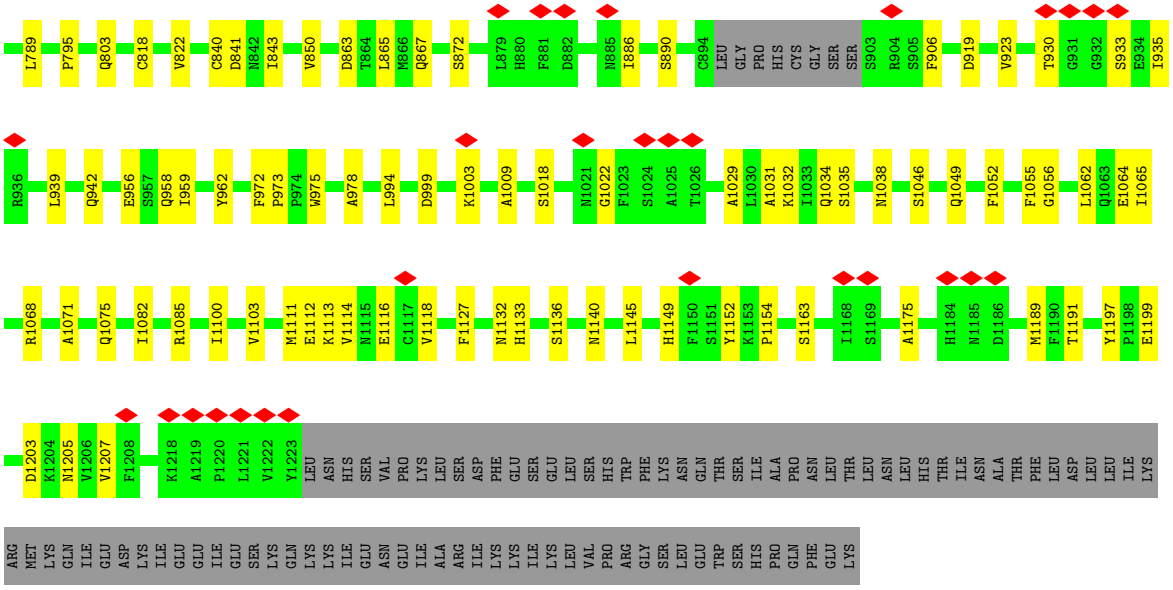




• Molecule 1: Spike glycoprotein,General control transcription factor GCN4

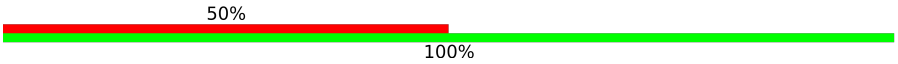
Chain C:





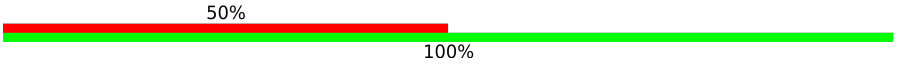
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:



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

Chain F:

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

Chain G:

• Molecule 3: 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-N-acetyl-alpha-neuraminic acid

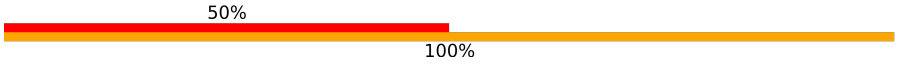
Chain H:

• Molecule 3: 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-N-acetyl-alpha-neuraminic acid

Chain I:

• Molecule 3: 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-N-acetyl-alpha-neuraminic acid

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.656	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.073	Depositor
Map size (Å)	332.00998, 332.00998, 332.00998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1067, 1.1067, 1.1067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG, 5N6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/9524	0.59	3/12961 (0.0%)
1	B	0.28	0/9551	0.59	3/12998 (0.0%)
1	C	0.29	0/9549	0.60	3/12995 (0.0%)
All	All	0.28	0/28624	0.59	9/38954 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	510	LEU	CA-CB-CG	7.21	131.89	115.30
1	A	1221	LEU	CA-CB-CG	7.07	131.56	115.30
1	C	272	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	610	LEU	CA-CB-CG	6.29	129.75	115.30
1	B	510	LEU	CA-CB-CG	5.48	127.90	115.30
1	C	546	CYS	CA-CB-SG	5.31	123.55	114.00
1	A	626	LEU	CA-CB-CG	5.20	127.27	115.30
1	B	1081	LEU	CA-CB-CG	5.04	126.88	115.30
1	B	1072	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9295	0	8943	156	0
1	B	9321	0	8968	152	0
1	C	9319	0	8966	144	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	H	44	0	17	1	0
3	I	44	0	17	1	0
3	J	44	0	17	3	0
4	A	98	0	91	1	0
4	B	168	0	156	1	0
4	C	98	0	91	0	0
All	All	28543	0	27366	433	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 8.

