Full wwPDB EM Validation Report ⓘ

May 13, 2024 – 02:55 pm BST

PDB ID	:	8OYU
EMDB ID	:	EMD-17296
Title	:	Stabilised BA.1 SARS-CoV-2 spike with H6 nanobodies in '2 up 1 down' RBD conformation
Authors	:	Weckener, M.; Naismith, J.H.; Owens, R.J.
Deposited on	:	2023-05-05
Resolution	:	4.00 Å(reported)
Based on initial models	:	7QO7, 8OWV

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

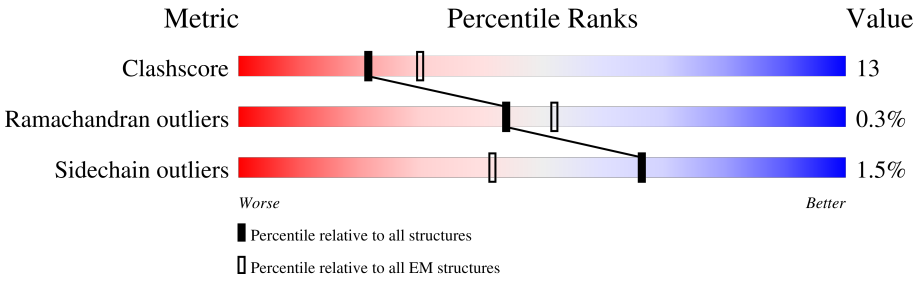
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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	1254	62% 24% • 12%
1	B	1254	61% 26% 13%
1	C	1254	• 61% 25% • 12%
2	D	126	7% 71% 29%
2	E	126	• 75% 23% •
3	F	2	100%
3	G	2	100%
3	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50%
3	J	2	100%
3	K	2	100%
3	L	2	100%
3	M	2	50% 50%
3	N	2	100%
3	O	2	50% 50%
3	P	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28223 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1098	Total	C	N	O	S	0	0
			8596	5496	1435	1626	39		
1	B	1096	Total	C	N	O	S	0	0
			8589	5492	1433	1625	39		
1	C	1098	Total	C	N	O	S	0	0
			8596	5496	1435	1626	39		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	variant	UNP P0DTC2
A	206	ILE	ASN	variant	UNP P0DTC2
A	207	VAL	LEU	variant	UNP P0DTC2
A	208	ARG	VAL	variant	UNP P0DTC2
A	209	GLU	ARG	variant	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	490	LYS	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	engineered mutation	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1229	LEU	PHE	engineered mutation	UNP P10104
A	1235	GLY	-	expression tag	UNP P10104
A	1236	ARG	-	expression tag	UNP P10104
A	1237	SER	-	expression tag	UNP P10104
A	1238	LEU	-	expression tag	UNP P10104
A	1239	GLU	-	expression tag	UNP P10104
A	1240	VAL	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	PHE	-	expression tag	UNP P10104
A	1243	GLN	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104
A	1245	PRO	-	expression tag	UNP P10104
A	1246	GLY	-	expression tag	UNP P10104
A	1247	HIS	-	expression tag	UNP P10104
A	1248	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	HIS	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	variant	UNP P0DTC2
B	206	ILE	ASN	variant	UNP P0DTC2
B	207	VAL	LEU	variant	UNP P0DTC2
B	208	ARG	VAL	variant	UNP P0DTC2
B	209	GLU	ARG	variant	UNP P0DTC2
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	LYS	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	680	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	engineered mutation	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	engineered mutation	UNP P0DTC2
B	896	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PRO	ALA	engineered mutation	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	1206	GLY	-	linker	UNP P0DTC2
B	1207	SER	-	linker	UNP P0DTC2
B	1229	LEU	PHE	engineered mutation	UNP P10104
B	1235	GLY	-	expression tag	UNP P10104
B	1236	ARG	-	expression tag	UNP P10104
B	1237	SER	-	expression tag	UNP P10104
B	1238	LEU	-	expression tag	UNP P10104
B	1239	GLU	-	expression tag	UNP P10104
B	1240	VAL	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	PHE	-	expression tag	UNP P10104
B	1243	GLN	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	PRO	-	expression tag	UNP P10104
B	1246	GLY	-	expression tag	UNP P10104
B	1247	HIS	-	expression tag	UNP P10104
B	1248	HIS	-	expression tag	UNP P10104
B	1249	HIS	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	variant	UNP P0DTC2
C	206	ILE	ASN	variant	UNP P0DTC2
C	207	VAL	LEU	variant	UNP P0DTC2
C	208	ARG	VAL	variant	UNP P0DTC2
C	209	GLU	ARG	variant	UNP P0DTC2
C	210	PRO	-	insertion	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	336	ASP	GLY	variant	UNP P0DTC2
C	368	LEU	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	490	LYS	GLN	variant	UNP P0DTC2
C	493	SER	GLY	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	544	LYS	THR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	680	SER	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	engineered mutation	UNP P0DTC2
C	853	LYS	ASN	variant	UNP P0DTC2
C	889	PRO	ALA	engineered mutation	UNP P0DTC2
C	896	PRO	ALA	engineered mutation	UNP P0DTC2
C	939	PRO	ALA	engineered mutation	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	978	PHE	LEU	variant	UNP P0DTC2
C	983	PRO	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	1206	GLY	-	linker	UNP P0DTC2
C	1207	SER	-	linker	UNP P0DTC2
C	1229	LEU	PHE	engineered mutation	UNP P10104
C	1235	GLY	-	expression tag	UNP P10104
C	1236	ARG	-	expression tag	UNP P10104
C	1237	SER	-	expression tag	UNP P10104
C	1238	LEU	-	expression tag	UNP P10104
C	1239	GLU	-	expression tag	UNP P10104
C	1240	VAL	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	PHE	-	expression tag	UNP P10104
C	1243	GLN	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	PRO	-	expression tag	UNP P10104
C	1246	GLY	-	expression tag	UNP P10104
C	1247	HIS	-	expression tag	UNP P10104
C	1248	HIS	-	expression tag	UNP P10104
C	1249	HIS	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104

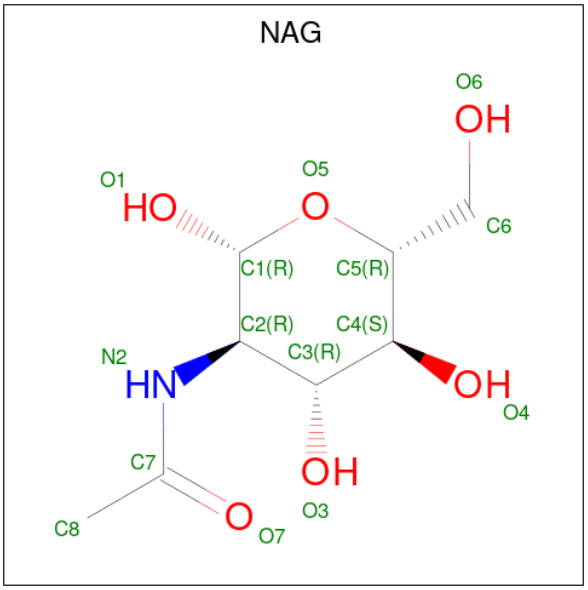
- Molecule 2 is a protein called H6 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	126	Total	C	N	O	S	2	0
			962	597	167	192	6		
2	D	126	Total	C	N	O	S	2	0
			962	597	167	192	6		

- Molecule 3 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
3	F	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0
3	H	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0
3	J	2	Total C N O 28 16 2 10	0	0
3	K	2	Total C N O 28 16 2 10	0	0
3	L	2	Total C N O 28 16 2 10	0	0
3	M	2	Total C N O 28 16 2 10	0	0
3	N	2	Total C N O 28 16 2 10	0	0
3	O	2	Total C N O 28 16 2 10	0	0
3	P	2	Total C N O 28 16 2 10	0	0