All (433) 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:1064:GLU:O	1:C:1068:ARG:HB3	1.89	0.73
1:A:131:ILE:HG13	1:A:133:ASN:H	1.56	0.69
1:B:320:ARG:HH21	1:B:627:TYR:H	1.39	0.69
1:B:423:CYS:HB2	1:B:594:PHE:HB2	1.73	0.69
1:B:104:SER:HB3	1:B:200:PHE:HB2	1.79	0.65
1:A:69:LYS:HE2	1:A:264:ARG:HH21	1.61	0.65
1:A:803:GLN:HB3	1:A:1149:HIS:HB2	1.79	0.64
1:C:131:ILE:HG13	1:C:133:ASN:H	1.62	0.64
1:A:942:GLN:HB3	1:A:947:ILE:HB	1.80	0.63
1:A:104:SER:HB3	1:A:200:PHE:HB2	1.81	0.63
1:A:1168:ILE:HG23	1:A:1170:GLY:H	1.64	0.63
1:A:789:LEU:HG	1:A:1163:SER:HB3	1.80	0.62
1:A:95:LEU:HD13	1:A:236:TYR:HB2	1.82	0.62
1:A:975:TRP:HB3	1:A:978:ALA:HB3	1.82	0.62
1:B:163:CYS:H	1:B:168:SER:HB2	1.63	0.62
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.82	0.62
1:C:339:PRO:HB3	1:C:437:ASN:HB3	1.81	0.61
1:C:162:ILE:H	1:C:172:GLU:HG3	1.65	0.61
1:C:201:HIS:HB3	1:C:212:TYR:HB2	1.83	0.61
1:A:682:ALA:HB3	1:A:691:ALA:HB3	1.82	0.61
1:A:871:LEU:HG	1:C:776:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:HA	1:C:227:TYR:HA	1.84	0.60
1:A:347:LYS:HB3	1:A:388:LEU:HB2	1.83	0.59
1:B:446:ARG:HD3	1:B:450:PHE:HB3	1.84	0.59
1:B:664:VAL:HG12	1:B:665:THR:HG23	1.83	0.59
1:A:735:CYS:SG	1:A:736:ALA:N	2.76	0.59
1:B:453:PHE:HB3	1:B:455:LEU:HD13	1.84	0.59
1:B:662:ASP:HB2	1:B:667:LYS:H	1.67	0.59
1:B:1079:ASP:HA	1:B:1082:ILE:HG12	1.84	0.59
1:C:726:ASN:HA	1:C:768:PHE:HB3	1.85	0.58
1:A:163:CYS:H	1:A:168:SER:HB2	1.68	0.58
1:B:814:VAL:HB	1:B:947:ILE:HD11	1.86	0.58
1:B:994:LEU:HB3	1:B:1132:ASN:HD21	1.68	0.58
1:A:67:PHE:O	1:A:264:ARG:NH1	2.37	0.58
1:C:1199:GLU:OE2	1:C:1205:ASN:ND2	2.36	0.58
1:B:975:TRP:HB3	1:B:978:ALA:HB3	1.84	0.57
1:C:453:PHE:HB3	1:C:455:LEU:HD13	1.86	0.57
1:B:990:ARG:NH1	1:B:1134:ILE:O	2.37	0.57
1:B:374:ASP:OD1	1:C:1068:ARG:NH2	2.37	0.57
1:B:50:TYR:HB2	1:B:221:THR:HA	1.86	0.57
1:A:367:SER:HB3	1:A:426:TYR:HB2	1.86	0.57
1:B:67:PHE:O	1:B:264:ARG:NH1	2.38	0.57
1:B:85:LEU:HD11	1:B:158:TYR:HB3	1.88	0.56
1:A:695:ARG:HA	1:A:719:GLY:HA3	1.87	0.56
1:B:1116:GLU:HG2	1:B:1124:ARG:HH21	1.70	0.56
1:A:1210:ASN:ND2	1:B:999:ASP:OD1	2.38	0.56
1:C:1112:GLU:O	1:C:1116:GLU:HB2	2.05	0.56
1:C:886:ILE:HD13	1:C:1009:ALA:HB1	1.86	0.56
1:C:939:LEU:O	1:C:942:GLN:NE2	2.38	0.55
1:B:796:THR:HG1	1:B:1156:SER:HG	1.52	0.55
1:A:814:VAL:HG12	1:A:949:VAL:HG22	1.88	0.55
1:B:397:ARG:HB3	1:B:400:ASP:HB2	1.89	0.55
1:A:652:ASP:HB2	1:A:656:ASN:HB2	1.88	0.54
1:C:67:PHE:O	1:C:264:ARG:NH1	2.39	0.54
1:C:370:CYS:HA	1:C:423:CYS:HA	1.88	0.54
1:C:466:CYS:SG	1:C:547:ALA:N	2.79	0.54
1:B:526:THR:HG22	1:C:361:ARG:HD2	1.89	0.54
1:B:1153:LYS:NZ	1:B:1154:PRO:O	2.41	0.54
1:A:315:ALA:H	1:A:622:VAL:HG13	1.71	0.54
1:C:104:SER:HB3	1:C:200:PHE:H	1.72	0.54
1:B:742:GLY:HA3	1:C:958:GLN:HE22	1.72	0.54
1:A:320:ARG:NH1	1:A:613:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:GLU:O	1:A:960:SER:HB3	2.08	0.54
1:C:694:TYR:HB3	1:C:697:LEU:HD12	1.89	0.53
1:C:85:LEU:HD11	1:C:158:TYR:HB3	1.89	0.53
1:A:107:LYS:NZ	1:A:108:ASN:O	2.42	0.53
1:A:740:GLY:HA2	1:B:953:ILE:HA	1.90	0.53
1:C:319:ARG:NH1	1:C:320:ARG:O	2.42	0.53
1:A:795:PRO:HA	1:A:1157:PHE:HA	1.91	0.53
1:B:1214:VAL:O	1:B:1218:LYS:NZ	2.42	0.53
1:C:537:LYS:NZ	1:C:538:SER:O	2.42	0.53
1:C:746:ASP:OD2	1:C:767:ARG:NH2	2.41	0.53
1:A:397:ARG:HH22	1:A:408:PHE:HB2	1.73	0.53
1:A:890:SER:HA	1:A:906:PHE:HB3	1.91	0.53
1:B:431:ALA:O	1:B:458:HIS:NE2	2.40	0.53
1:C:1191:THR:HG23	1:C:1197:TYR:H	1.74	0.53
1:B:342:LEU:O	1:B:545:HIS:ND1	2.41	0.52
1:B:1132:ASN:HB3	1:B:1152:TYR:HB3	1.90	0.52
1:C:395:ASN:ND2	1:C:583:VAL:O	2.41	0.52
1:C:715:ASP:HA	1:C:720:CYS:HA	1.92	0.52
1:A:809:THR:O	1:A:858:GLN:NE2	2.43	0.52
1:B:651:TYR:O	1:C:54:ARG:NH2	2.38	0.52
1:A:17:ASP:HB3	1:A:131:ILE:HG22	1.92	0.52
1:B:320:ARG:NH2	1:B:625:ASP:O	2.43	0.52
1:C:692:LEU:HB2	1:C:722:PHE:HB2	1.91	0.52
1:C:699:CYS:HA	1:C:702:VAL:HG12	1.90	0.52
1:B:746:ASP:OD2	1:B:767:ARG:NH2	2.42	0.52
1:B:847:LEU:O	1:B:851:ASN:ND2	2.42	0.52
1:A:830:HIS:HA	1:A:833:LEU:HG	1.92	0.52
1:C:841:ASP:OD1	1:C:841:ASP:N	2.43	0.52
1:B:213:TYR:HE1	1:B:223:LEU:HD13	1.75	0.52
1:C:1034:GLN:O	1:C:1038:ASN:ND2	2.43	0.52
1:A:24:ALA:O	1:A:170:ARG:NH2	2.42	0.51
1:B:999:ASP:O	1:B:1003:LYS:NZ	2.43	0.51
1:B:1212:CYS:HB2	1:B:1216:PHE:HD2	1.76	0.51
1:B:430:PRO:HA	1:B:587:ARG:HA	1.93	0.51
1:C:105:ARG:HB3	1:C:257:TRP:HB2	1.92	0.51
1:C:695:ARG:HA	1:C:719:GLY:HA3	1.92	0.51
1:A:215:ASP:N	1:A:215:ASP:OD1	2.44	0.51
1:C:1113:LYS:NZ	1:C:1127:PHE:O	2.44	0.51
1:A:85:LEU:HD11	1:A:158:TYR:HB3	1.92	0.51
1:A:370:CYS:HA	1:A:423:CYS:HA	1.93	0.51
1:A:1158:LYS:NZ	1:A:1159:THR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ASP:HB2	1:C:593:ASN:HB3	1.92	0.51
1:C:1175:ALA:HB3	1:C:1207:VAL:HB	1.92	0.51
1:A:19:ASN:ND2	1:A:22:ASN:OD1	2.44	0.51
1:A:397:ARG:NH1	1:A:400:ASP:OD2	2.43	0.51
1:B:119:SER:HB3	1:B:193:VAL:HG22	1.93	0.51
1:C:64:THR:OG1	1:C:265:GLN:OE1	2.28	0.51
1:B:39:VAL:HB	1:B:71:GLY:HA2	1.92	0.51
1:A:624:TYR:HB3	1:A:635:PHE:HZ	1.76	0.50
1:B:1062:LEU:HD13	1:B:1065:ILE:HD11	1.93	0.50
1:C:330:ASP:OD1	1:C:330:ASP:N	2.43	0.50
1:C:1049:GLN:HA	1:C:1052:PHE:HD2	1.75	0.50
1:A:1022:GLY:O	1:A:1027:ASN:ND2	2.44	0.50
1:B:658:ILE:HG22	1:C:935:ILE:HD13	1.93	0.50
1:B:682:ALA:HB3	1:B:691:ALA:HB3	1.92	0.50
1:B:1034:GLN:HA	1:B:1037:VAL:HG22	1.93	0.50
1:B:1118:VAL:HG11	1:B:1138:VAL:HG23	1.92	0.50
1:A:160:HIS:NE2	1:A:173:SER:OG	2.44	0.50
1:B:339:PRO:HG3	1:B:345:GLU:HB2	1.94	0.50
1:B:460:VAL:N	1:B:580:ASP:O	2.44	0.50
1:B:537:LYS:NZ	1:B:538:SER:O	2.44	0.50
1:C:446:ARG:HD3	1:C:450:PHE:HB3	1.93	0.50
1:B:950:LEU:HD12	1:B:951:PRO:HD2	1.92	0.50
1:C:795:PRO:HB3	1:C:1154:PRO:HB3	1.92	0.50
1:A:489:LYS:NZ	1:A:490:PRO:O	2.43	0.50
1:C:387:VAL:HG13	1:C:595:ILE:HB	1.93	0.50
1:A:30:THR:HG1	1:A:89:TRP:HE1	1.57	0.50
1:B:69:LYS:HG3	1:B:72:ALA:HB2	1.94	0.50
1:A:351:ASN:ND2	1:B:186:LYS:O	2.45	0.50
1:A:836:TYR:HB3	1:A:839:PHE:HB3	1.94	0.50
1:B:24:ALA:O	1:B:170:ARG:NH2	2.40	0.50
1:B:204:GLN:NE2	1:B:232:LEU:O	2.45	0.50
1:B:415:LYS:HD2	1:B:542:VAL:HG12	1.94	0.50
1:C:919:ASP:OD1	1:C:919:ASP:N	2.44	0.50
1:A:310:THR:O	1:A:312:LYS:NZ	2.45	0.49
1:B:143:ASN:HB2	1:B:164:LYS:HD3	1.94	0.49
1:B:555:LYS:HD2	1:B:573:ALA:HA	1.94	0.49
1:B:692:LEU:HB2	1:B:722:PHE:HB2	1.94	0.49
1:A:387:VAL:HB	1:A:595:ILE:HB	1.94	0.49
1:C:446:ARG:HE	1:C:450:PHE:HD2	1.60	0.49
1:C:323:ASP:OD1	1:C:323:ASP:N	2.45	0.49
1:A:311:VAL:HG23	1:A:313:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HB2	1:B:241:THR:HB	1.95	0.49
1:C:125:VAL:HG23	1:C:138:VAL:HG22	1.95	0.49
1:A:972:PHE:HB3	1:A:974:PRO:HD2	1.95	0.49
1:C:1018:SER:O	1:C:1022:GLY:N	2.45	0.49
1:B:27:ASP:OD1	1:B:27:ASP:N	2.46	0.49
1:B:215:ASP:OD1	1:B:215:ASP:N	2.45	0.49
1:C:163:CYS:H	1:C:168:SER:HB2	1.78	0.49
1:C:472:THR:OG1	1:C:500:ASN:OD1	2.30	0.49
1:C:1100:ILE:HA	1:C:1103:VAL:HG12	1.94	0.49
1:C:930:THR:O	1:C:933:SER:OG	2.31	0.48
1:C:1133:HIS:NE2	1:C:1136:SER:OG	2.42	0.48
1:A:636:LYS:HB3	1:A:670:ASN:HB2	1.95	0.48
1:A:836:TYR:HE1	1:C:1055:PHE:HA	1.78	0.48
1:A:1063:GLN:HE22	1:C:630:THR:HG23	1.78	0.48
1:B:907:PHE:HD2	1:B:1139:GLN:HG2	1.77	0.48
1:B:696:ASN:HD21	1:C:923:VAL:HG23	1.77	0.48
1:B:799:THR:HG23	1:B:1155:ILE:HD13	1.95	0.48
1:C:382:CYS:HA	1:C:605:CYS:HA	1.96	0.48
1:C:739:MET:SD	1:C:739:MET:N	2.86	0.48
1:C:1046:SER:O	1:C:1049:GLN:NE2	2.46	0.48
1:B:1050:GLN:NE2	1:B:1053:ASN:OD1	2.46	0.48
1:C:1140:ASN:HA	1:C:1145:LEU:HD13	1.96	0.48
1:B:1030:LEU:HD13	1:B:1033:ILE:HD11	1.95	0.48
1:A:778:PHE:HB3	1:B:873:SER:HB3	1.96	0.48
1:C:300:ASN:O	1:C:304:TYR:OH	2.31	0.48
1:A:402:GLN:O	1:A:410:GLN:NE2	2.46	0.48
1:B:339:PRO:HA	1:B:437:ASN:HB3	1.96	0.48
1:B:343:ASN:ND2	1:B:439:TYR:O	2.47	0.48
1:C:341:PRO:HB2	1:C:413:ASN:HB3	1.96	0.48
1:A:169:SER:HB2	1:A:241:THR:HB	1.96	0.48
1:C:27:ASP:OD1	1:C:27:ASP:N	2.47	0.48
1:A:301:THR:HG22	1:A:684:HIS:HA	1.95	0.48
1:A:319:ARG:NH1	1:A:320:ARG:O	2.47	0.48
1:A:95:LEU:HD11	1:A:234:HIS:HB3	1.96	0.47
1:A:384:LYS:HG3	1:A:598:GLY:HA3	1.94	0.47
1:C:137:ILE:HA	1:C:150:ALA:HA	1.96	0.47
1:C:343:ASN:HB3	1:C:441:PRO:HD3	1.95	0.47
1:C:384:LYS:HG2	1:C:598:GLY:HA3	1.95	0.47
1:C:863:ASP:O	1:C:867:GLN:NE2	2.43	0.47
1:B:370:CYS:HA	1:B:423:CYS:HA	1.96	0.47
1:C:394:PRO:HB3	1:C:580:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ILE:HD13	1:A:947:ILE:HG13	1.96	0.47
1:C:383:PHE:O	1:C:604:THR:N	2.46	0.47
1:A:640:ALA:HB3	1:A:668:THR:HG21	1.95	0.47
1:C:662:ASP:HB3	1:C:666:ASN:H	1.79	0.47
1:C:994:LEU:HD13	1:C:1132:ASN:HB3	1.95	0.47
1:B:438:ASN:HB3	1:B:453:PHE:HB2	1.96	0.47
1:C:1062:LEU:HA	1:C:1065:ILE:HD12	1.96	0.47
1:B:301:THR:HG22	1:B:684:HIS:HA	1.96	0.47
1:B:317:VAL:HG12	1:B:626:LEU:HD21	1.97	0.47
1:B:795:PRO:HB3	1:B:1154:PRO:HB3	1.97	0.47
1:A:791:GLU:OE2	1:A:1159:THR:OG1	2.33	0.47
1:B:88:LEU:HD21	4:B:1412:NAG:H82	1.96	0.47
1:B:1203:ASP:HB3	1:B:1224:LEU:HD21	1.96	0.47
1:C:518:CYS:H	1:C:521:LEU:HD11	1.80	0.47
1:A:428:SER:OG	1:A:589:ASN:ND2	2.47	0.46
1:A:623:ASP:HB3	1:A:630:THR:HB	1.97	0.46
1:A:880:HIS:NE2	1:A:882:ASP:O	2.48	0.46
1:B:735:CYS:O	1:B:738:ARG:NH1	2.48	0.46
1:A:320:ARG:NE	1:A:625:ASP:O	2.48	0.46
1:A:664:VAL:O	4:A:1402:NAG:O6	2.33	0.46
1:A:882:ASP:OD1	1:A:882:ASP:N	2.47	0.46
1:B:248:ASN:HA	3:I:1:SIA:H111	1.97	0.46
1:B:698:LYS:HB3	1:B:701:TYR:HB3	1.97	0.46
1:C:999:ASP:O	1:C:1003:LYS:NZ	2.49	0.46
1:A:847:LEU:HA	1:A:850:VAL:HG12	1.98	0.46
1:A:372:ASN:ND2	1:A:418:THR:O	2.40	0.46
1:A:1057:ALA:N	1:A:1080:ARG:HH12	2.14	0.46
1:C:63:PHE:H	1:C:265:GLN:HE22	1.63	0.46
1:A:346:ARG:HH22	1:A:348:ILE:HD13	1.80	0.46
1:A:382:CYS:HA	1:A:605:CYS:HA	1.97	0.46
1:B:341:PRO:HB2	1:B:413:ASN:HB3	1.97	0.46
1:B:523:ASP:OD1	1:B:523:ASP:N	2.48	0.46
1:C:975:TRP:HB3	1:C:978:ALA:HB3	1.97	0.46
1:A:487:SER:OG	1:A:512:HIS:ND1	2.48	0.46
1:A:847:LEU:O	1:A:851:ASN:ND2	2.49	0.46
1:C:284:SER:OG	1:C:285:SER:N	2.48	0.46
1:B:328:ASP:OD1	1:B:331:LYS:NZ	2.41	0.46
1:C:1132:ASN:HB2	1:C:1152:TYR:HB3	1.96	0.46
1:B:476:CYS:N	1:B:567:CYS:SG	2.89	0.46
1:B:1068:ARG:HG3	1:B:1069:LEU:HD12	1.97	0.46
1:A:649:LEU:HD11	1:A:657:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:SER:OG	1:B:457:SER:N	2.49	0.45
1:B:558:VAL:HG21	1:B:565:VAL:HB	1.98	0.45
1:A:835:GLU:OE2	1:C:1056:GLY:N	2.49	0.45
1:A:1210:ASN:OD1	1:A:1211:THR:N	2.49	0.45
1:C:1071:ALA:O	1:C:1075:GLN:NE2	2.49	0.45
1:B:31:THR:HB	1:B:89:TRP:HD1	1.81	0.45
1:B:393:ILE:HD11	1:B:589:ASN:HB2	1.98	0.45
1:B:806:PHE:HB3	1:B:1032:LYS:HE3	1.98	0.45
1:B:1162:VAL:HG12	1:B:1182:ILE:HB	1.98	0.45
1:A:209:PHE:N	1:A:226:LEU:O	2.43	0.45
1:A:291:GLN:NE2	1:A:297:LEU:O	2.49	0.45
1:A:1090:ASN:HA	1:A:1093:VAL:HG22	1.98	0.45
1:B:504:CYS:HA	1:B:518:CYS:HA	1.99	0.45
1:B:826:TYR:HB2	1:B:829:CYS:HB3	1.98	0.45
1:A:624:TYR:HD2	1:A:626:LEU:H	1.63	0.45
1:A:695:ARG:HG2	1:A:718:LEU:HB3	1.99	0.45
1:B:208:THR:HA	1:B:227:TYR:HA	1.98	0.45
1:B:1177:LYS:HE2	1:B:1205:ASN:HA	1.97	0.45
1:A:1100:ILE:HA	1:A:1103:VAL:HG12	1.98	0.45
1:B:937:ASP:N	1:B:937:ASP:OD1	2.49	0.45
1:C:301:THR:HG22	1:C:685:GLN:H	1.82	0.45
1:A:75:ARG:HH21	1:A:77:LEU:HD22	1.81	0.45
1:B:1107:ALA:O	1:B:1111:MET:HG2	2.16	0.45
1:C:397:ARG:NH2	1:C:400:ASP:OD2	2.46	0.45
1:A:333:LEU:HD12	1:A:359:LEU:HD11	1.99	0.45
1:A:472:THR:HA	1:A:499:THR:HA	1.98	0.45
1:A:1064:GLU:O	1:A:1068:ARG:HB2	2.17	0.45
1:B:107:LYS:O	1:B:255:GLN:NE2	2.50	0.45
1:C:425:LEU:HB3	1:C:592:SER:HB2	1.99	0.45
1:C:695:ARG:NH2	1:C:739:MET:O	2.44	0.45
1:A:1202:SER:OG	1:A:1203:ASP:N	2.50	0.45