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



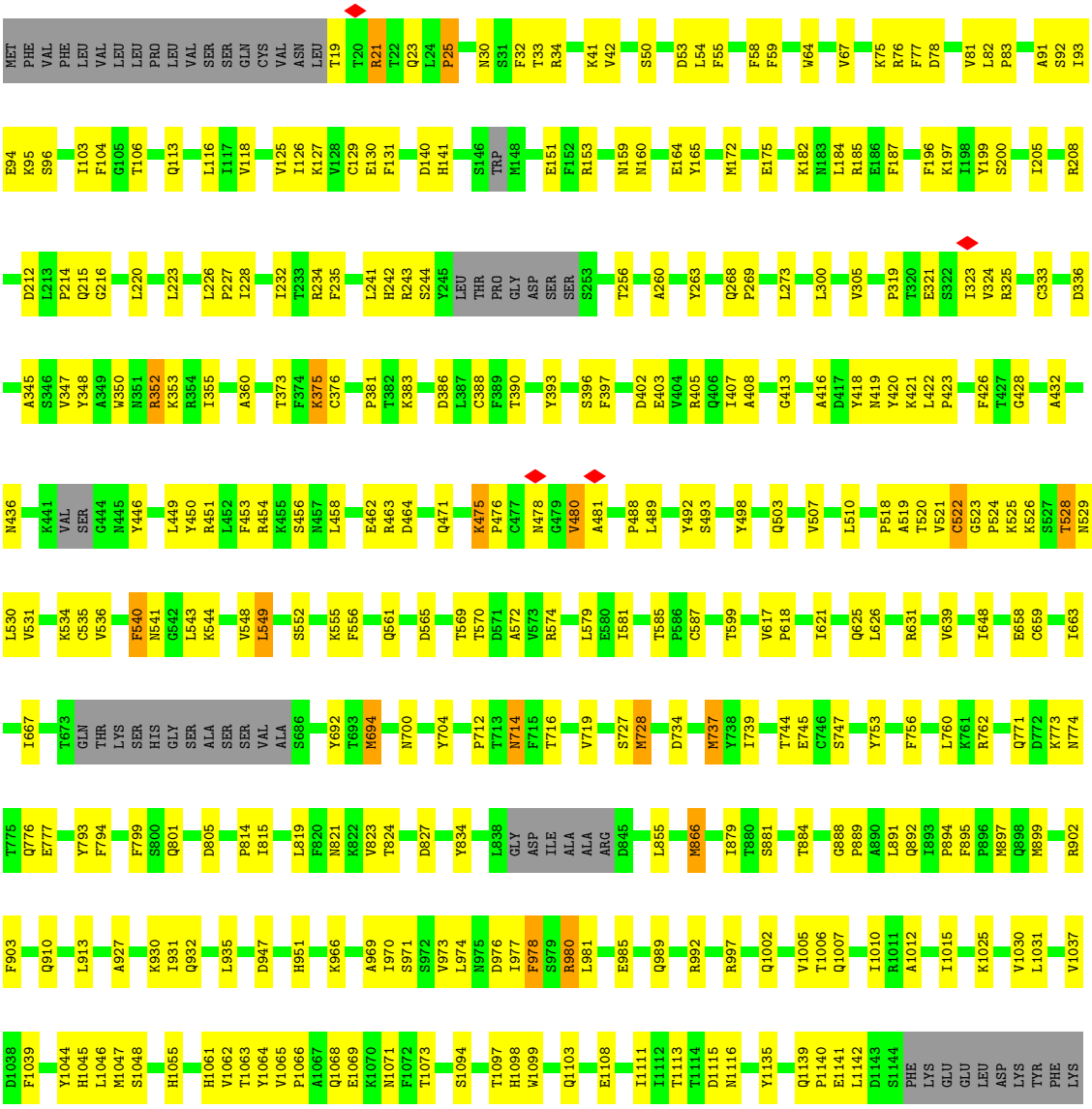
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	B	1	14	8	1	5	0
4	B	1	14	8	1	5	0
4	B	1	14	8	1	5	0
4	B	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8	1	5	0
4	C	1	14	8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

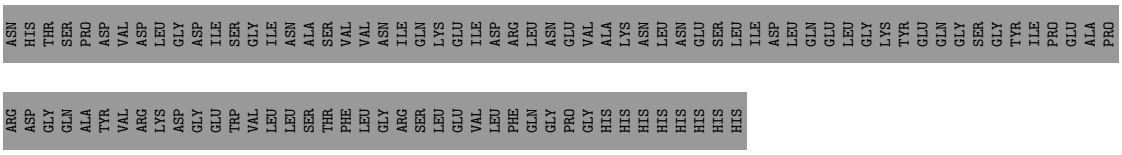
3 Residue-property plots (i)

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,Fibritin

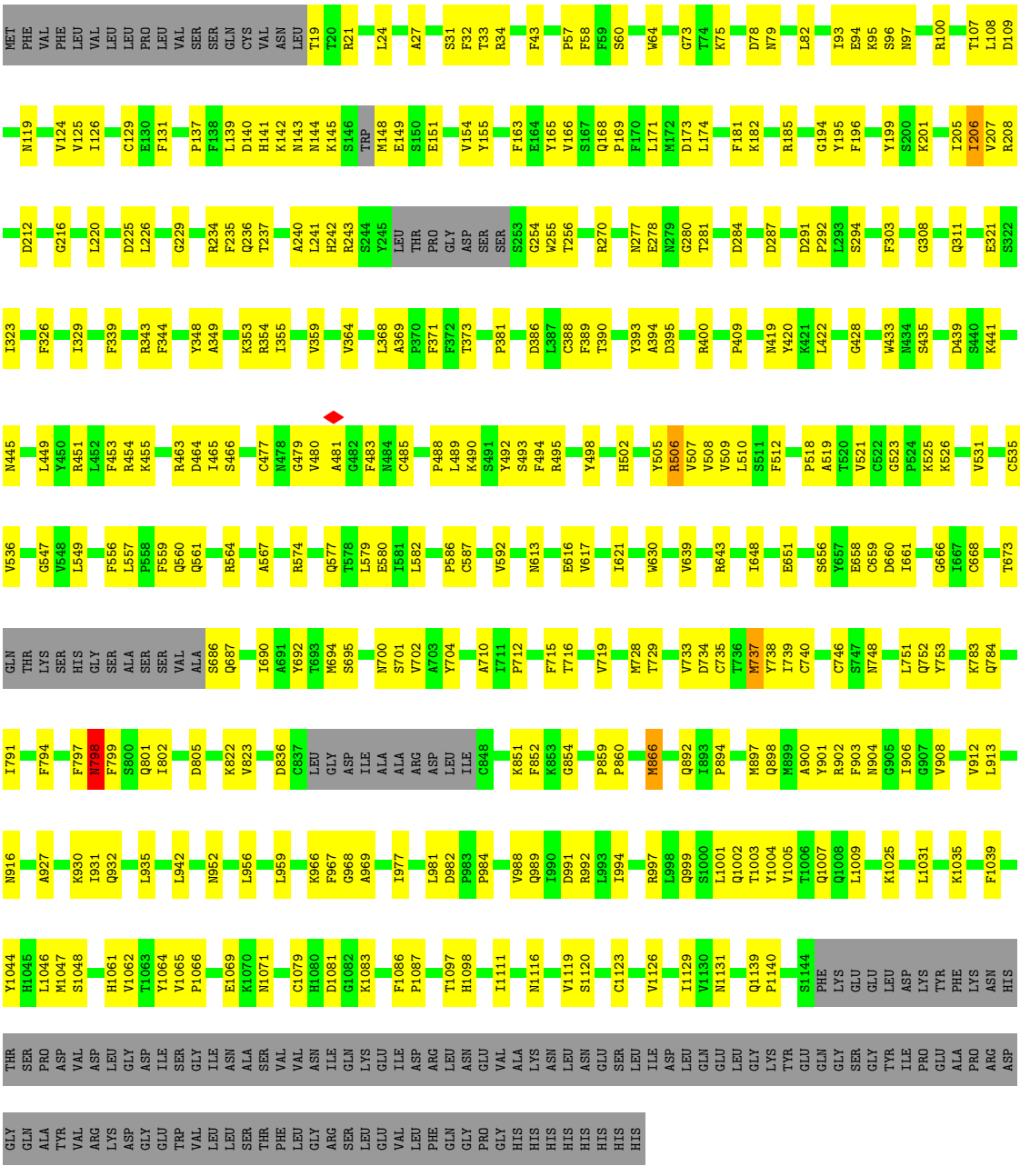
Chain A:





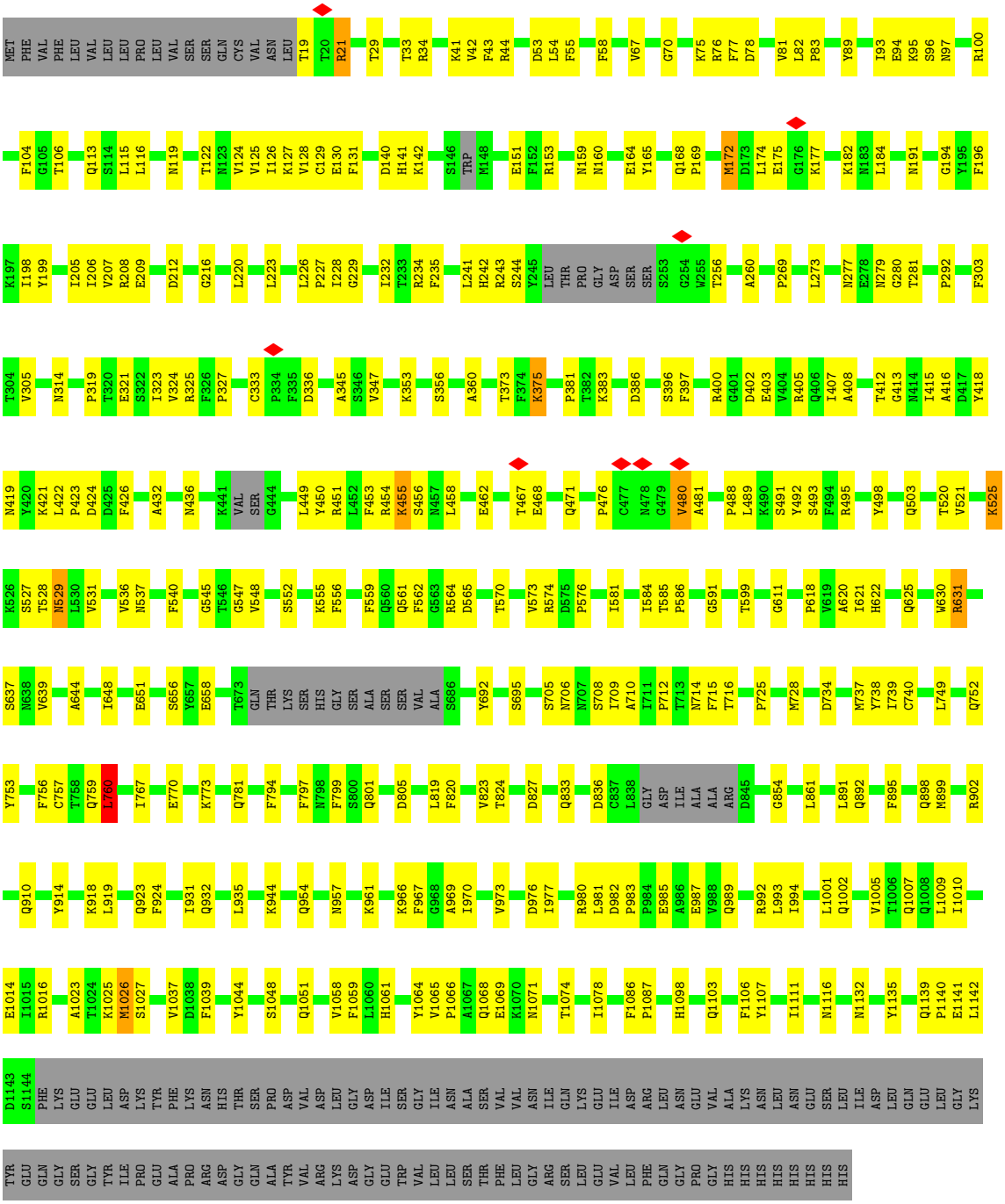
• Molecule 1: Spike glycoprotein,Fibritin

Chain B:

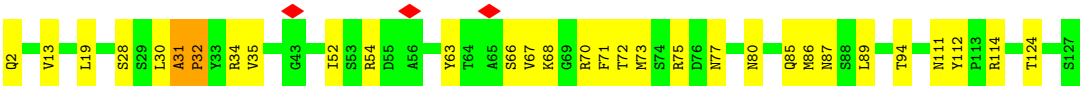


• Molecule 1: Spike glycoprotein,Fibritin

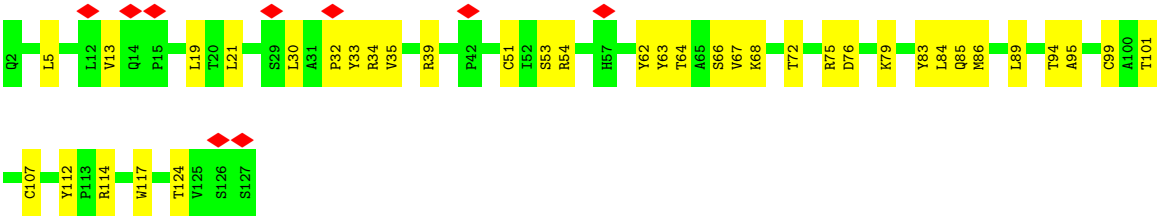
Chain C:



• Molecule 2: H6 nanobody

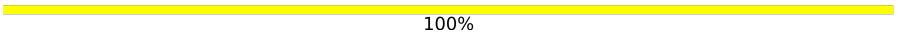


• Molecule 2: H6 nanobody



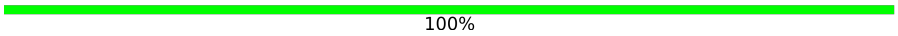
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

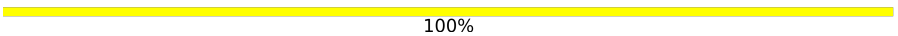
Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

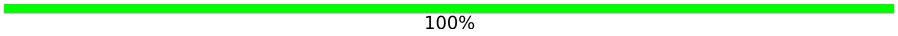


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

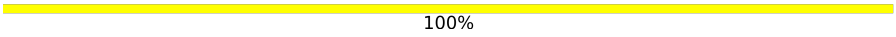


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

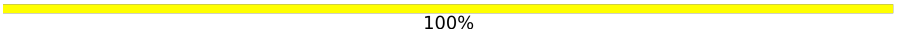


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/8802	0.51	1/11976 (0.0%)
1	B	0.26	0/8796	0.50	1/11969 (0.0%)
1	C	0.26	0/8802	0.50	1/11976 (0.0%)
2	D	0.26	0/990	0.55	0/1347
2	E	1.05	3/990 (0.3%)	0.96	6/1347 (0.4%)
All	All	0.32	3/28380 (0.0%)	0.53	9/38615 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	32	PRO	CG-CD	-26.57	0.62	1.50
2	E	32	PRO	CB-CG	12.19	2.10	1.50
2	E	32	PRO	N-CD	11.20	1.63	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	32	PRO	CA-N-CD	-15.59	89.68	111.50
2	E	32	PRO	N-CD-CG	-13.58	82.83	103.20
2	E	32	PRO	CB-CG-CD	-10.59	65.19	106.50
2	E	32	PRO	N-CA-CB	-10.40	90.82	103.30
2	E	32	PRO	CA-CB-CG	-10.21	84.61	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	PRO	CA-N-CD	-8.35	99.81	111.50
2	E	31	ALA	C-N-CD	6.89	142.87	128.40
1	B	798	ASN	C-N-CA	6.07	136.88	121.70
1	C	760	LEU	CA-CB-CG	5.77	128.57	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	323	ILE	Peptide

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	A	8596	0	8391	242	0
1	B	8589	0	8397	222	0
1	C	8596	0	8387	230	0
2	D	962	0	920	23	0
2	E	962	0	920	36	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	3	0
3	J	28	0	25	0	0
3	K	28	0	25	4	0
3	L	28	0	25	0	0
3	M	28	0	25	4	0
3	N	28	0	25	3	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
4	A	42	0	39	3	0
4	B	56	0	52	4	0
4	C	112	0	104	2	0
All	All	28223	0	27485	728	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 13.