1:B:1041:ALA:O	1:B:1045:ASN:ND2	2.49	0.45
1:C:43:SER:O	1:C:278:ASN:ND2	2.37	0.45
1:C:332:TRP:O	1:C:390:LYS:NZ	2.50	0.45
1:A:30:THR:OG1	1:A:89:TRP:NE1	2.41	0.44
1:A:66:TYR:HB3	1:A:261:LEU:HD23	1.99	0.44
1:A:143:ASN:HB2	1:A:164:LYS:HD3	1.99	0.44
1:A:357:SER:N	1:A:608:ASP:OD2	2.49	0.44
1:C:129:VAL:HG13	1:C:131:ILE:HG12	1.99	0.44
1:C:300:ASN:OD1	1:C:304:TYR:OH	2.33	0.44
1:C:506:SER:HA	1:C:516:CYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ASN:HA	1:A:768:PHE:HB3	1.97	0.44
1:B:130:PHE:HB3	1:B:155:MET:HG3	1.99	0.44
1:B:389:ASP:HB2	1:B:593:ASN:HB3	2.00	0.44
1:B:1071:ALA:HA	1:B:1074:ALA:HB3	1.99	0.44
1:B:1031:ALA:O	1:B:1035:SER:HB3	2.17	0.44
1:B:1058:ILE:HD11	1:B:1069:LEU:HD11	1.99	0.44
1:C:54:ARG:NH2	1:C:55:VAL:O	2.37	0.44
1:A:541:GLY:H	1:A:544:GLU:HB2	1.82	0.44
1:A:549:PHE:HB2	1:A:574:PHE:HD2	1.81	0.44
1:B:98:PHE:N	1:B:233:SER:O	2.47	0.44
1:A:60:THR:HG22	1:A:269:LYS:HG3	2.00	0.44
1:A:659:GLY:HA2	1:A:671:ILE:HG13	2.00	0.44
1:C:50:TYR:HB2	1:C:221:THR:HA	2.00	0.44
1:A:662:ASP:OD2	1:A:665:THR:OG1	2.30	0.44
1:B:269:LYS:HD3	1:B:277:THR:HB	1.98	0.44
1:B:1000:VAL:HA	1:B:1003:LYS:HZ2	1.82	0.44
1:C:1082:ILE:HA	1:C:1085:ARG:HG2	2.00	0.44
1:A:262:SER:OG	1:A:263:LYS:N	2.50	0.44
1:C:140:GLN:HG2	1:C:147:GLU:HB2	1.98	0.44
1:A:98:PHE:N	1:A:233:SER:O	2.51	0.44
1:A:781:ASP:O	1:B:872:SER:OG	2.36	0.44
1:A:850:VAL:HG21	1:A:1100:ILE:HG21	1.99	0.44
1:C:372:ASN:HB3	1:C:421:SER:HA	2.00	0.44
1:C:1114:VAL:O	1:C:1118:VAL:HB	2.18	0.44
1:A:967:THR:HG22	1:A:1137:LEU:HD11	1.99	0.44
1:B:857:THR:HG21	1:B:1104:LYS:HG2	1.98	0.44
1:C:82:THR:OG1	3:J:2:5N6:O8	2.36	0.44
1:A:82:THR:OG1	3:H:2:5N6:O8	2.36	0.43
1:B:1046:SER:O	1:B:1049:GLN:NE2	2.51	0.43
1:C:248:ASN:HA	3:J:1:SIA:H111	2.00	0.43
1:A:301:THR:HB	1:A:737:LEU:HD11	1.98	0.43
1:A:529:ASP:OD1	1:A:529:ASP:N	2.51	0.43
1:A:829:CYS:SG	1:A:830:HIS:N	2.91	0.43
1:B:128:SER:HB2	1:B:232:LEU:HA	2.00	0.43
1:B:653:PHE:HB2	1:C:61:ILE:HD12	2.01	0.43
1:B:809:THR:H	1:B:1144:GLY:HA2	1.83	0.43
1:C:153:TYR:HB3	1:C:181:PRO:HB3	2.00	0.43
1:A:647:GLN:HB3	1:B:55:VAL:HG21	2.00	0.43
1:A:860:HIS:O	1:A:864:THR:OG1	2.22	0.43
1:B:642:TYR:CZ	1:C:57:LEU:HD11	2.54	0.43
1:B:702:VAL:HG12	1:B:706:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HB3	1:C:280:VAL:HB	1.99	0.43
1:A:384:LYS:NZ	1:A:601:SER:OG	2.51	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.91	0.43
1:A:1114:VAL:HG12	1:A:1138:VAL:HG21	2.01	0.43
1:C:262:SER:OG	1:C:263:LYS:N	2.51	0.43
1:A:129:VAL:HG23	1:A:131:ILE:HG12	2.00	0.43
1:B:341:PRO:HG2	1:B:462:TYR:HB3	2.00	0.43
1:C:818:CYS:HB3	1:C:840:CYS:HB2	1.74	0.43
1:A:792:ILE:HD12	1:B:974:PRO:HB3	2.00	0.43
1:B:511:ASP:OD1	1:B:511:ASP:N	2.48	0.43
1:C:785:SER:O	1:C:785:SER:OG	2.35	0.43
1:A:336:PHE:HB3	1:A:434:VAL:HA	2.00	0.43
1:A:660:PHE:HD1	1:A:671:ILE:HD11	1.84	0.43
1:B:478:LYS:HA	1:B:479:PRO:HD3	1.93	0.43
1:C:74:PHE:HB3	1:C:257:TRP:HB3	2.00	0.43
1:A:682:ALA:HB1	1:A:737:LEU:HD23	2.00	0.43
1:A:765:SER:OG	1:A:766:TYR:N	2.43	0.43
1:B:156:CYS:SG	1:B:157:GLU:N	2.92	0.43
1:B:781:ASP:O	1:C:872:SER:OG	2.30	0.43
1:C:456:SER:OG	1:C:457:SER:N	2.52	0.43
1:C:840:CYS:HA	1:C:843:ILE:HD12	2.01	0.43
1:C:1111:MET:HA	1:C:1114:VAL:HG22	2.00	0.43
1:C:1203:ASP:OD1	1:C:1203:ASP:N	2.49	0.43
1:A:918:SER:OG	1:A:919:ASP:N	2.52	0.42
1:B:584:SER:HB2	1:B:589:ASN:HD21	1.83	0.42
1:C:192:ASN:N	1:C:215:ASP:OD2	2.51	0.42
1:B:796:THR:OG1	1:B:1156:SER:OG	2.27	0.42
1:C:213:TYR:HE1	1:C:223:LEU:HD13	1.84	0.42
1:C:431:ALA:O	1:C:458:HIS:NE2	2.52	0.42
1:A:84:LYS:HA	1:A:170:ARG:HH21	1.85	0.42
1:A:504:CYS:HA	1:A:518:CYS:HA	2.01	0.42
1:A:982:PRO:O	1:A:986:ASN:N	2.47	0.42
1:B:397:ARG:HH21	1:B:462:TYR:HH	1.67	0.42
1:B:644:ASN:H	1:B:647:GLN:HB2	1.83	0.42
1:A:27:ASP:N	1:A:27:ASP:OD1	2.53	0.42
1:A:74:PHE:HB3	1:A:257:TRP:HB3	2.00	0.42
1:B:91:GLN:HA	1:B:95:LEU:HD23	2.01	0.42
1:B:125:VAL:HG23	1:B:138:VAL:HG22	2.01	0.42
1:B:890:SER:HA	1:B:906:PHE:HB3	2.02	0.42
1:C:24:ALA:O	1:C:170:ARG:NH2	2.49	0.42
1:A:809:THR:H	1:A:1144:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:TYR:HB2	1:B:626:LEU:HG	2.00	0.42
1:B:634:ILE:HG13	1:B:674:CYS:HB3	2.01	0.42
1:C:369:SER:O	1:C:424:GLN:N	2.44	0.42
1:A:393:ILE:HD12	1:A:589:ASN:HB3	2.00	0.42
1:A:667:LYS:NZ	1:A:669:TYR:OH	2.51	0.42
1:B:87:THR:HA	1:B:90:TYR:HD2	1.83	0.42
1:A:106:VAL:HB	1:A:198:LEU:HB2	2.01	0.42
1:C:73:ASN:OD1	1:C:73:ASN:N	2.52	0.42
1:A:1113:LYS:NZ	1:A:1127:PHE:O	2.43	0.42
3:J:1:SIA:O9	3:J:1:SIA:O7	2.38	0.42
1:A:572:ASP:OD1	1:A:572:ASP:N	2.53	0.42
1:A:1174:ILE:HG23	1:A:1206:VAL:HG21	2.01	0.42
1:B:1002:ASN:HA	1:B:1005:GLN:HE22	1.85	0.42
1:C:428:SER:HB2	1:C:587:ARG:HB3	2.01	0.42
1:C:627:TYR:OH	1:C:662:ASP:OD1	2.36	0.42
1:B:620:VAL:HG23	1:B:622:VAL:HG23	2.01	0.41
1:A:942:GLN:O	1:A:947:ILE:N	2.53	0.41
1:B:77:LEU:HB3	1:B:256:TYR:HD2	1.85	0.41
1:B:112:TYR:HD1	1:B:117:LEU:HD12	1.86	0.41
1:B:818:CYS:HB3	1:B:840:CYS:HB2	1.83	0.41
1:B:890:SER:O	1:B:907:PHE:N	2.48	0.41
1:C:647:GLN:NE2	1:C:649:LEU:O	2.49	0.41
1:C:850:VAL:HG13	1:C:1100:ILE:HD12	2.03	0.41
1:C:972:PHE:HD1	1:C:973:PRO:HD2	1.85	0.41
1:B:18:PHE:O	1:B:157:GLU:N	2.48	0.41
1:B:107:LYS:HB3	1:B:255:GLN:HE21	1.84	0.41
1:B:430:PRO:HB2	1:B:432[B]:ILE:HG12	2.03	0.41
1:B:484:SER:O	1:B:486:LYS:NZ	2.52	0.41
1:C:789:LEU:HD13	1:C:1163:SER:HB3	2.02	0.41
1:C:822:VAL:HA	1:C:1085:ARG:HD2	2.02	0.41
1:C:1189:MET:HB3	1:C:1199:GLU:H	1.85	0.41
1:C:240:LEU:HG	1:C:242:CYS:HB2	2.03	0.41
1:C:1029:ALA:HA	1:C:1032:LYS:HD3	2.02	0.41
1:A:123:THR:HB	1:A:238:LEU:HB2	2.01	0.41
1:B:1205:ASN:OD1	1:B:1205:ASN:N	2.53	0.41
1:C:865:LEU:HD23	1:C:962:TYR:HB3	2.03	0.41
1:C:1031:ALA:O	1:C:1035:SER:HB3	2.20	0.41
1:A:397:ARG:HB3	1:A:400:ASP:HB2	2.01	0.41
1:B:1004:ASN:HB2	1:B:1007:LEU:HB2	2.02	0.41
1:B:1167:CYS:HB3	1:B:1212:CYS:HB3	1.50	0.41
1:C:42:VAL:HG21	1:C:266:TYR:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HD21	1:C:292:CYS:HB2	2.03	0.41
1:A:383:PHE:HE1	1:A:599:ILE:HG13	1.85	0.41
1:A:1079:ASP:OD1	1:A:1080:ARG:N	2.51	0.41
1:B:34:ARG:HH12	1:B:78:SER:HB2	1.86	0.41
1:A:79:LEU:HD11	1:A:89:TRP:CD2	2.56	0.41
1:A:997:THR:HG21	1:A:1197:TYR:HD2	1.85	0.41
1:A:1078:ILE:HD12	1:A:1081:LEU:HD23	2.01	0.41
1:B:160:HIS:H	1:B:174:TRP:HB3	1.85	0.41
1:A:411:SER:HB2	1:A:539:LEU:HD22	2.03	0.41
1:A:692:LEU:HB2	1:A:722:PHE:HB2	2.02	0.41
1:A:744:CYS:SG	1:A:745:VAL:N	2.94	0.41
1:B:96:SER:OG	1:B:97:ASP:N	2.54	0.41
1:B:109:THR:OG1	1:B:120:GLU:O	2.37	0.41
1:B:796:THR:HG21	1:B:1158:LYS:HE3	2.02	0.41
1:C:42:VAL:HG22	1:C:279:ALA:HB3	2.02	0.41
1:C:223:LEU:HG	1:C:224:PHE:HD1	1.86	0.41
1:A:208:THR:HA	1:A:227:TYR:HA	2.02	0.41
1:B:1116:GLU:OE1	1:B:1122:SER:OG	2.38	0.41
1:C:382:CYS:HB2	1:C:628:GLY:HA3	2.02	0.41
1:C:1064:GLU:O	1:C:1068:ARG:CB	2.63	0.41
1:A:816:ILE:HD11	1:A:821:PHE:HB2	2.02	0.40
1:A:1064:GLU:O	1:A:1068:ARG:CB	2.69	0.40
1:C:332:TRP:HZ3	1:C:388:LEU:HB3	1.85	0.40
1:A:889:LYS:HD2	1:A:889:LYS:HA	1.91	0.40
1:A:909:ASP:N	1:A:909:ASP:OD1	2.54	0.40
1:A:1099:ASP:HA	1:A:1102:LEU:HG	2.02	0.40
1:B:430:PRO:HB2	1:B:432[A]:ILE:HG12	2.03	0.40
1:C:95:LEU:HD11	1:C:234:HIS:HB3	2.04	0.40
1:A:66:TYR:HE1	1:A:263:LYS:HG2	1.87	0.40
1:A:727:LEU:N	1:A:768:PHE:O	2.54	0.40
1:A:782:SER:OG	1:A:783:ILE:N	2.54	0.40
1:C:623:ASP:HA	1:C:632:GLN:HA	2.02	0.40
1:A:799:THR:HB	1:A:1154:PRO:HA	2.02	0.40
1:B:198:LEU:HG	1:B:215:ASP:HA	2.04	0.40
1:C:523:ASP:OD1	1:C:526:THR:OG1	2.31	0.40
1:A:269:LYS:HE2	1:A:297:LEU:HD23	2.04	0.40
1:A:284:SER:OG	1:A:285:SER:N	2.55	0.40
1:A:794:ILE:O	1:A:1158:LYS:N	2.46	0.40
1:B:1097:LEU:HA	1:B:1100:ILE:HG12	2.03	0.40
1:C:103:PHE:HB2	1:C:261:LEU:HD11	2.04	0.40
1:C:803:GLN:HG2	1:C:1149:HIS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:SER:HB2	1:C:906:PHE:HB3	2.03	0.40
1:C:956:GLU:HA	1:C:959:ILE:HG12	2.04	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	A	1178/1326 (89%)	1093 (93%)	84 (7%)	1 (0%)	51 85
1	B	1181/1326 (89%)	1098 (93%)	81 (7%)	2 (0%)	47 81
1	C	1181/1326 (89%)	1111 (94%)	68 (6%)	2 (0%)	47 81
All	All	3540/3978 (89%)	3302 (93%)	233 (7%)	5 (0%)	54 85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	ILE
1	A	166	ILE
1	B	166	ILE
1	B	184	LEU
1	C	245	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1063/1190 (89%)	1060 (100%)	3 (0%)	92 95
1	B	1066/1190 (90%)	1065 (100%)	1 (0%)	93 97
1	C	1066/1190 (90%)	1065 (100%)	1 (0%)	93 97
All	All	3195/3570 (90%)	3190 (100%)	5 (0%)	93 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	654	ASN
1	A	767	ARG
1	A	1068	ARG
1	B	1158	LYS
1	C	319	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	ASN
1	B	1050	GLN
1	C	1038	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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	$\#\|Z\|>2$
2	NAG	D	1	2,1	14,14,15	0.26	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	0.44	0
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	F	1	2,1	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
2	NAG	F	2	2	14,14,15	0.34	0	17,19,21	0.61	0
2	NAG	G	1	2,1	14,14,15	0.36	0	17,19,21	0.65	1 (5%)
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.54	0
3	SIA	H	1	3	21,21,21	1.54	2 (9%)	25,31,31	1.91	4 (16%)
3	5N6	H	2	3	23,23,24	2.60	6 (26%)	28,32,35	1.46	3 (10%)
3	SIA	I	1	3	21,21,21	1.55	2 (9%)	25,31,31	1.85	2 (8%)
3	5N6	I	2	3	23,23,24	2.36	5 (21%)	28,32,35	1.39	4 (14%)
3	SIA	J	1	3	21,21,21	1.54	2 (9%)	25,31,31	1.84	1 (4%)
3	5N6	J	2	3	23,23,24	2.36	6 (26%)	28,32,35	1.43	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	SIA	H	1	3	-	12/20/38/38	0/1/1/1
3	5N6	H	2	3	-	8/21/37/41	0/1/1/1
3	SIA	I	1	3	-	9/20/38/38	0/1/1/1
3	5N6	I	2	3	-	8/21/37/41	0/1/1/1
3	SIA	J	1	3	-	13/20/38/38	0/1/1/1
3	5N6	J	2	3	-	6/21/37/41	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	5N6	C2-C1	9.17	1.60	1.52
3	I	2	5N6	C2-C1	7.95	1.59	1.52
3	J	2	5N6	C2-C1	7.79	1.59	1.52
3	I	1	SIA	O6-C2	4.71	1.48	1.43
3	J	1	SIA	O6-C2	4.66	1.47	1.43
3	H	1	SIA	O6-C2	4.55	1.47	1.43
3	H	2	5N6	C4-C5	3.97	1.56	1.53
3	H	2	5N6	C9-C8	3.56	1.56	1.51
3	J	2	5N6	C9-C8	3.53	1.56	1.51
3	I	2	5N6	C4-C5	3.50	1.56	1.53
3	H	1	SIA	C2-C1	3.35	1.58	1.53
3	J	2	5N6	C7-C6	3.25	1.57	1.53
3	I	1	SIA	C2-C1	3.24	1.58	1.53
3	J	1	SIA	C2-C1	3.23	1.58	1.53
3	I	2	5N6	C9-C8	3.20	1.56	1.51
3	J	2	5N6	C4-C5	3.15	1.55	1.53
3	H	2	5N6	C7-C6	3.08	1.56	1.53
3	I	2	5N6	C7-C6	3.03	1.56	1.53
3	H	2	5N6	C6-C5	2.55	1.57	1.53
3	H	2	5N6	C8-C7	2.54	1.58	1.53
3	J	2	5N6	C8-C7	2.48	1.58	1.53
3	I	2	5N6	C8-C7	2.47	1.58	1.53
3	J	2	5N6	C6-C5	2.13	1.56	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	SIA	O1A-C1-C2	-7.51	112.21	123.59
3	J	1	SIA	O1A-C1-C2	-7.47	112.28	123.59
3	H	1	SIA	O1A-C1-C2	-7.21	112.67	123.59
3	H	2	5N6	C6-O6-C2	4.08	120.07	111.34
3	J	2	5N6	C6-O6-C2	3.70	119.25	111.34
3	I	2	5N6	C6-O6-C2	3.59	119.03	111.34
2	F	1	NAG	C2-N2-C7	3.07	127.27	122.90
3	J	2	5N6	O1A-C1-C2	-2.87	115.79	122.57
3	I	2	5N6	O1A-C1-C2	-2.84	115.86	122.57
3	H	2	5N6	O1A-C1-C2	-2.83	115.89	122.57
3	H	2	5N6	O6-C2-C1	2.66	112.92	107.70
3	J	2	5N6	C3-C4-C5	-2.57	108.36	111.46
3	I	2	5N6	C3-C4-C5	-2.32	108.66	111.46
2	G	1	NAG	C1-O5-C5	2.25	115.25	112.19
3	J	2	5N6	O6-C2-C1	2.17	111.95	107.70
3	I	2	5N6	O6-C2-C1	2.14	111.90	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	SIA	O6-C6-C5	2.10	111.83	109.78
3	H	1	SIA	O2-C2-C1	-2.06	106.58	110.76
3	H	1	SIA	C8-C7-C6	-2.05	109.14	113.03
3	I	1	SIA	O6-C6-C7	-2.04	104.15	107.29

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	SIA	C5-C6-C7-C8
3	H	1	SIA	C5-C6-C7-O7
3	H	1	SIA	O6-C6-C7-C8
3	H	1	SIA	O6-C6-C7-O7
3	H	1	SIA	C6-C7-C8-C9
3	H	1	SIA	C6-C7-C8-O8
3	H	1	SIA	O7-C7-C8-C9
3	H	1	SIA	O7-C7-C8-O8
3	H	1	SIA	C7-C8-C9-O9
3	H	1	SIA	O8-C8-C9-O9
3	H	2	5N6	C7-C8-C9-O9
3	H	2	5N6	O8-C8-C9-O9
3	H	2	5N6	C6-C7-C8-O8
3	H	2	5N6	O7-C7-C8-O8
3	I	1	SIA	O1A-C1-C2-C3
3	I	1	SIA	C6-C7-C8-C9
3	I	1	SIA	C6-C7-C8-O8
3	I	1	SIA	O7-C7-C8-C9
3	I	1	SIA	O7-C7-C8-O8
3	I	2	5N6	C7-C8-C9-O9
3	I	2	5N6	O8-C8-C9-O9
3	I	2	5N6	C6-C7-C8-C9
3	I	2	5N6	O7-C7-C8-C9
3	I	2	5N6	C6-C7-C8-O8
3	I	2	5N6	O7-C7-C8-O8
3	J	1	SIA	O1B-C1-C2-O6
3	J	1	SIA	C5-C6-C7-O7
3	J	1	SIA	O6-C6-C7-C8
3	J	1	SIA	O6-C6-C7-O7
3	J	1	SIA	C6-C7-C8-O8
3	J	1	SIA	O7-C7-C8-C9
3	J	1	SIA	O7-C7-C8-O8
3	J	2	5N6	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
3	J	2	5N6	O7-C7-C8-O8
2	G	1	NAG	O5-C5-C6-O6
3	I	2	5N6	OBJ-CAG-O9-C9
3	H	2	5N6	OBJ-CAG-O9-C9
3	J	2	5N6	OBJ-CAG-O9-C9
2	G	2	NAG	O5-C5-C6-O6
3	I	2	5N6	CAF-CAG-O9-C9
3	J	2	5N6	CAF-CAG-O9-C9
2	E	2	NAG	C4-C5-C6-O6
3	H	2	5N6	CAF-CAG-O9-C9
2	G	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	H	2	5N6	O7-C7-C8-C9
3	J	2	5N6	O7-C7-C8-C9
3	H	2	5N6	C6-C7-C8-C9
3	J	1	SIA	C6-C7-C8-C9
3	J	2	5N6	C6-C7-C8-C9
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	H	1	SIA	C11-C10-N5-C5
3	H	1	SIA	O10-C10-N5-C5
3	I	1	SIA	C11-C10-N5-C5
3	I	1	SIA	O10-C10-N5-C5
3	J	1	SIA	C11-C10-N5-C5
3	J	1	SIA	O10-C10-N5-C5
2	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	J	1	SIA	C5-C6-C7-C8
3	J	1	SIA	O1A-C1-C2-C3
3	I	1	SIA	O1A-C1-C2-O6
3	I	1	SIA	O1A-C1-C2-O2
3	J	1	SIA	O1A-C1-C2-O2
2	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	SIA	1	0