All (728) 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:E:32:PRO:CG	2:E:32:PRO:N	1.67	1.50
2:E:32:PRO:CG	2:E:32:PRO:CB	2.10	1.27
2:E:32:PRO:CG	2:E:32:PRO:CA	2.45	0.95
2:E:32:PRO:N	2:E:32:PRO:HG3	1.48	0.94
1:A:525:LYS:HD3	1:A:526:LYS:H	1.35	0.91
2:E:32:PRO:CD	2:E:32:PRO:HG2	1.39	0.90
2:E:32:PRO:CG	2:E:32:PRO:HD2	1.37	0.89
2:E:32:PRO:HG3	2:E:32:PRO:CD	1.39	0.89
2:E:32:PRO:CG	2:E:32:PRO:HD3	1.37	0.88
2:E:72:THR:HB	2:E:85:GLN:HB3	1.63	0.79
1:B:968:GLY:H	1:C:752:GLN:HE22	1.31	0.79
1:A:522:CYS:SG	1:A:523:GLY:N	2.57	0.78
1:B:354:ARG:NH2	1:C:227:PRO:O	2.15	0.77
1:B:710:ALA:HB3	1:C:891:LEU:HB3	1.66	0.77
1:A:704:TYR:HA	1:B:892:GLN:HG3	1.67	0.75
1:B:489:LEU:HD12	1:B:490:LYS:HG3	1.69	0.75
1:C:449:LEU:HD21	1:C:489:LEU:HA	1.70	0.73
1:A:1048:SER:OG	1:A:1061:HIS:ND1	2.22	0.73
1:A:196:PHE:HB2	1:A:226:LEU:HB3	1.71	0.73
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.21	0.73
1:C:739:ILE:HD11	1:C:994:ILE:HA	1.72	0.71
1:B:477:CYS:HB3	1:B:483:PHE:HB2	1.72	0.71
1:C:168:GLN:NE2	1:C:169:PRO:O	2.22	0.71
1:C:1048:SER:OG	1:C:1061:HIS:ND1	2.23	0.71
1:A:454:ARG:HH12	1:A:458:LEU:HG	1.54	0.70
1:A:34:ARG:HH12	1:A:216:GLY:H	1.37	0.70
1:C:753:TYR:HB3	1:C:756:PHE:HE2	1.57	0.70
1:A:103:ILE:HG12	1:A:116:LEU:HD13	1.74	0.70
1:B:1098:HIS:H	3:M:1:NAG:H81	1.57	0.70
1:C:528:THR:HG22	1:C:529:ASN:H	1.56	0.69
2:E:31:ALA:C	2:E:32:PRO:HG3	2.13	0.69
1:A:319:PRO:HB3	1:A:536:VAL:HA	1.74	0.69
1:B:141:HIS:HB3	1:B:240:ALA:HB1	1.73	0.69
1:C:714:ASN:HB2	1:C:1068:GLN:HB2	1.73	0.69
1:A:390:THR:HB	1:A:519:ALA:HA	1.74	0.69
1:B:967:PHE:O	1:B:992:ARG:NH1	2.26	0.69
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.26	0.69
1:B:894:PRO:HB2	1:B:897:MET:HG2	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:LYS:NZ	1:B:1039:PHE:O	2.25	0.68
2:D:21:LEU:HD12	2:D:84:LEU:HD23	1.76	0.68
1:A:525:LYS:HD3	1:A:526:LYS:N	2.07	0.68
1:A:910:GLN:HE21	1:C:1086:PHE:HB3	1.60	0.67
1:A:408:ALA:HA	1:A:422:LEU:HD12	1.76	0.67
1:C:454:ARG:HH12	1:C:458:LEU:HG	1.60	0.67
1:A:700:ASN:ND2	1:B:784:GLN:OE1	2.27	0.67
1:A:449:LEU:HD21	1:A:489:LEU:HA	1.78	0.66
1:B:493:SER:HA	1:B:495:ARG:HH22	1.60	0.66
1:B:798:ASN:OD1	1:B:798:ASN:N	2.27	0.66
1:A:526:LYS:HD3	1:A:543:LEU:HB2	1.78	0.66
1:B:798:ASN:HB3	3:K:1:NAG:HN2	1.61	0.66
1:C:491:SER:OG	1:C:495:ARG:NH2	2.28	0.66
1:B:480:VAL:HA	1:B:485:CYS:HB2	1.78	0.66
1:A:352:ARG:HH11	1:A:463:ARG:HH21	1.44	0.66
2:E:66:SER:O	2:E:70:ARG:NH2	2.29	0.66
1:A:83:PRO:HA	1:A:234:ARG:HA	1.78	0.65
2:E:2:GLN:NE2	2:E:28:SER:OG	2.27	0.65
1:A:969:ALA:HA	1:A:992:ARG:HH21	1.60	0.65
1:A:1031:LEU:HB3	1:C:1037:VAL:HG11	1.78	0.65
1:B:182:LYS:HG2	1:B:208:ARG:HD3	1.76	0.65
1:C:421:LYS:HB3	1:C:458:LEU:HD13	1.78	0.65
1:C:525:LYS:NZ	1:C:527:SER:O	2.28	0.65
1:B:639:VAL:HG12	1:B:648:ILE:HG12	1.78	0.64
1:A:205:ILE:O	1:A:208:ARG:NH2	2.30	0.64
1:A:548:VAL:N	1:A:585:THR:O	2.30	0.64
2:E:30:LEU:O	2:E:75:ARG:NH2	2.30	0.64
1:C:413:GLY:H	1:C:416:ALA:HB3	1.61	0.64
1:A:973:VAL:HG12	1:A:976:ASP:H	1.62	0.64
1:C:421:LYS:HD3	1:C:458:LEU:HD22	1.79	0.64
1:A:739:ILE:O	1:A:997:ARG:NH1	2.31	0.64
1:B:348:TYR:HB2	1:B:464:ASP:HB3	1.80	0.64
2:D:30:LEU:O	2:D:75:ARG:NH2	2.31	0.64
1:C:333:CYS:HB3	1:C:360:ALA:HB2	1.80	0.64
1:B:557:LEU:HB2	1:B:560:GLN:HG3	1.79	0.63
1:B:968:GLY:N	1:C:752:GLN:HE22	1.97	0.63
1:C:205:ILE:O	1:C:208:ARG:NH2	2.29	0.63
1:C:767:ILE:HD11	1:C:1009:LEU:HD23	1.78	0.63
1:A:1097:THR:OG1	1:A:1098:HIS:ND1	2.32	0.63
1:B:277:ASN:HB2	4:B:1303:NAG:H81	1.80	0.63
1:B:999:GLN:OE1	1:B:1002:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:PRO:HG2	1:A:541:ASN:HA	1.80	0.63
1:A:528:THR:HA	1:A:543:LEU:HD23	1.80	0.63
1:B:435:SER:HB3	1:B:439:ASP:HB2	1.81	0.63
1:C:115:LEU:HD11	1:C:128:VAL:HG22	1.81	0.63
1:B:126:ILE:N	1:B:165:TYR:O	2.31	0.62
1:B:241:LEU:HB3	1:B:255:TRP:HB3	1.80	0.62
2:E:32:PRO:CG	2:E:32:PRO:CD	0.63	0.62
1:B:82:LEU:O	1:B:235:PHE:N	2.30	0.62
1:C:970:ILE:HD12	1:C:981:LEU:HD11	1.80	0.62
1:B:1111:ILE:O	1:B:1116:ASN:ND2	2.32	0.62
1:B:798:ASN:HB3	3:K:1:NAG:N2	2.14	0.62
1:A:375:LYS:HA	1:A:381:PRO:HB3	1.82	0.62
1:B:449:LEU:HD22	1:B:489:LEU:HD13	1.79	0.62
1:B:79:ASN:ND2	1:B:237:THR:O	2.34	0.61
1:B:93:ILE:O	1:B:208:ARG:NH1	2.33	0.61
1:B:148:MET:SD	1:B:149:GLU:N	2.72	0.61
1:B:959:LEU:HD21	1:B:1004:TYR:HB2	1.83	0.61
1:A:95:LYS:NZ	1:A:175:GLU:OE2	2.29	0.61
1:C:756:PHE:HA	1:C:759:GLN:NE2	2.15	0.61
1:A:760:LEU:HG	1:A:1005:VAL:HG21	1.81	0.61
1:A:325:ARG:HH11	1:A:531:VAL:HG23	1.66	0.60
1:B:196:PHE:HB2	1:B:226:LEU:HB2	1.82	0.60
1:B:716:THR:N	1:B:1065:VAL:O	2.33	0.60
1:C:95:LYS:NZ	1:C:175:GLU:OE2	2.31	0.60
1:A:1113:THR:OG1	1:A:1115:ASP:OD2	2.20	0.60
1:C:408:ALA:HA	1:C:422:LEU:HD12	1.82	0.60
1:C:454:ARG:HH22	1:C:458:LEU:HG	1.66	0.60
1:A:716:THR:N	1:A:1065:VAL:O	2.34	0.60
1:B:386:ASP:O	1:B:525:LYS:NZ	2.35	0.60
1:B:1097:THR:N	3:M:1:NAG:O7	2.34	0.60
2:E:34:ARG:NH2	2:E:111:ASN:OD1	2.31	0.60
1:A:773:LYS:O	1:A:776:GLN:HG2	2.02	0.60
1:B:173:ASP:HB2	1:B:185:ARG:HH21	1.66	0.60
1:C:172:MET:SD	1:C:172:MET:N	2.71	0.60
1:B:388:CYS:SG	1:B:523:GLY:N	2.70	0.60
2:E:30:LEU:N	2:E:80:ASN:OD1	2.24	0.59
1:C:67:VAL:HB	1:C:260:ALA:HB3	1.83	0.59
1:C:83:PRO:HA	1:C:234:ARG:HA	1.82	0.59
1:A:910:GLN:HE22	1:C:1087:PRO:HD2	1.68	0.59
1:B:927:ALA:HA	1:B:930:LYS:HD2	1.84	0.59
1:B:739:ILE:O	1:B:997:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:PRO:HB2	1:A:897:MET:HG2	1.84	0.59