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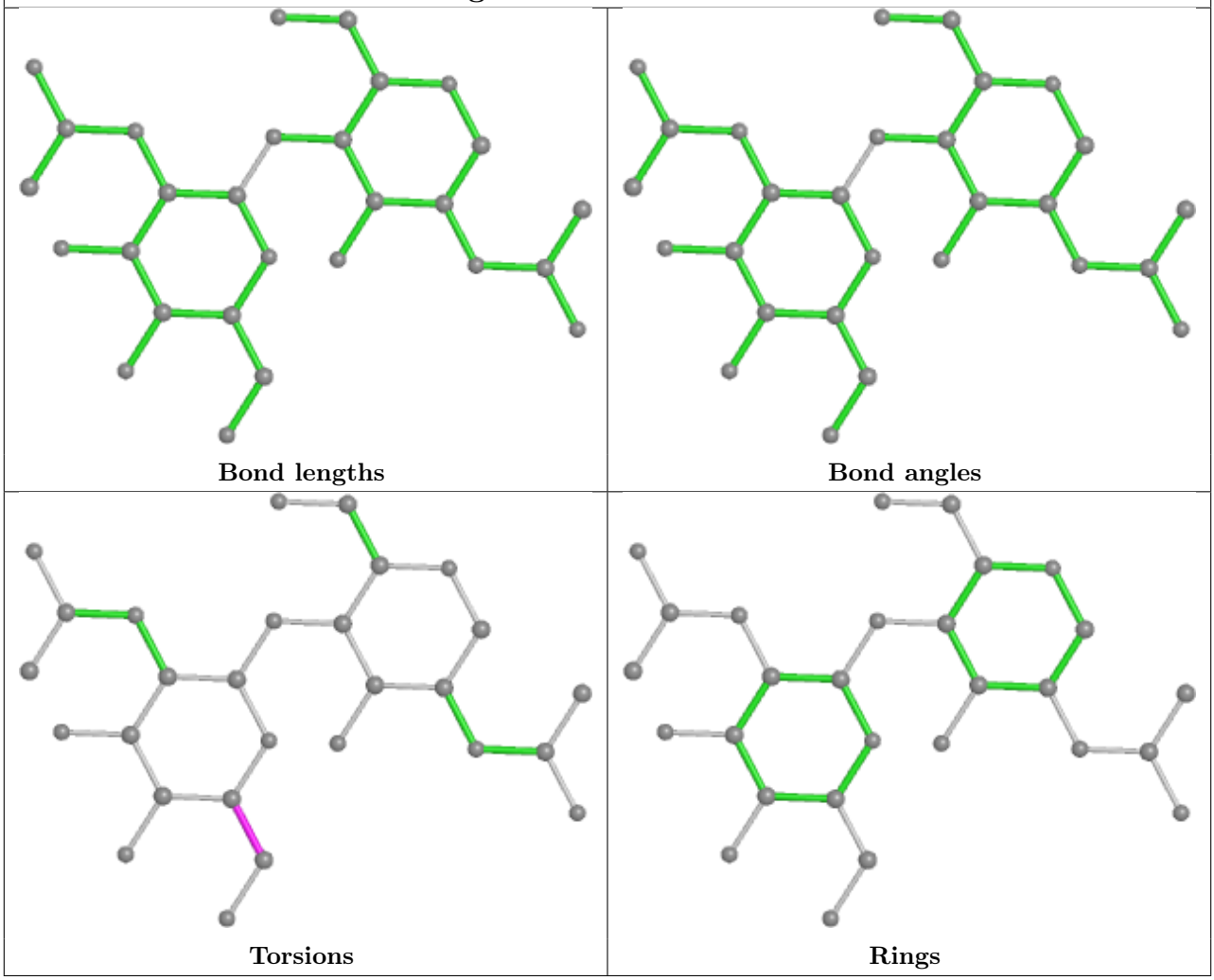
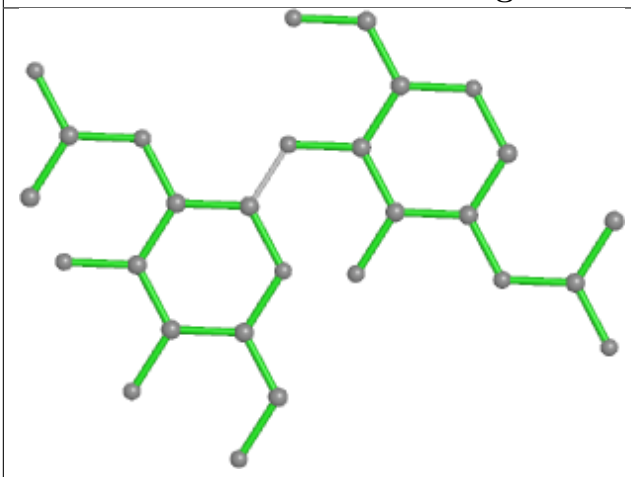
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	5N6	1	0
3	J	1	SIA	2	0
3	J	2	5N6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

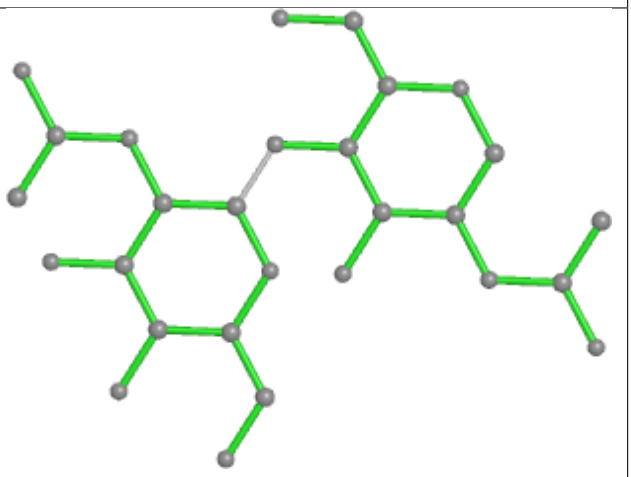
Oligosaccharide Chain D



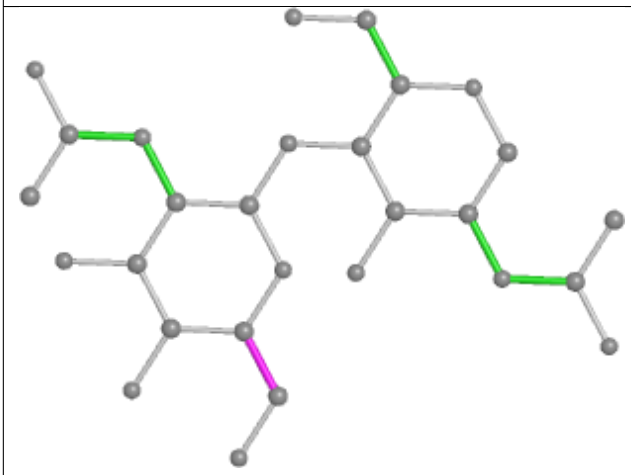
Oligosaccharide Chain E



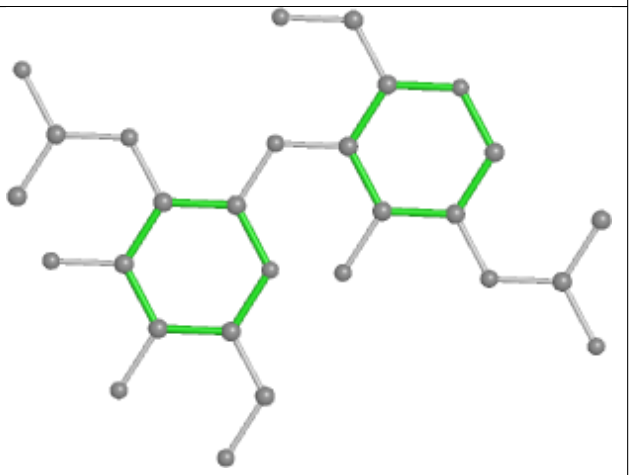
Bond lengths



Bond angles

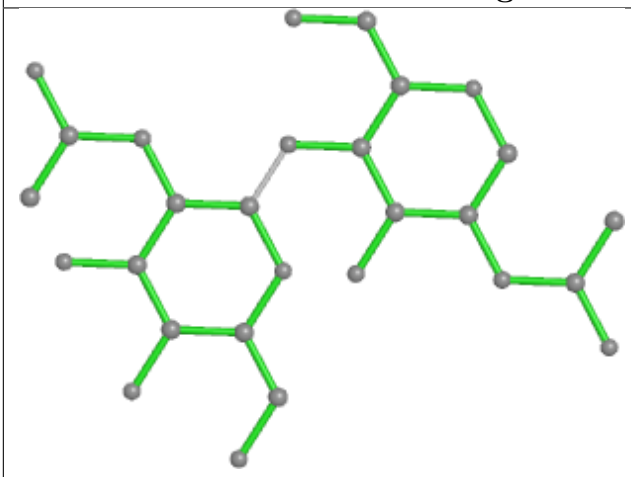


Torsions

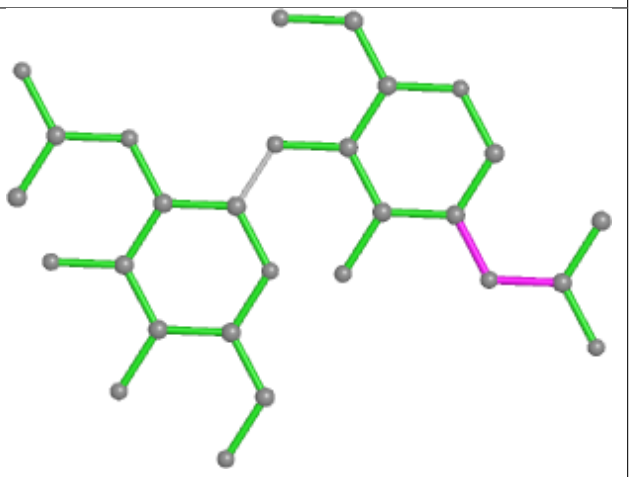


Rings

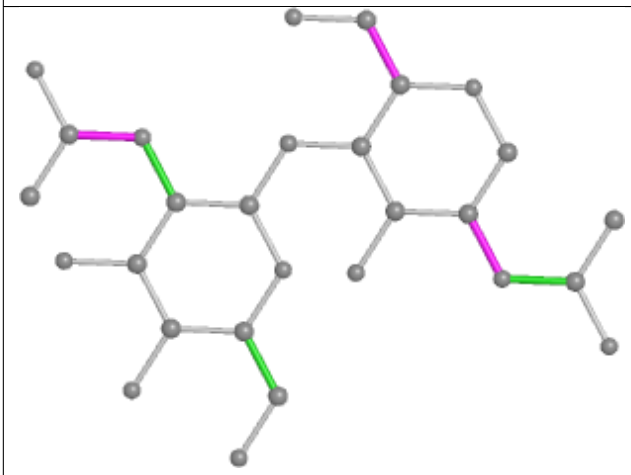
Oligosaccharide Chain F



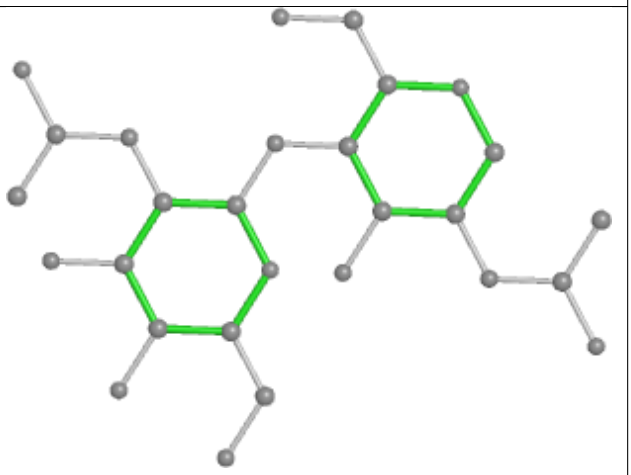
Bond lengths



Bond angles

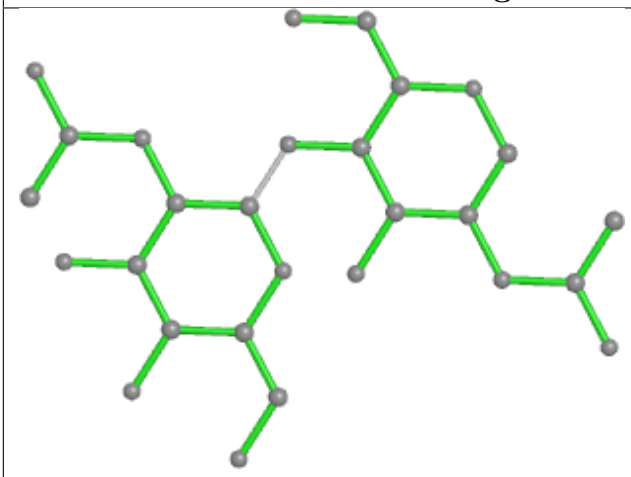


Torsions

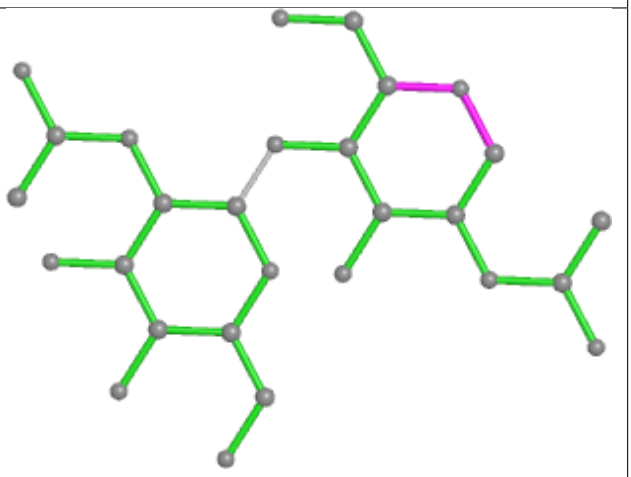


Rings

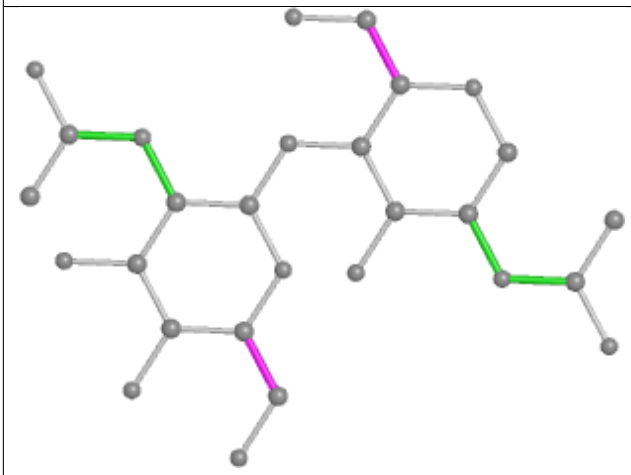
Oligosaccharide Chain G



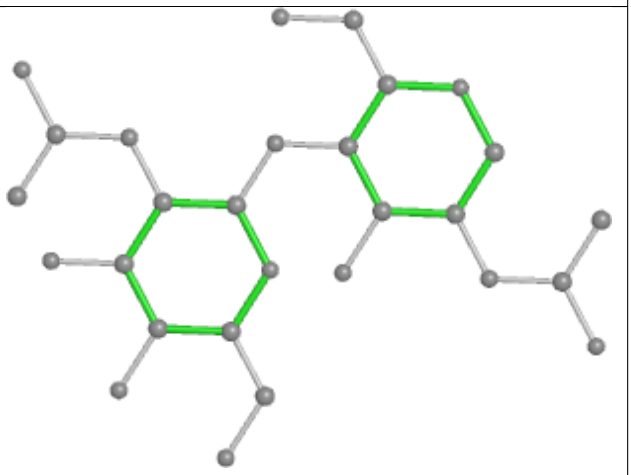
Bond lengths



Bond angles

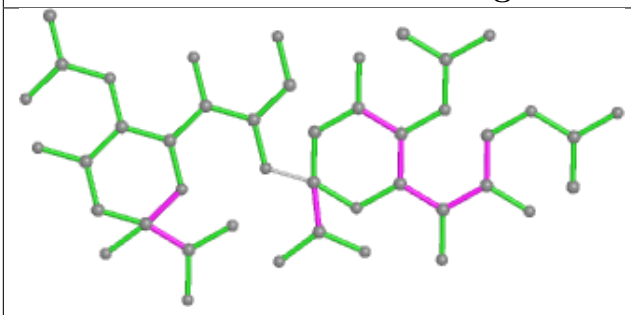


Torsions

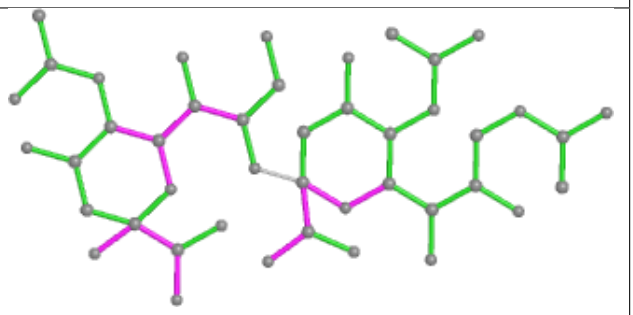


Rings

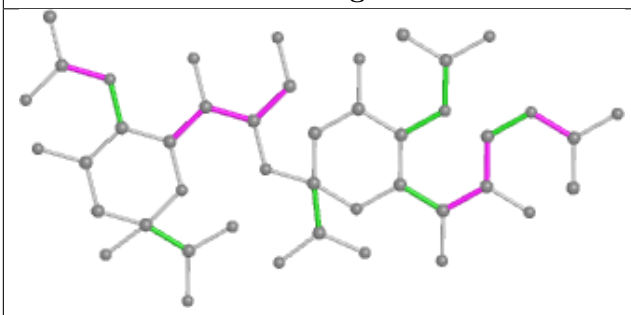
Oligosaccharide Chain H



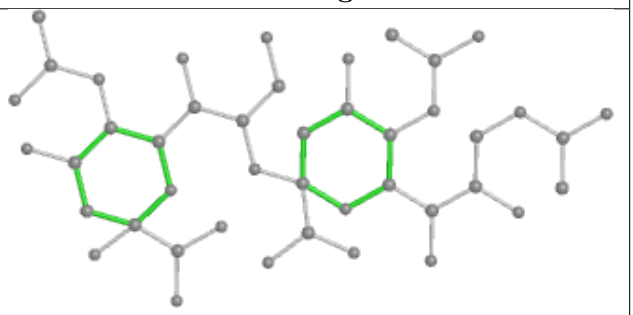
Bond lengths



Bond angles

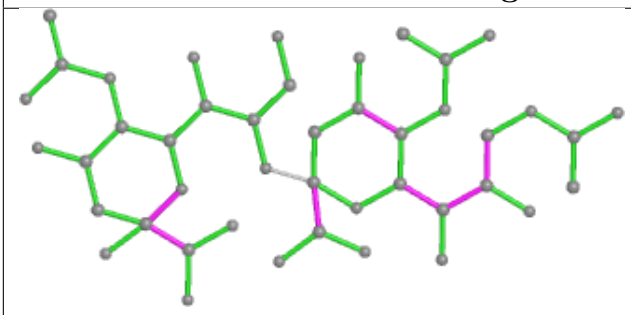


Torsions

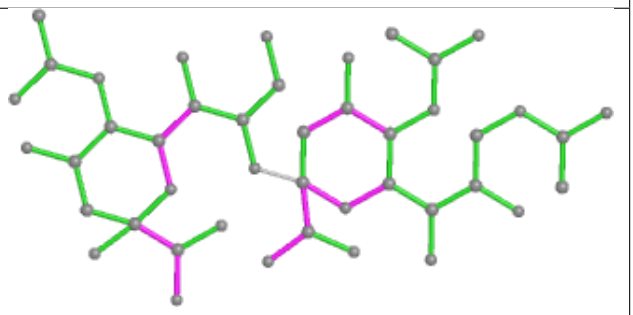


Rings

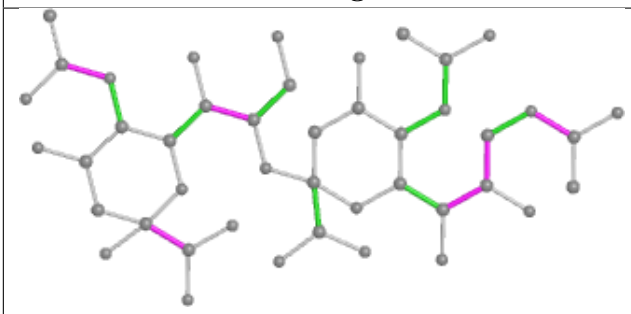
Oligosaccharide Chain I



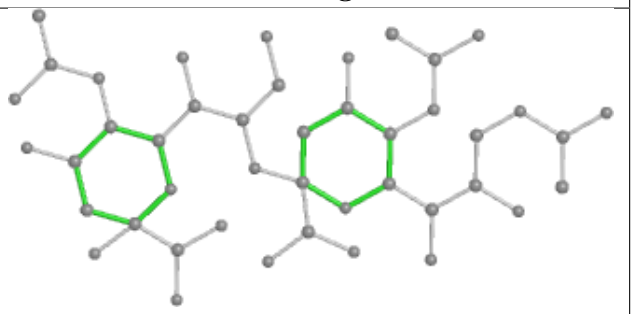
Bond lengths



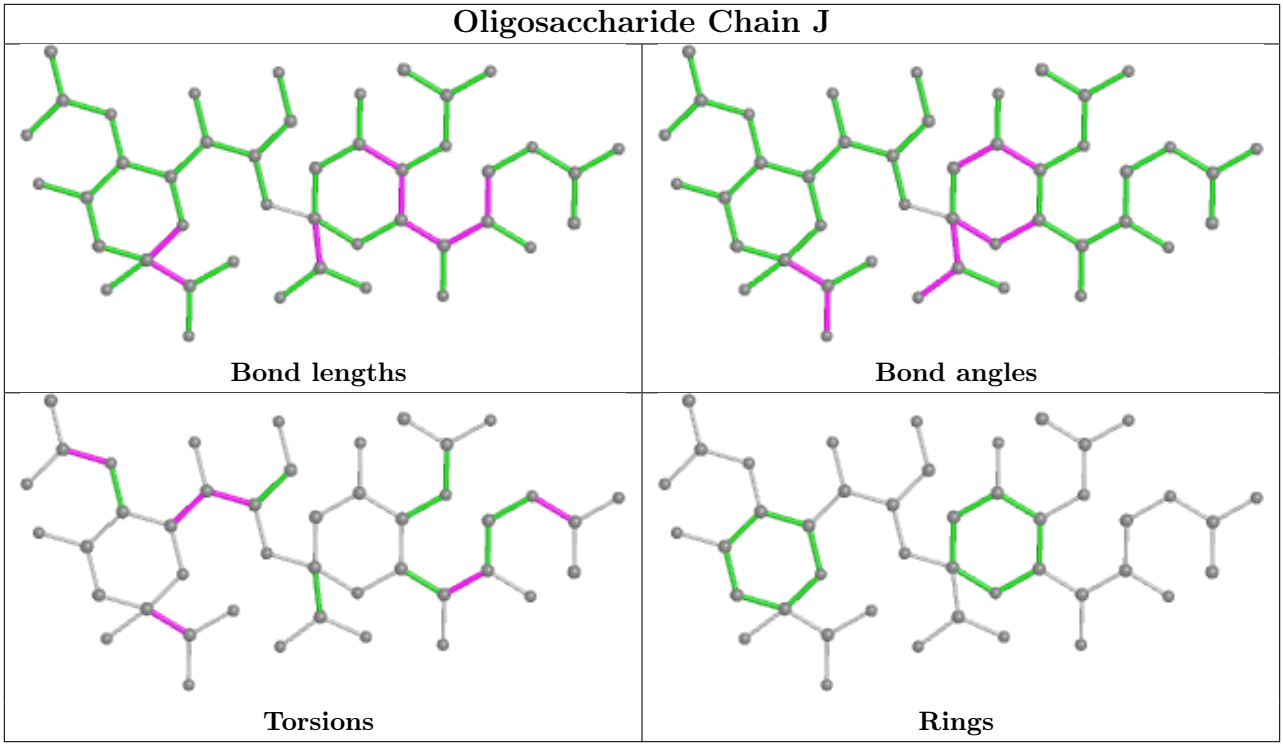
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1407	1	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
4	NAG	C	1405	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
4	NAG	B	1409	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	A	1402	1	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
4	NAG	B	1410	1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
4	NAG	C	1404	1	14,14,15	0.36	0	17,19,21	0.58	0
4	NAG	C	1402	1	14,14,15	0.34	0	17,19,21	0.56	0
4	NAG	A	1403	1	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	C	1407	1	14,14,15	0.37	0	17,19,21	0.44	0
4	NAG	C	1406	1	14,14,15	0.41	0	17,19,21	0.44	0
4	NAG	B	1411	1	14,14,15	0.34	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1403	1	14,14,15	0.38	0	17,19,21	0.58	1 (5%)
4	NAG	A	1401	1	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
4	NAG	B	1408	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	A	1404	1	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
4	NAG	B	1405	1	14,14,15	0.53	0	17,19,21	1.02	2 (11%)
4	NAG	A	1405	1	14,14,15	0.39	0	17,19,21	0.53	0
4	NAG	B	1402	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	1404	1	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	C	1401	1	14,14,15	0.53	0	17,19,21	0.49	0
4	NAG	B	1412	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	B	1403	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	1406	1	14,14,15	0.48	0	17,19,21	0.97	1 (5%)
4	NAG	A	1407	1	14,14,15	0.35	0	17,19,21	0.54	0
4	NAG	B	1406	1	14,14,15	0.40	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	B	1407	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1412	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1401	NAG	C2-N2-C7	3.05	127.24	122.90
4	C	1405	NAG	C2-N2-C7	3.02	127.21	122.90
4	A	1406	NAG	C2-N2-C7	3.02	127.21	122.90
4	A	1402	NAG	C2-N2-C7	3.01	127.19	122.90
4	A	1404	NAG	C2-N2-C7	2.99	127.16	122.90
4	B	1405	NAG	C2-N2-C7	2.98	127.14	122.90
4	B	1410	NAG	C1-O5-C5	2.22	115.20	112.19
4	C	1403	NAG	C1-O5-C5	2.06	114.98	112.19
4	B	1405	NAG	C1-O5-C5	2.01	114.92	112.19
4	B	1407	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1405	NAG	O5-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1407	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	B	1409	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1407	NAG	C4-C5-C6-O6
4	B	1410	NAG	O5-C5-C6-O6
4	A	1403	NAG	C8-C7-N2-C2
4	A	1403	NAG	O7-C7-N2-C2
4	B	1401	NAG	C8-C7-N2-C2
4	B	1401	NAG	O7-C7-N2-C2
4	B	1407	NAG	C8-C7-N2-C2
4	B	1407	NAG	O7-C7-N2-C2
4	C	1404	NAG	C8-C7-N2-C2
4	C	1404	NAG	O7-C7-N2-C2
4	A	1403	NAG	C4-C5-C6-O6
4	B	1410	NAG	C4-C5-C6-O6
4	B	1409	NAG	C4-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	B	1407	NAG	O5-C5-C6-O6
4	C	1407	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	B	1412	NAG	C4-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	B	1412	NAG	O5-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	A	1401	NAG	C3-C2-N2-C7
4	A	1402	NAG	C3-C2-N2-C7
4	A	1404	NAG	C3-C2-N2-C7
4	A	1406	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1402	NAG	1	0
4	B	1412	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.

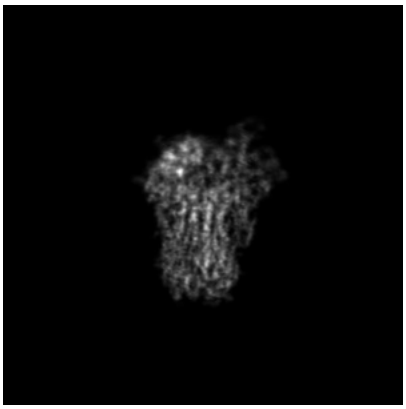
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17077. These allow visual inspection of the internal detail of the map and identification of artifacts.

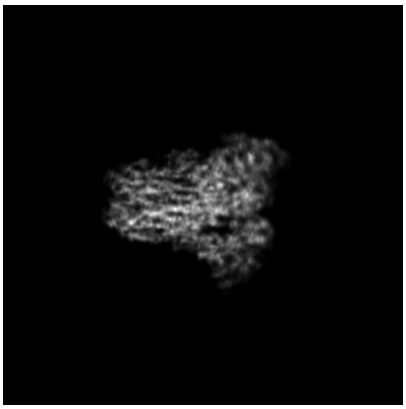
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

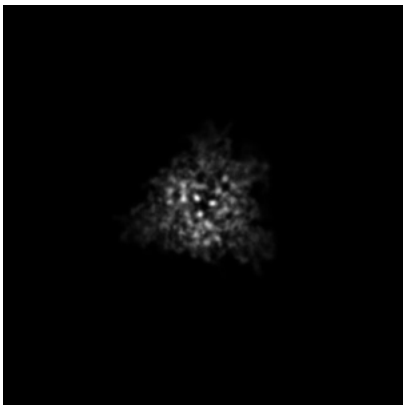
6.1.1 Primary map



X

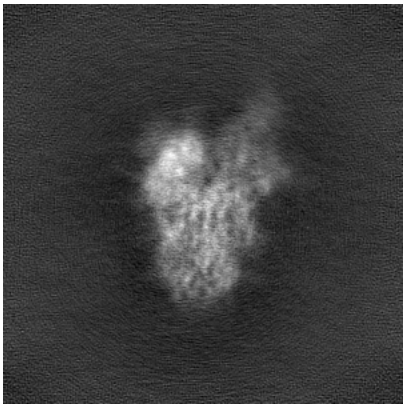


Y

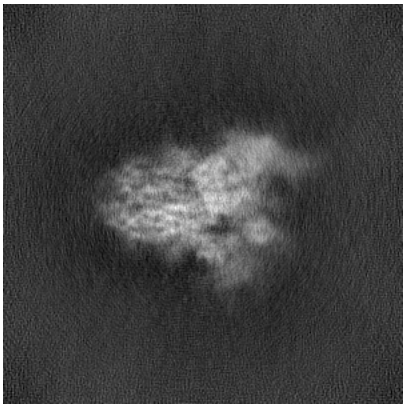


Z

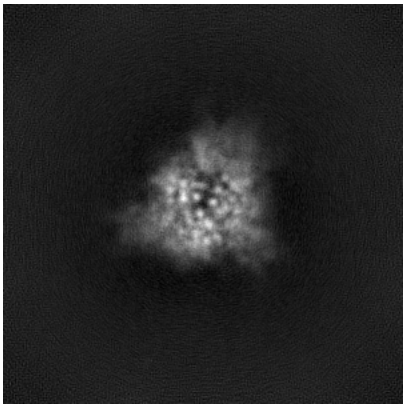
6.1.2 Raw map



X



Y



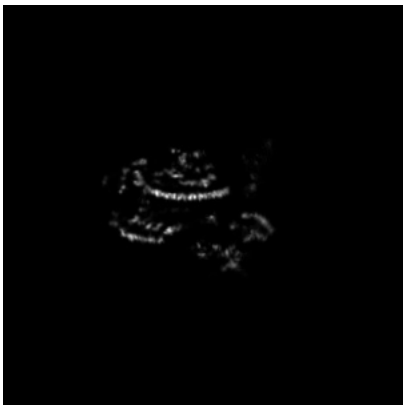
Z

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

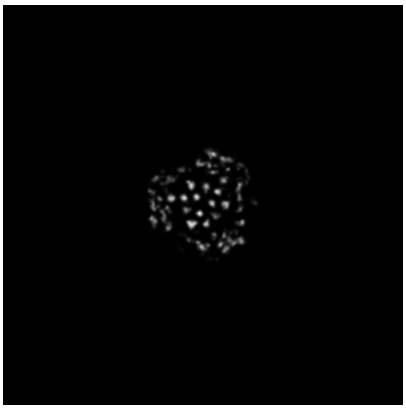
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150

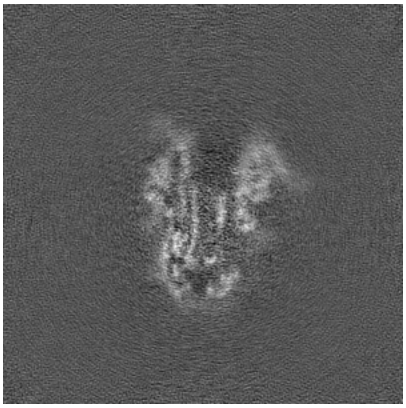


Y Index: 150

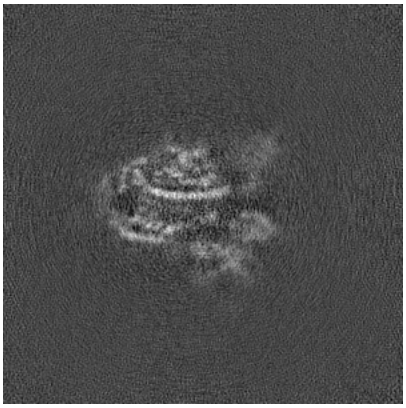


Z Index: 150

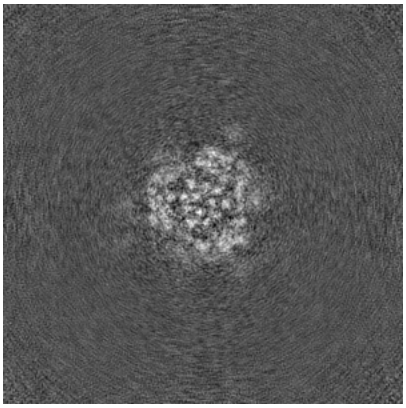
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

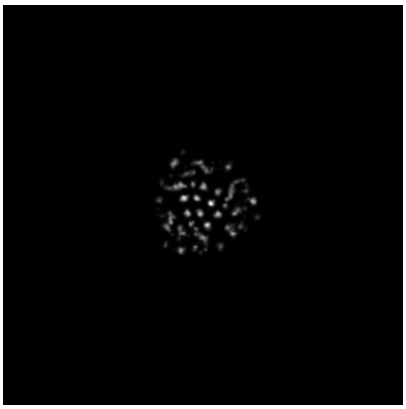
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

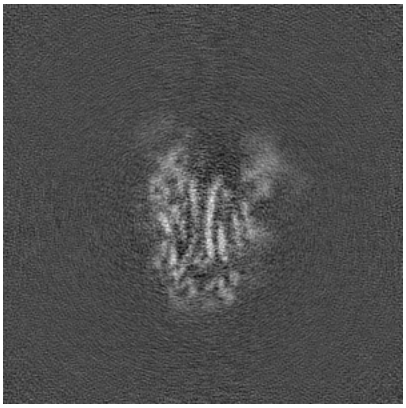
X Index: 145

Y Index: 154

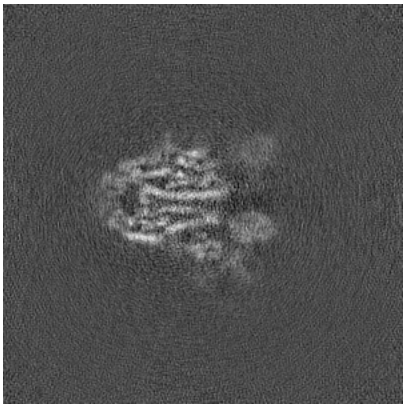


Z Index: 143

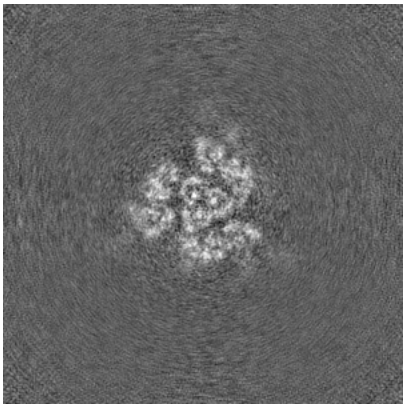
6.3.2 Raw map



X Index: 145



Y Index: 152

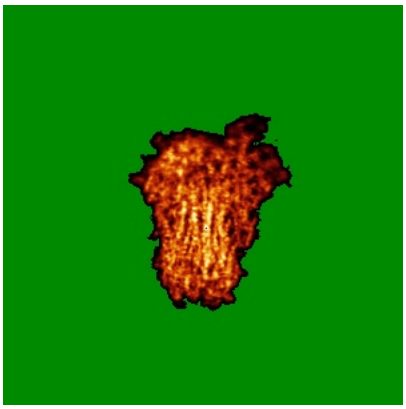


Z Index: 156

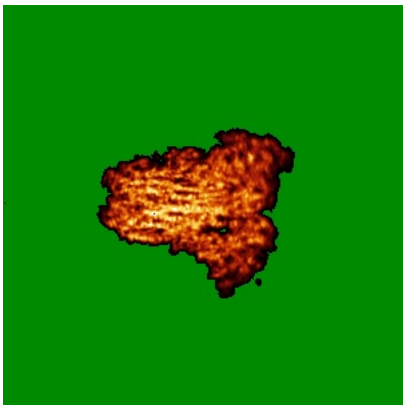
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