1:B:409:PRO:HB3	1:B:422:LEU:HD22	1.84	0.59
1:C:345:ALA:HB3	1:C:396:SER:HB2	1.83	0.59
1:C:1111:ILE:O	1:C:1116:ASN:ND2	2.35	0.59
1:B:738:TYR:CE2	1:B:1001:LEU:HD21	2.38	0.59
1:C:140:ASP:OD1	1:C:153:ARG:NH2	2.34	0.59
1:A:727:SER:HG	1:A:1055:HIS:HD1	1.50	0.59
1:A:1111:ILE:O	1:A:1116:ASN:ND2	2.35	0.59
1:B:658:GLU:O	1:B:692:TYR:OH	2.17	0.58
1:C:321:GLU:H	1:C:536:VAL:HG12	1.68	0.58
1:A:574:ARG:NH1	1:A:579:LEU:O	2.35	0.58
1:A:719:VAL:HG22	1:A:1062:VAL:HG12	1.85	0.58
1:B:199:TYR:HB3	1:B:220:LEU:HB3	1.86	0.58
1:B:902:ARG:NH1	1:B:1046:LEU:O	2.36	0.58
2:D:34:ARG:HH22	2:D:112:TYR:HA	1.68	0.58
1:B:465:ILE:HD12	1:B:465:ILE:H	1.68	0.58
1:C:383:LYS:HG2	1:C:386:ASP:HB2	1.86	0.58
1:C:931:ILE:O	1:C:935:LEU:HG	2.04	0.58
1:C:1141:GLU:HG2	1:C:1142:LEU:HD12	1.85	0.58
1:A:531:VAL:H	1:A:549:LEU:HD13	1.68	0.58
1:A:67:VAL:HB	1:A:260:ALA:HB3	1.86	0.58
1:C:34:ARG:HH12	1:C:216:GLY:H	1.51	0.58
1:A:531:VAL:O	1:A:549:LEU:HB2	2.04	0.58
1:B:464:ASP:OD1	1:B:466:SER:OG	2.19	0.58
1:C:21:ARG:HE	1:C:77:PHE:HB3	1.69	0.57
1:B:143:ASN:O	1:B:145:LYS:NZ	2.36	0.57
1:A:1044:TYR:HB2	1:A:1064:TYR:HB3	1.86	0.57
1:B:1044:TYR:HB2	1:B:1064:TYR:HB3	1.85	0.57
1:C:898:GLN:O	1:C:902:ARG:HG3	2.03	0.57
1:B:353:LYS:HB3	1:B:394:ALA:HB3	1.86	0.57
1:C:182:LYS:HG3	1:C:208:ARG:HH11	1.69	0.57
1:C:705:SER:HB3	1:C:708:SER:HB3	1.87	0.57
1:C:1014:GLU:OE1	1:C:1014:GLU:N	2.28	0.57
1:A:352:ARG:NH1	1:A:463:ARG:HH21	2.02	0.57
1:A:518:PRO:HG3	1:B:195:TYR:CZ	2.40	0.57
1:A:974:LEU:HD21	1:A:997:ARG:HH12	1.69	0.57
1:B:277:ASN:OD1	1:B:281:THR:N	2.33	0.57
1:C:770:GLU:OE2	1:C:1016:ARG:NH1	2.38	0.57
1:A:226:LEU:HD12	1:A:227:PRO:HD2	1.86	0.57
1:A:714:ASN:HB3	1:A:1068:GLN:HB2	1.87	0.57
1:B:329:ILE:HB	1:B:359:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HG23	1:C:325:ARG:HD2	1.87	0.57
1:A:42:VAL:HG22	1:C:562:PHE:HB2	1.85	0.56
1:A:529:ASN:HB3	1:A:549:LEU:HD21	1.87	0.56
1:C:801:GLN:NE2	1:C:932:GLN:OE1	2.38	0.56
1:A:126:ILE:HB	1:A:165:TYR:HB3	1.87	0.56
1:A:902:ARG:NH1	1:A:1046:LEU:O	2.39	0.56
1:B:1098:HIS:N	3:M:1:NAG:H81	2.19	0.56
1:C:982:ASP:N	1:C:982:ASP:OD1	2.39	0.56
1:A:453:PHE:H	1:A:488:PRO:HB3	1.69	0.56
1:B:1048:SER:OG	1:B:1061:HIS:ND1	2.32	0.56
1:B:1126:VAL:HG13	1:C:914:TYR:HB3	1.87	0.56
1:C:1026:MET:SD	1:C:1027:SER:N	2.79	0.56
3:I:2:NAG:H3	3:I:2:NAG:H83	1.87	0.56
1:A:82:LEU:O	1:A:235:PHE:N	2.34	0.56
2:E:31:ALA:CA	2:E:32:PRO:HG3	2.35	0.56
1:B:353:LYS:N	1:B:394:ALA:O	2.32	0.56
1:A:25:PRO:HD2	1:A:25:PRO:O	2.05	0.56
1:B:142:LYS:HB2	1:B:242:HIS:CG	2.41	0.56
1:B:321:GLU:HG3	1:B:536:VAL:HG23	1.88	0.56
2:E:85:GLN:NE2	2:E:87:ASN:OD1	2.34	0.56
1:A:92:SER:HB3	1:A:185:ARG:HB2	1.88	0.56
2:D:32:PRO:HA	2:D:54:ARG:HD3	1.88	0.55
1:B:243:ARG:NH1	1:B:254:GLY:O	2.39	0.55
1:B:454:ARG:HD3	1:B:455:LYS:H	1.71	0.55
1:A:127:LYS:HG2	1:A:131:PHE:HZ	1.71	0.55
4:A:1302:NAG:H3	4:A:1302:NAG:H83	1.88	0.55
1:B:126:ILE:HB	1:B:165:TYR:HB3	1.88	0.55
1:A:421:LYS:HD3	1:A:458:LEU:HD22	1.89	0.55
1:A:104:PHE:HB3	1:A:232:ILE:HG12	1.87	0.55
1:B:479:GLY:O	1:B:481:ALA:N	2.35	0.55
1:B:798:ASN:HA	1:B:799:PHE:HB2	1.88	0.55
1:A:67:VAL:O	1:A:260:ALA:N	2.37	0.55
1:A:352:ARG:HD2	1:A:393:TYR:OH	2.07	0.55
1:A:423:PRO:HG2	1:A:426:PHE:HA	1.88	0.55
1:A:801:GLN:NE2	1:A:932:GLN:OE1	2.32	0.55
1:A:140:ASP:OD1	1:A:153:ARG:NH2	2.37	0.55
1:B:349:ALA:HA	1:B:463:ARG:HB3	1.89	0.55
1:C:182:LYS:H	1:C:208:ARG:HH12	1.54	0.55
1:A:383:LYS:HG2	1:A:386:ASP:HB2	1.88	0.54
1:A:1030:VAL:HA	1:A:1047:MET:HE1	1.88	0.54
1:B:660:ASP:H	1:B:668:CYS:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:SER:HB3	1:C:498:TYR:HD2	1.73	0.54
1:C:314:ASN:HA	1:C:591:GLY:HA2	1.90	0.54
1:C:781:GLN:NE2	1:C:1026:MET:SD	2.80	0.54
1:B:952:ASN:O	1:B:956:LEU:HG	2.07	0.54
1:C:424:ASP:OD1	1:C:424:ASP:N	2.40	0.54
4:A:1302:NAG:H61	1:B:791:ILE:HG21	1.89	0.54
1:C:29:THR:OG1	1:C:212:ASP:OD1	2.25	0.54
1:A:323:ILE:HG22	1:A:325:ARG:HH12	1.71	0.54
1:C:277:ASN:OD1	1:C:281:THR:N	2.39	0.54
2:E:13:VAL:HG21	2:E:89:LEU:HD13	1.88	0.54
1:B:836:ASP:OD1	1:B:836:ASP:N	2.40	0.54
2:E:70:ARG:HG3	2:E:87:ASN:O	2.08	0.54
1:B:419:ASN:OD1	1:B:420:TYR:N	2.41	0.54
1:A:493:SER:HB3	1:A:498:TYR:HD2	1.73	0.54
1:B:449:LEU:HD13	1:B:489:LEU:HB2	1.89	0.54
1:B:19:THR:HG23	1:B:75:LYS:HD3	1.89	0.53
1:B:559:PHE:O	1:B:561:GLN:NE2	2.34	0.53
2:E:75:ARG:NE	2:E:77:ASN:OD1	2.41	0.53
1:A:927:ALA:HA	1:A:930:LYS:HD3	1.90	0.53
1:B:1131:ASN:H	4:B:1301:NAG:H83	1.74	0.53
1:A:182:LYS:H	1:A:208:ARG:HH12	1.54	0.53
1:B:194:GLY:HA2	1:B:229:GLY:HA2	1.90	0.53
1:B:390:THR:HG22	1:B:519:ALA:HA	1.90	0.53
1:C:196:PHE:N	1:C:226:LEU:O	2.41	0.53
1:C:520:THR:HG23	1:C:521:VAL:HG23	1.90	0.53
1:A:714:ASN:HA	3:H:1:NAG:H83	1.91	0.53
1:A:762:ARG:NH1	1:C:954:GLN:OE1	2.41	0.53
1:B:666:GLY:N	1:C:861:LEU:O	2.41	0.53
1:A:1141:GLU:HG2	1:A:1142:LEU:HD12	1.91	0.53
1:A:892:GLN:NE2	1:C:1071:ASN:OD1	2.42	0.53
1:A:734:ASP:HB3	1:A:737:MET:SD	2.49	0.52
1:C:621:ILE:HD12	1:C:625:GLN:HG2	1.90	0.52
1:C:918:LYS:H	1:C:918:LYS:HD3	1.74	0.52
1:A:534:LYS:HD3	1:A:535:CYS:N	2.24	0.52
1:A:977:ILE:HA	1:A:980:ARG:HH21	1.73	0.52
2:E:94:THR:HG23	2:E:124:THR:HA	1.91	0.52
2:E:70:ARG:HG2	2:E:71:PHE:HD1	1.74	0.52
2:D:5:LEU:HD11	2:D:101:THR:HG22	1.90	0.52
1:B:34:ARG:NH1	1:B:216:GLY:O	2.42	0.52
1:C:1098:HIS:CG	3:N:1:NAG:H5	2.44	0.52
1:B:326:PHE:O	1:B:577:GLN:NE2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:PHE:HA	1:B:498:TYR:HD2	1.74	0.52