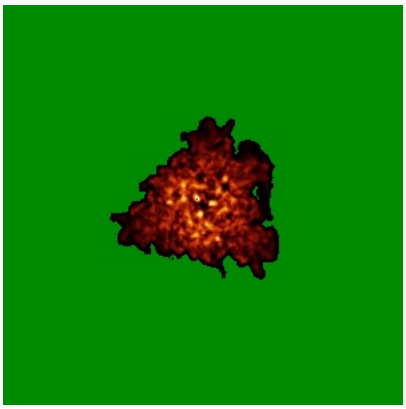
6.4.1 Primary map



X

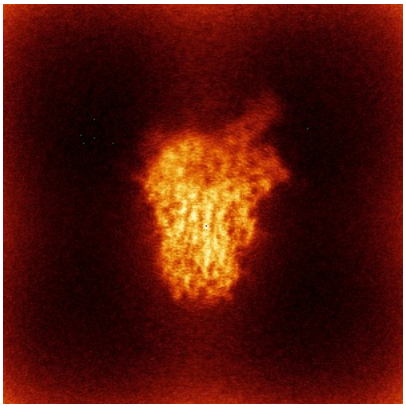


Y

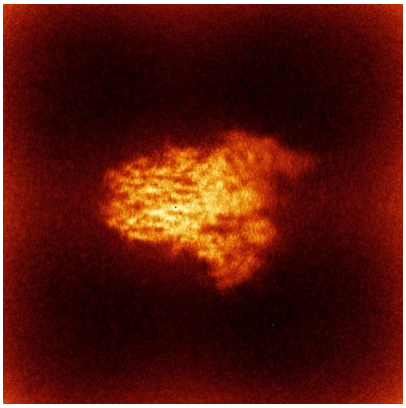


Z

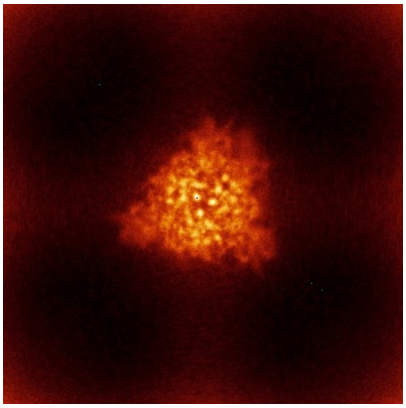
6.4.2 Raw map



X



Y

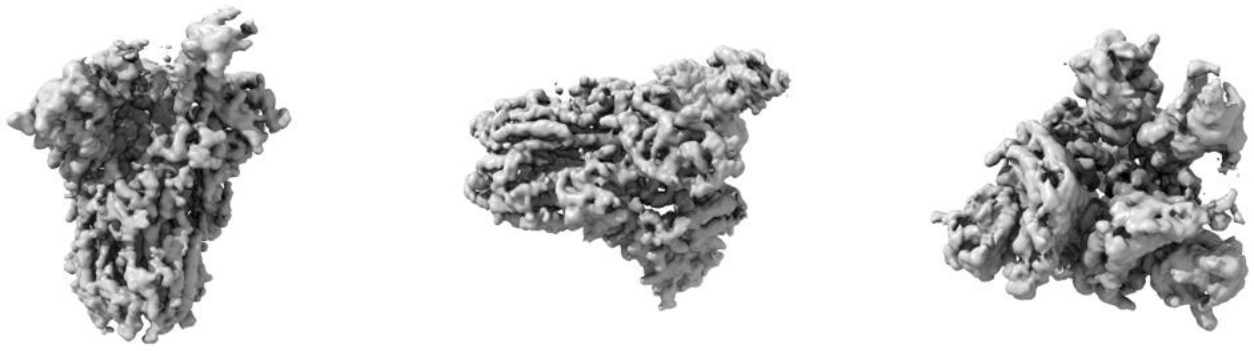


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.073. 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

X Y Z

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.

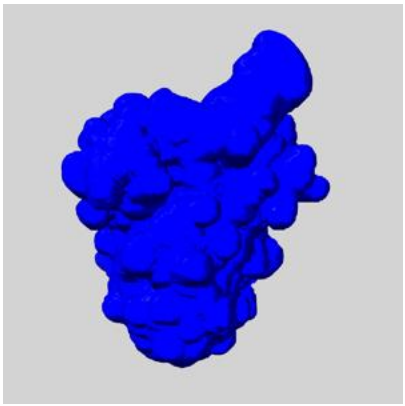
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

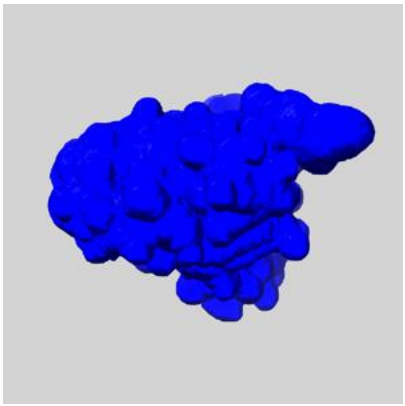
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

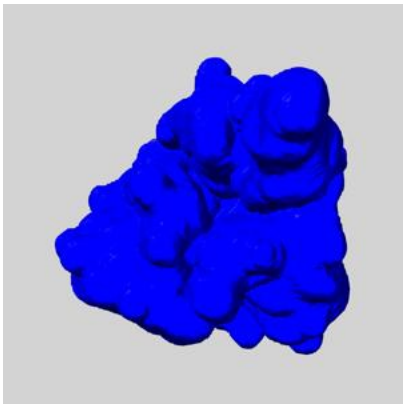
6.6.1 emd_17077_msk_1.map (i)



X



Y

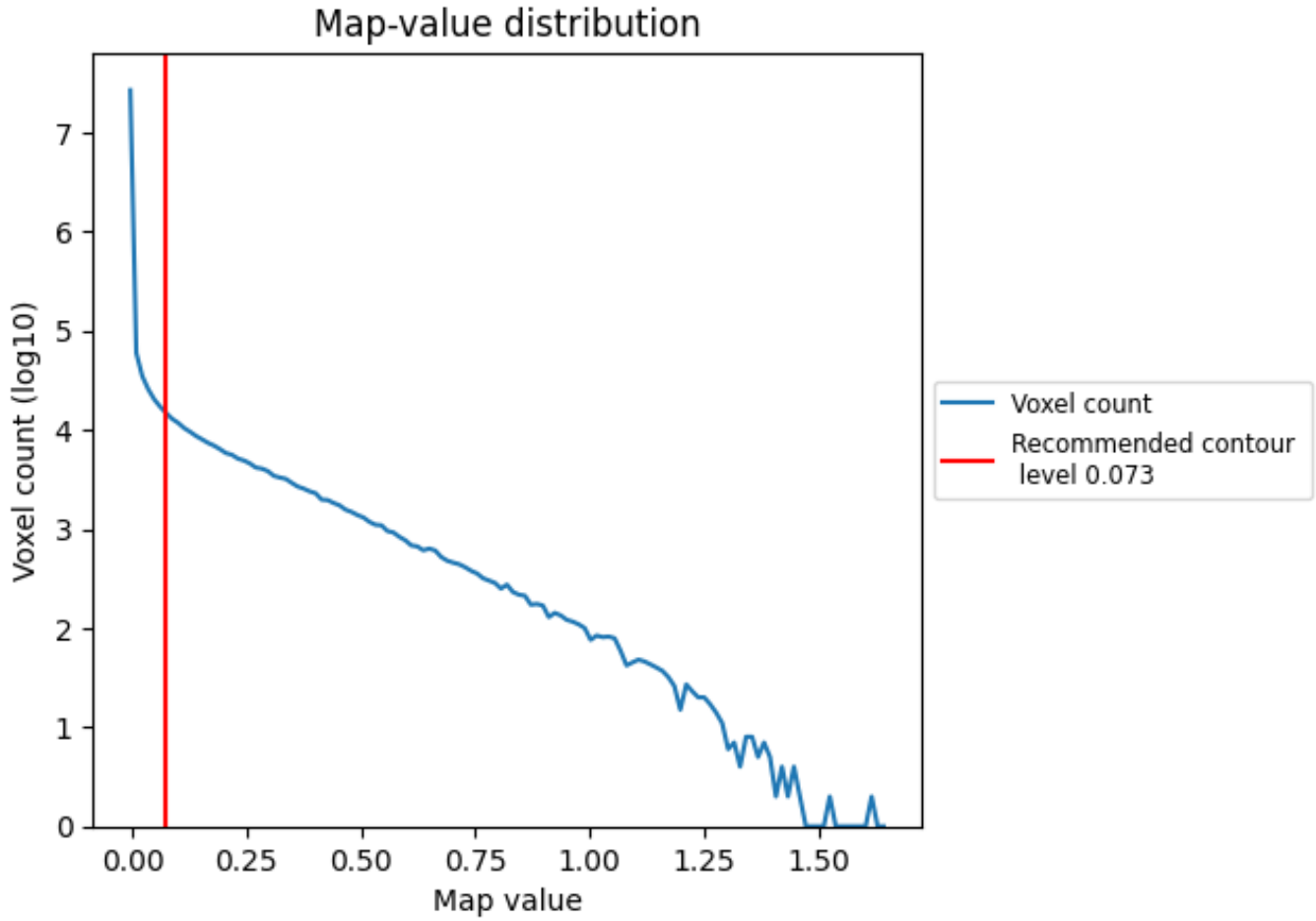


Z

7 Map analysis

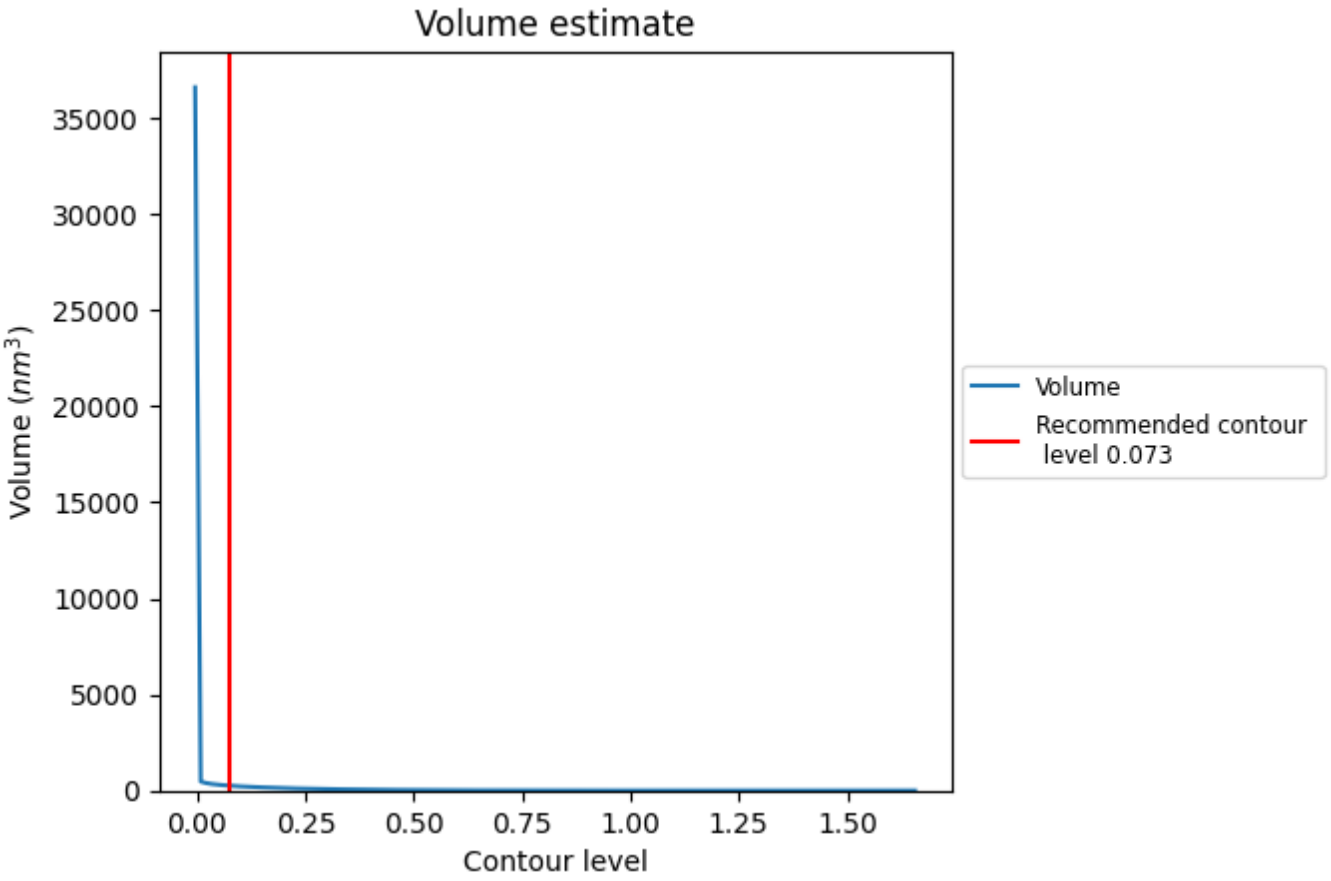
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

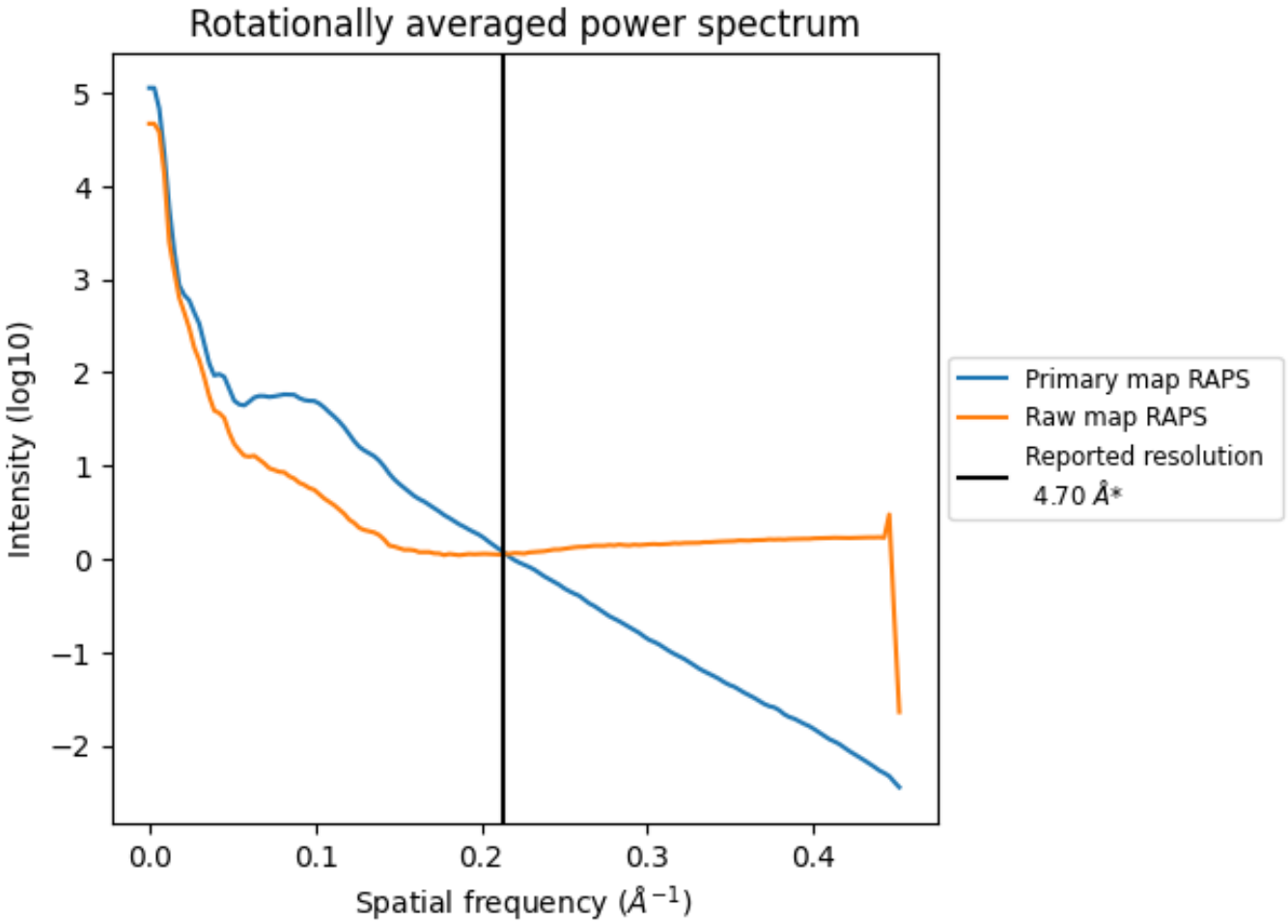
7.2 Volume estimate



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 (i)