1:C:106:THR:O	1:C:234:ARG:NH1	2.42	0.52
1:C:325:ARG:HA	1:C:325:ARG:CZ	2.40	0.52
1:A:141:HIS:CD2	1:A:242:HIS:H	2.28	0.52
1:A:347:VAL:HG12	1:A:397:PHE:HB2	1.91	0.52
1:C:34:ARG:NH1	1:C:216:GLY:O	2.43	0.52
1:C:327:PRO:HA	1:C:528:THR:HG23	1.91	0.52
1:B:801:GLN:HG3	1:B:932:GLN:NE2	2.24	0.52
1:A:373:THR:OG1	1:A:432:ALA:N	2.43	0.51
1:A:388:CYS:HA	1:A:522:CYS:HB2	1.92	0.51
1:A:794:PHE:HB2	1:A:799:PHE:HE2	1.75	0.51
1:C:127:LYS:HG2	1:C:131:PHE:HZ	1.75	0.51
1:C:423:PRO:HG2	1:C:426:PHE:HA	1.90	0.51
1:C:969:ALA:HA	1:C:992:ARG:HH21	1.74	0.51
1:C:1005:VAL:O	1:C:1009:LEU:HG	2.10	0.51
1:A:21:ARG:HE	1:A:77:PHE:HB3	1.75	0.51
1:C:104:PHE:HB3	1:C:232:ILE:HG12	1.92	0.51
1:A:528:THR:OG1	1:A:529:ASN:N	2.41	0.51
1:B:912:VAL:O	1:B:916:ASN:ND2	2.36	0.51
1:C:42:VAL:HB	1:C:44:ARG:HH21	1.74	0.51
1:C:82:LEU:O	1:C:235:PHE:N	2.38	0.51
1:C:1103:GLN:HE21	1:C:1106:PHE:HB3	1.75	0.51
1:B:560:GLN:O	1:B:574:ARG:NH2	2.42	0.51
2:E:52:ILE:HB	2:E:73:MET:HG3	1.92	0.51
1:A:1094:SER:HB2	1:A:1099:TRP:CD2	2.45	0.51
1:B:125:VAL:HA	1:B:166:VAL:HG22	1.92	0.51
1:B:439:ASP:OD2	1:B:506:ARG:NH2	2.41	0.51
1:B:656:SER:HB3	1:B:695:SER:HB3	1.91	0.51
1:C:116:LEU:HD21	1:C:127:LYS:HB3	1.92	0.51
1:B:291:ASP:OD1	1:B:291:ASP:N	2.44	0.51
1:A:1047:MET:O	1:A:1062:VAL:HG22	2.11	0.51
1:C:421:LYS:NZ	1:C:462:GLU:O	2.31	0.51
2:E:31:ALA:N	2:E:32:PRO:HG3	2.25	0.51
1:A:78:ASP:OD1	1:A:78:ASP:N	2.44	0.51
1:A:421:LYS:HB3	1:A:458:LEU:HD13	1.92	0.51
1:A:520:THR:HG23	1:A:521:VAL:HG23	1.92	0.51
1:B:31:SER:OG	1:B:60:SER:N	2.30	0.51
2:E:70:ARG:HG2	2:E:71:PHE:CD1	2.46	0.51
1:B:95:LYS:HG3	1:B:182:LYS:HE3	1.92	0.51
1:C:347:VAL:HG12	1:C:397:PHE:HB2	1.92	0.51
1:B:124:VAL:HG13	1:B:169:PRO:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:ILE:O	1:B:981:LEU:HB3	2.11	0.51
1:A:355:ILE:HG22	1:A:521:VAL:HG21	1.93	0.50
1:C:273:LEU:HD22	1:C:303:PHE:HE1	1.75	0.50
1:B:364:VAL:O	1:B:368:LEU:HB2	2.11	0.50
1:C:709:ILE:HD11	1:C:1074:THR:HG21	1.93	0.50
2:D:21:LEU:HB2	2:D:84:LEU:HB3	1.93	0.50
1:B:168:GLN:HG3	1:B:169:PRO:HD2	1.94	0.50
1:B:393:TYR:O	1:B:510:LEU:HA	2.12	0.50
1:A:716:THR:HB	1:A:1065:VAL:HB	1.93	0.50
1:B:353:LYS:O	1:B:394:ALA:N	2.37	0.50
1:C:552:SER:OG	1:C:581:ILE:HG13	2.12	0.50
1:A:663:ILE:HD12	1:A:663:ILE:H	1.77	0.50
1:A:1047:MET:SD	1:A:1048:SER:N	2.81	0.50
1:C:93:ILE:HG22	1:C:182:LYS:HE2	1.93	0.50
1:C:207:VAL:HG22	1:C:209:GLU:H	1.76	0.50
3:M:1:NAG:H83	3:M:1:NAG:H3	1.94	0.50
1:A:243:ARG:NH1	1:A:244:SER:OG	2.45	0.50
1:A:325:ARG:HB2	1:A:530:LEU:HD22	1.94	0.50
1:A:985:GLU:OE2	1:A:989:GLN:HG2	2.11	0.50
2:E:67:VAL:HG12	2:E:70:ARG:HH21	1.77	0.50
1:A:1007:GLN:HA	1:A:1010:ILE:HG12	1.94	0.50
1:A:891:LEU:HB3	1:C:710:ALA:HB3	1.93	0.50
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.12	0.50
1:B:94:GLU:HB3	1:B:96:SER:O	2.12	0.50
1:B:659:CYS:HB2	1:B:694:MET:SD	2.51	0.50
1:A:376:CYS:SG	1:A:381:PRO:HA	2.52	0.49
1:B:140:ASP:HB2	1:B:151:GLU:HG2	1.94	0.49
1:B:348:TYR:O	1:B:464:ASP:N	2.40	0.49
1:B:901:TYR:HA	1:B:904:ASN:HD22	1.77	0.49
2:D:13:VAL:HG21	2:D:19:LEU:HG	1.93	0.49
1:A:480:VAL:HG22	1:A:481:ALA:H	1.76	0.49
1:C:199:TYR:HB3	1:C:220:LEU:HB3	1.93	0.49
1:C:705:SER:OG	1:C:706:ASN:N	2.45	0.49
1:A:421:LYS:NZ	1:A:462:GLU:O	2.37	0.49
1:A:989:GLN:OE1	1:A:992:ARG:NH2	2.43	0.49
1:C:973:VAL:HB	1:C:976:ASP:HB3	1.95	0.49
1:B:129:CYS:HB2	1:B:131:PHE:CE2	2.48	0.49
1:B:344:PHE:CD1	1:B:506:ARG:HG2	2.48	0.49
1:B:1071:ASN:ND2	1:C:892:GLN:HE22	2.10	0.49
1:C:305:VAL:O	1:C:599:THR:N	2.32	0.49
1:A:773:LYS:HG2	1:A:777:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:O	1:B:241:LEU:N	2.34	0.49
1:B:715:PHE:HA	1:B:1066:PRO:HA	1.95	0.49
1:A:182:LYS:HG3	1:A:208:ARG:HH11	1.78	0.49
1:A:407:ILE:HG22	1:A:416:ALA:HB2	1.94	0.49
1:A:970:ILE:HG12	1:A:989:GLN:HE21	1.78	0.49
1:B:1071:ASN:HD21	1:C:892:GLN:HE22	1.60	0.49
1:C:81:VAL:HG23	1:C:81:VAL:O	2.13	0.49
1:C:637:SER:HB2	1:C:651:GLU:OE1	2.13	0.49
1:A:543:LEU:HD12	1:A:544:LYS:H	1.78	0.49
1:A:1037:VAL:HG11	1:B:1031:LEU:HB3	1.93	0.49
1:A:1046:LEU:HB2	1:A:1062:VAL:HG23	1.95	0.49
1:B:323:ILE:HD13	1:B:531:VAL:H	1.78	0.49
1:C:174:LEU:O	1:C:177:LYS:NZ	2.46	0.49
1:C:639:VAL:HG12	1:C:648:ILE:HG12	1.94	0.49
1:A:32:PHE:HB3	1:A:215:GLN:HE22	1.78	0.48
1:A:658:GLU:O	1:A:692:TYR:OH	2.18	0.48
1:A:1071:ASN:ND2	4:A:1303:NAG:O3	2.45	0.48
1:A:33:THR:HA	1:A:58:PHE:HD1	1.77	0.48
1:C:540:PHE:CE2	1:C:573:VAL:HG11	2.48	0.48
1:C:895:PHE:O	1:C:899:MET:HG2	2.12	0.48
1:A:552:SER:OG	1:A:581:ILE:HG13	2.13	0.48
1:B:205:ILE:O	1:B:207:VAL:N	2.46	0.48
1:B:702:VAL:HG12	1:C:892:GLN:HB3	1.95	0.48
1:C:421:LYS:HE3	1:C:462:GLU:H	1.79	0.48
1:A:184:LEU:HD21	1:A:205:ILE:HD12	1.95	0.48
1:A:895:PHE:O	1:A:899:MET:HE3	2.13	0.48
1:B:277:ASN:ND2	4:B:1303:NAG:O7	2.47	0.48
1:C:480:VAL:HG22	1:C:481:ALA:H	1.77	0.48
1:A:42:VAL:HG11	1:C:564:ARG:HG2	1.95	0.48
1:A:793:TYR:CE2	4:C:1306:NAG:H5	2.47	0.48
1:B:1005:VAL:O	1:B:1009:LEU:HG	2.14	0.48
1:A:81:VAL:HB	1:A:234:ARG:HD3	1.95	0.48
1:A:106:THR:O	1:A:234:ARG:NH1	2.47	0.48
1:A:531:VAL:N	1:A:549:LEU:HD13	2.28	0.48
2:D:34:ARG:NH2	2:D:51:CYS:SG	2.77	0.48
1:A:405:ARG:O	1:A:405:ARG:NE	2.47	0.48
1:A:947:ASP:O	1:A:951:HIS:ND1	2.46	0.48
1:B:343:ARG:HH21	1:B:441:LYS:HD3	1.78	0.48
1:B:799:PHE:HD2	1:B:802:ILE:HD11	1.77	0.48
1:C:127:LYS:HD2	1:C:164:GLU:OE1	2.14	0.48
1:C:989:GLN:OE1	1:C:992:ARG:NH2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:LEU:HB2	2:E:86:MET:HE1	1.94	0.48