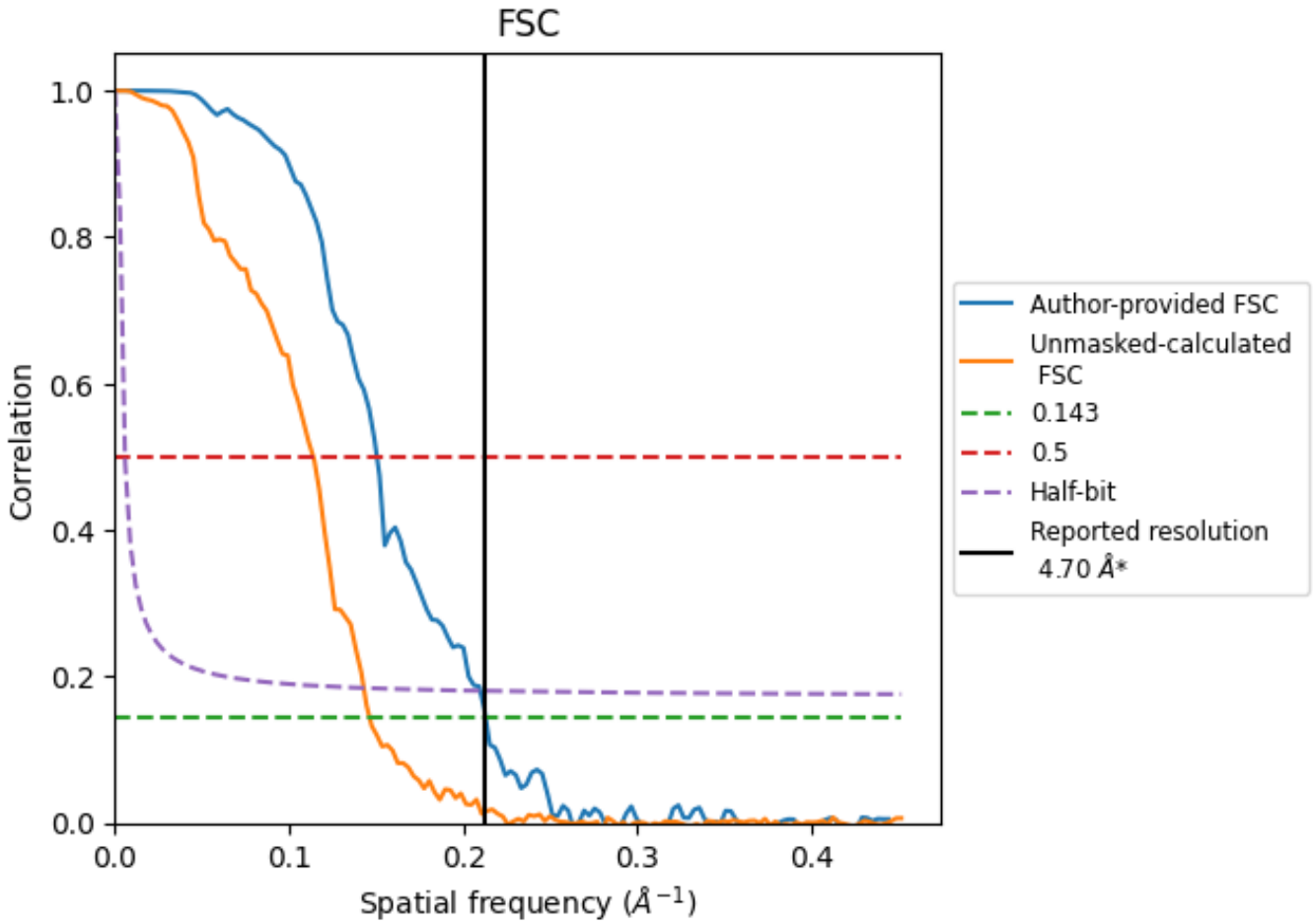


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

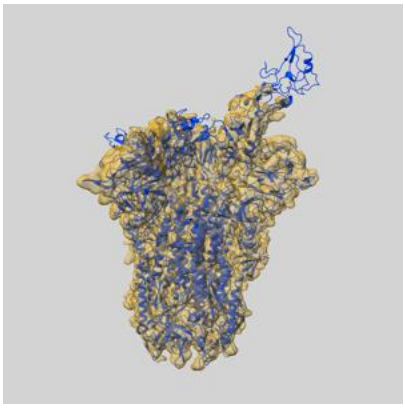
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	6.64	4.76
Unmasked-calculated*	6.83	8.77	6.99

*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 6.83 differs from the reported value 4.7 by more than 10 %

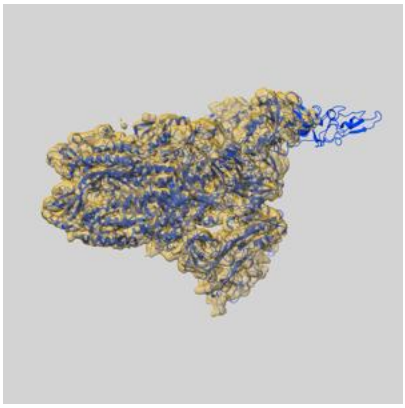
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17077 and PDB model 8OPN. Per-residue inclusion information can be found in section 3 on page 11.

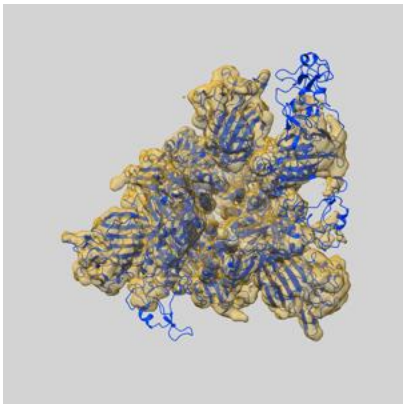
9.1 Map-model overlay



X



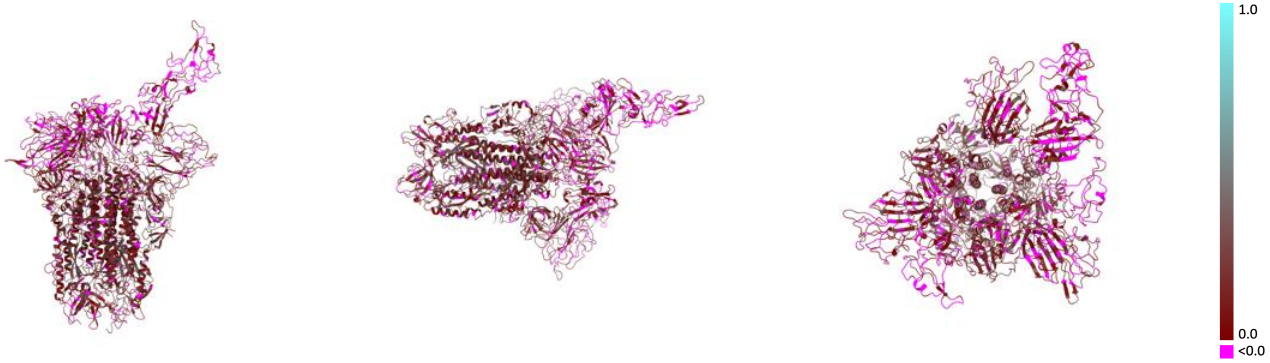
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.073 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.

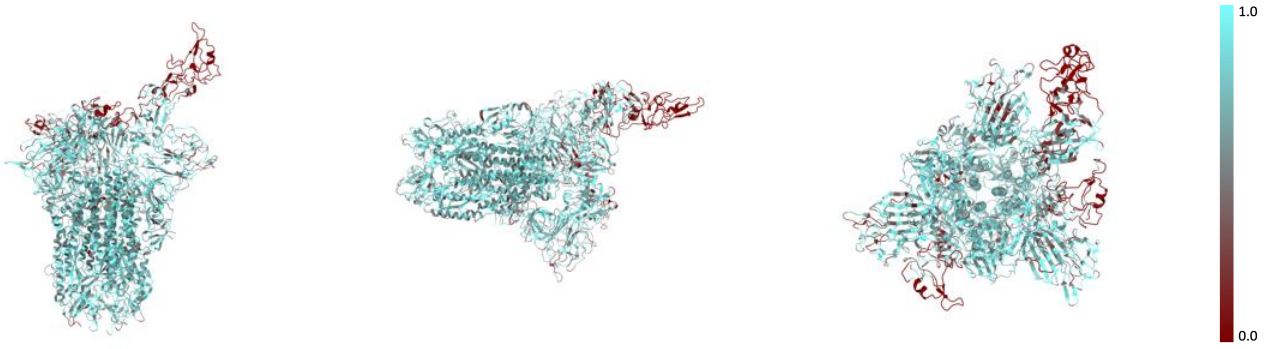
9.2 Q-score mapped to coordinate model



X Y Z

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.

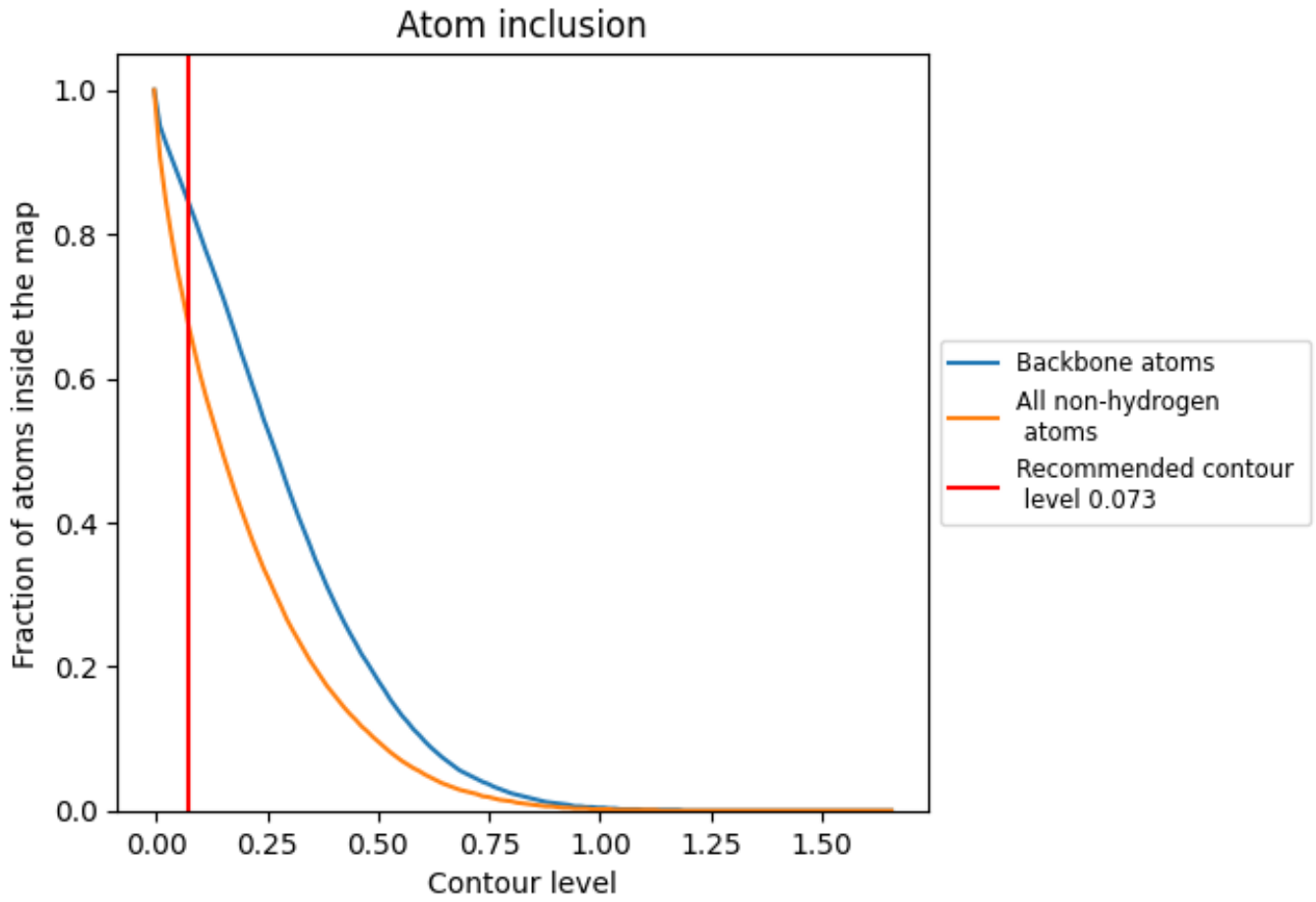
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.073).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.1330
A	0.6450	0.1240
B	0.6900	0.1450
C	0.6910	0.1300
D	0.2500	0.0590
E	0.4290	0.1400
F	0.5710	0.2010
G	0.4640	0.1100
H	0.6820	0.0860
I	0.3180	0.0150
J	0.2730	0.0590