1:A:333:CYS:HB3	1:A:360:ALA:HB2	1.96	0.48
1:B:518:PRO:HD3	1:B:561:GLN:HG3	1.96	0.48
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.96	0.48
1:B:371:PHE:HB3	1:B:433:TRP:HA	1.96	0.48
1:C:407:ILE:HG22	1:C:416:ALA:HB2	1.94	0.48
1:C:454:ARG:NE	1:C:456:SER:O	2.47	0.48
1:A:345:ALA:HB3	1:A:396:SER:HB2	1.96	0.48
1:A:529:ASN:HB3	1:A:549:LEU:HD11	1.96	0.48
1:A:621:ILE:HD12	1:A:625:GLN:HG2	1.96	0.48
1:A:744:THR:O	1:A:747:SER:OG	2.25	0.48
1:A:903:PHE:CD2	1:A:913:LEU:HB2	2.49	0.47
1:B:33:THR:HA	1:B:58:PHE:CD1	2.49	0.47
1:B:97:ASN:HB3	1:B:100:ARG:HH11	1.79	0.47
2:E:30:LEU:HD13	2:E:35:VAL:HG21	1.96	0.47
1:A:34:ARG:NH2	1:A:214:PRO:O	2.46	0.47
1:A:91:ALA:HB3	1:A:263:TYR:HB2	1.96	0.47
1:B:354:ARG:HH12	1:C:228:ILE:HA	1.79	0.47
1:B:389:PHE:N	1:B:521:VAL:O	2.47	0.47
1:B:733:VAL:HA	1:B:854:GLY:O	2.14	0.47
1:C:977:ILE:HD11	1:C:989:GLN:HE21	1.79	0.47
1:B:171:LEU:HD23	1:B:185:ARG:HG2	1.96	0.47
1:C:419:ASN:HD21	1:C:451:ARG:N	2.12	0.47
1:B:966:LYS:HB3	1:C:752:GLN:OE1	2.15	0.47
1:A:471:GLN:NE2	1:A:475:LYS:O	2.47	0.47
1:A:659:CYS:N	1:A:694:MET:SD	2.88	0.47
1:C:753:TYR:HB3	1:C:756:PHE:CE2	2.45	0.47
1:B:704:TYR:HA	1:C:892:GLN:HB2	1.96	0.47
1:C:184:LEU:HD21	1:C:205:ILE:HD12	1.95	0.47
1:C:403:GLU:HG3	1:C:415:ILE:HG22	1.97	0.47
1:C:716:THR:N	1:C:1065:VAL:O	2.47	0.47
1:C:739:ILE:HG23	1:C:740:CYS:SG	2.54	0.47
1:A:30:ASN:OD1	1:A:59:PHE:HA	2.15	0.47
1:A:352:ARG:HH11	1:A:463:ARG:NH2	2.11	0.47
1:A:419:ASN:HD21	1:A:451:ARG:N	2.12	0.47
1:A:1103:GLN:HG2	1:A:1108:GLU:OE1	2.14	0.47
1:B:453:PHE:HB3	1:B:488:PRO:HA	1.97	0.47
1:C:556:PHE:CD2	1:C:581:ILE:HG21	2.49	0.47
1:C:712:PRO:HA	1:C:1069:GLU:HA	1.96	0.47
2:D:53:SER:O	2:D:75:ARG:NH1	2.47	0.47
3:N:1:NAG:H4	3:N:2:NAG:H83	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PHE:HA	1:B:206:ILE:HA	1.97	0.47
1:B:900:ALA:O	1:B:904:ASN:ND2	2.48	0.47
1:C:353:LYS:HA	1:C:353:LYS:HD2	1.74	0.47
1:C:529:ASN:OD1	1:C:576:PRO:HD2	2.15	0.47
1:A:226:LEU:HG	1:A:228:ILE:HG12	1.97	0.47
1:A:534:LYS:HG3	1:A:536:VAL:HG13	1.95	0.47
1:A:639:VAL:HG12	1:A:648:ILE:HG12	1.96	0.47
1:B:564:ARG:HB2	1:C:42:VAL:HG11	1.97	0.46
1:B:579:LEU:HD12	1:B:580:GLU:N	2.30	0.46
1:C:124:VAL:HG13	1:C:169:PRO:HA	1.97	0.46
1:C:129:CYS:HB2	1:C:131:PHE:CZ	2.50	0.46
1:A:534:LYS:HD3	1:A:535:CYS:H	1.80	0.46
1:B:734:ASP:HB3	1:B:737:MET:SD	2.56	0.46
1:B:997:ARG:O	1:B:1001:LEU:HG	2.15	0.46
1:A:413:GLY:H	1:A:416:ALA:HB3	1.80	0.46
1:A:659:CYS:HB2	1:A:694:MET:SD	2.54	0.46
1:B:903:PHE:CD2	1:B:913:LEU:HB2	2.50	0.46
1:B:988:VAL:HG13	1:B:989:GLN:HE21	1.79	0.46
1:C:537:ASN:HA	1:C:545:GLY:O	2.15	0.46
2:E:86:MET:HE3	2:E:89:LEU:HD21	1.98	0.46
1:B:107:THR:OG1	1:B:109:ASP:OD1	2.31	0.46
1:C:468:GLU:OE1	1:C:468:GLU:N	2.45	0.46
1:A:30:ASN:HB3	1:A:32:PHE:CE2	2.50	0.46
1:A:212:ASP:OD1	1:A:212:ASP:N	2.48	0.46
1:A:745:GLU:HG3	1:A:978:PHE:CE2	2.50	0.46
1:B:445:ASN:HA	1:B:495:ARG:HH21	1.80	0.46
1:C:561:GLN:HA	1:C:574:ARG:HG3	1.97	0.46
1:B:560:GLN:HA	1:C:41:LYS:HG3	1.97	0.46
1:C:141:HIS:CD2	1:C:242:HIS:H	2.33	0.46
1:C:191:ASN:HB2	1:C:196:PHE:CE1	2.51	0.46
1:C:319:PRO:HB3	1:C:536:VAL:HA	1.97	0.46
1:C:820:PHE:O	1:C:824:THR:HB	2.15	0.46
1:A:32:PHE:HB3	1:A:215:GLN:NE2	2.31	0.46
1:A:403:GLU:O	1:A:407:ILE:HG23	2.16	0.46
1:B:613:ASN:HB3	1:B:616:GLU:OE1	2.16	0.46
1:A:32:PHE:CZ	1:A:212:ASP:HB2	2.51	0.46
1:A:140:ASP:H	1:A:151:GLU:HG2	1.80	0.46
1:A:773:LYS:HB3	1:A:773:LYS:HE2	1.79	0.46
1:B:73:GLY:HA2	1:B:256:THR:HG21	1.97	0.46
1:B:287:ASP:O	1:B:294:SER:HB3	2.16	0.46
1:B:783:LYS:HG3	1:B:784:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:H	1:C:21:ARG:HD3	1.81	0.46
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.51	0.46
1:C:631:ARG:HD3	1:C:631:ARG:H	1.79	0.46
2:D:64[A]:THR:HG22	2:D:67:VAL:HG22	1.97	0.46
1:A:819:LEU:O	1:A:823:VAL:HG23	2.16	0.46
1:A:910:GLN:NE2	1:C:1086:PHE:HB3	2.28	0.46
1:C:827:ASP:N	1:C:827:ASP:OD1	2.46	0.46
1:A:454:ARG:NE	1:A:456:SER:O	2.49	0.46
1:C:402:ASP:O	1:C:405:ARG:NH2	2.48	0.46
1:C:1007:GLN:HA	1:C:1010:ILE:HG12	1.98	0.46
1:C:1051:GLN:N	1:C:1058:VAL:O	2.41	0.46
1:C:43:PHE:CE1	1:C:280:GLY:HA3	2.51	0.45
1:C:277:ASN:HD21	1:C:279:ASN:HB2	1.82	0.45
1:C:547:GLY:HA2	1:C:586:PRO:HA	1.98	0.45
1:A:116:LEU:HG	1:A:118:VAL:HG13	1.98	0.45
1:A:350:TRP:HZ2	1:A:420:TYR:HA	1.81	0.45
1:A:528:THR:CA	1:A:543:LEU:HD23	2.46	0.45
1:A:556:PHE:CZ	1:A:572:ALA:HB3	2.51	0.45
1:B:21:ARG:HH22	1:B:24:LEU:HB2	1.81	0.45
1:B:137:PRO:HB2	1:B:154:VAL:HG12	1.98	0.45
1:A:753:TYR:HB2	1:A:756:PHE:CE2	2.50	0.45
1:C:70:GLY:HA3	1:C:76:ARG:HG3	1.98	0.45
1:C:336:ASP:OD1	1:C:336:ASP:N	2.48	0.45
1:C:706:ASN:OD1	4:C:1306:NAG:N2	2.50	0.45
1:A:561:GLN:HA	1:A:574:ARG:HG3	1.98	0.45
1:A:199:TYR:HB3	1:A:220:LEU:HB3	1.98	0.45
1:A:773:LYS:HA	1:A:776:GLN:CD	2.37	0.45
1:C:33:THR:HA	1:C:58:PHE:CD1	2.52	0.45
1:C:895:PHE:O	1:C:899:MET:HE3	2.17	0.45
2:D:39:ARG:HB2	2:D:95:ALA:HB3	1.98	0.45
3:I:1:NAG:H4	3:I:2:NAG:C7	2.46	0.45
1:A:159:ASN:OD1	1:A:159:ASN:N	2.49	0.45
1:A:548:VAL:HG23	1:A:587:CYS:HB3	1.99	0.45
1:B:651:GLU:HG3	1:B:690:ILE:HG22	1.98	0.45
1:B:739:ILE:HD11	1:B:994:ILE:HA	1.98	0.45
1:B:201:LYS:HG2	1:B:220:LEU:HG	1.99	0.45
2:D:63:TYR:HB3	2:D:67:VAL:HG23	1.99	0.45
1:A:348:TYR:HB2	1:A:464:ASP:O	2.17	0.45
1:A:454:ARG:HH22	1:A:458:LEU:HG	1.81	0.45
1:B:395:ASP:OD1	1:B:509:VAL:N	2.34	0.45
1:B:567:ALA:HA	1:C:961:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:PHE:CE2	1:B:1120:SER:HB3	2.52	0.45
1:C:33:THR:HA	1:C:58:PHE:HD1	1.81	0.45
1:A:185:ARG:HB3	1:A:187:PHE:CE2	2.52	0.45
1:A:805:ASP:OD1	1:A:805:ASP:N	2.46	0.45
1:B:549:LEU:HB3	1:B:582:LEU:HD21	1.99	0.45
1:B:1003:THR:O	1:B:1007:GLN:HG2	2.17	0.45
1:B:686:SER:OG	1:B:687:GLN:N	2.50	0.44
1:B:791:ILE:H	1:B:791:ILE:HD12	1.81	0.44
1:B:1087:PRO:HD2	1:C:910:GLN:OE1	2.15	0.44
1:C:737:MET:SD	1:C:854:GLY:HA3	2.57	0.44
1:A:129:CYS:HB2	1:A:131:PHE:CZ	2.52	0.44
1:A:353:LYS:HA	1:A:353:LYS:HD2	1.80	0.44
1:A:626:LEU:HD12	1:A:626:LEU:HA	1.85	0.44
1:B:535:CYS:HB2	1:B:587:CYS:HB3	1.55	0.44
1:A:428:GLY:HA3	1:A:510:LEU:O	2.17	0.44
1:B:78:ASP:OD1	1:B:78:ASP:N	2.48	0.44
1:B:616:GLU:OE1	1:B:616:GLU:N	2.51	0.44
1:C:1078:ILE:HD13	1:C:1132:ASN:HD22	1.81	0.44
1:A:21:ARG:H	1:A:21:ARG:HD3	1.83	0.44
1:A:32:PHE:HZ	1:A:212:ASP:HB2	1.82	0.44
1:A:419:ASN:ND2	1:A:450:TYR:HB2	2.33	0.44
1:B:643:ARG:HD3	1:C:833:GLN:HE22	1.83	0.44
1:B:673:THR:HA	1:B:687:GLN:HA	2.00	0.44
1:A:41:LYS:HD2	1:C:559:PHE:O	2.16	0.44
1:A:94:GLU:HB3	1:A:96:SER:O	2.18	0.44
1:B:27:ALA:HB3	1:B:64:TRP:HE1	1.82	0.44
1:B:43:PHE:CE1	1:B:280:GLY:HA3	2.53	0.44
1:B:700:ASN:OD1	1:B:701:SER:N	2.51	0.44
1:C:738:TYR:CE2	1:C:1001:LEU:HD21	2.53	0.44
1:A:617:VAL:HA	1:A:621:ILE:HG21	2.00	0.44
1:B:339:PHE:CE1	1:B:508:VAL:HB	2.52	0.44
1:C:419:ASN:ND2	1:C:450:TYR:HB2	2.32	0.44
1:C:451:ARG:HH12	1:C:467:THR:HG23	1.83	0.44
2:D:39:ARG:NH2	2:D:66:SER:OG	2.50	0.44
1:A:801:GLN:O	1:A:815:ILE:HG12	2.17	0.44
1:B:354:ARG:NH2	1:B:393:TYR:OH	2.44	0.44
1:C:198:ILE:HG23	1:C:223:LEU:HB2	1.98	0.44
1:C:403:GLU:O	1:C:407:ILE:HG23	2.18	0.44
2:D:86:MET:SD	2:D:89:LEU:HD21	2.57	0.44
1:A:54:LEU:HA	1:A:269:PRO:HA	1.98	0.44
1:A:794:PHE:HB2	1:A:799:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:LEU:HD23	1:A:935:LEU:HA	1.87	0.44
1:B:174:LEU:H	1:B:174:LEU:HD23	1.82	0.44
1:B:740:CYS:HB3	1:B:746:CYS:HB3	1.90	0.44
1:C:1044:TYR:HB2	1:C:1064:TYR:HB3	2.00	0.44
2:E:63:TYR:HB2	2:E:68:LYS:HG2	2.00	0.44
1:B:348:TYR:CE1	1:B:449:LEU:HD21	2.52	0.43
1:C:243:ARG:NH1	1:C:244:SER:OG	2.52	0.43
1:C:418:TYR:HA	1:C:454:ARG:NH2	2.32	0.43
1:B:308:GLY:HA2	1:B:661:ILE:HG12	2.00	0.43
1:B:712:PRO:HA	1:B:1069:GLU:HA	2.00	0.43
1:B:748:ASN:HA	1:B:751:LEU:HG	2.00	0.43
1:C:570:THR:HG22	1:C:584:ILE:HG21	1.99	0.43
1:C:819:LEU:O	1:C:823:VAL:HG23	2.18	0.43
2:D:114:ARG:HD2	2:D:117:TRP:HE1	1.83	0.43
1:B:556:PHE:HB3	1:B:574:ARG:NH2	2.33	0.43
1:B:906:ILE:HG13	1:B:908:VAL:HG23	2.01	0.43
1:C:159:ASN:OD1	1:C:159:ASN:N	2.51	0.43
1:C:436:ASN:HB2	1:C:503:GLN:OE1	2.19	0.43
1:A:127:LYS:HD2	1:A:164:GLU:OE1	2.18	0.43
1:A:402:ASP:OD1	1:A:402:ASP:N	2.52	0.43
1:A:927:ALA:O	1:A:931:ILE:HG12	2.19	0.43
1:B:57:PRO:HG3	1:B:270:ARG:HE	1.84	0.43
1:B:79:ASN:HB3	1:B:236:GLN:HE21	1.84	0.43
1:B:719:VAL:HG22	1:B:1062:VAL:HG13	2.01	0.43
1:C:969:ALA:HA	1:C:992:ARG:NH2	2.33	0.43
1:A:432:ALA:HB2	1:A:507:VAL:HG13	2.00	0.43
1:B:126:ILE:HD12	1:B:165:TYR:HD2	1.83	0.43
1:B:1139:GLN:HG3	1:B:1140:PRO:HD3	2.00	0.43
1:C:142:LYS:HB2	1:C:242:HIS:CG	2.53	0.43
1:C:548:VAL:N	1:C:585:THR:O	2.30	0.43
1:A:1113:THR:HG22	1:A:1135:TYR:HB3	2.00	0.43
1:C:241:LEU:HD22	1:C:256:THR:HA	2.01	0.43
1:C:454:ARG:NH1	1:C:458:LEU:HG	2.30	0.43
1:C:1002:GLN:HA	1:C:1005:VAL:HG12	2.01	0.43
1:A:67:VAL:HA	1:A:76:ARG:HH22	1.83	0.43
1:B:348:TYR:HD1	1:B:449:LEU:HD11	1.84	0.43
1:B:898:GLN:O	1:B:902:ARG:HG3	2.18	0.43
1:C:656:SER:HB3	1:C:695:SER:HB3	2.00	0.43
1:C:734:ASP:HB3	1:C:737:MET:SD	2.59	0.43
1:C:919:LEU:HG	1:C:923:GLN:HE21	1.84	0.43
1:A:34:ARG:NH1	1:A:216:GLY:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HG22	1:A:182:LYS:HE2	2.00	0.43
1:A:324:VAL:HG11	1:A:540:PHE:CE1	2.53	0.43
1:B:1081:ASP:HB2	1:B:1083:LYS:NZ	2.34	0.43
1:B:1083:LYS:HD2	1:B:1119:VAL:HG11	2.00	0.43
1:C:574:ARG:HA	1:C:581:ILE:HG22	2.01	0.43
1:A:305:VAL:HB	1:A:599:THR:HG23	2.01	0.43
1:B:144:ASN:H	1:B:149:GLU:HG2	1.83	0.43
1:C:620:ALA:HA	1:C:622:HIS:CE1	2.53	0.43
2:D:94:THR:OG1	2:D:124:THR:HA	2.19	0.43
1:B:108:LEU:HG	1:B:234:ARG:HH12	1.84	0.42
1:C:400:ARG:NH1	1:C:492:TYR:O	2.52	0.42
2:E:112:TYR:O	2:E:114:ARG:NE	2.42	0.42
1:A:555:LYS:HE2	1:A:555:LYS:HB2	1.89	0.42
1:A:1139:GLN:HG3	1:A:1140:PRO:HD3	2.02	0.42
1:B:163:PHE:CE2	1:B:165:TYR:HB2	2.54	0.42
1:B:284:ASP:HB3	1:B:303:PHE:HE2	1.83	0.42
1:C:305:VAL:N	1:C:599:THR:OG1	2.44	0.42
1:C:918:LYS:H	1:C:918:LYS:CD	2.32	0.42
1:A:970:ILE:HD13	1:A:981:LEU:HD13	2.01	0.42
1:B:927:ALA:O	1:B:931:ILE:HG12	2.20	0.42
1:B:982:ASP:HB2	1:B:984:PRO:HD2	2.01	0.42
1:C:67:VAL:O	1:C:260:ALA:N	2.52	0.42
1:C:658:GLU:O	1:C:692:TYR:OH	2.25	0.42
1:B:805:ASP:OD1	1:B:805:ASP:N	2.46	0.42
3:I:1:NAG:O6	3:I:2:NAG:N2	2.52	0.42
1:A:618:PRO:O	1:A:621:ILE:HG12	2.19	0.42
1:B:512:PHE:HE2	1:C:980:ARG:HH12	1.68	0.42
1:C:19:THR:HG23	1:C:75:LYS:HE2	1.99	0.42
1:C:618:PRO:O	1:C:621:ILE:HG12	2.20	0.42
2:D:79:LYS:NZ	2:D:83:TYR:OH	2.43	0.42
1:A:436:ASN:HB2	1:A:503:GLN:OE1	2.19	0.42
1:A:888:GLY:HA3	1:A:889:PRO:HD3	1.95	0.42
1:B:126:ILE:O	1:B:165:TYR:N	2.52	0.42
1:B:355:ILE:HG22	1:B:521:VAL:HG21	2.02	0.42
1:B:851:LYS:HG3	1:B:852:PHE:H	1.85	0.42
1:C:194:GLY:HA2	1:C:229:GLY:HA2	2.01	0.42
1:C:565:ASP:N	1:C:565:ASP:OD1	2.53	0.42
1:C:757:CYS:O	1:C:760:LEU:HD12	2.20	0.42
1:C:957:ASN:O	1:C:961:LYS:HG2	2.19	0.42
1:A:1108:GLU:N	1:A:1108:GLU:OE2	2.53	0.42
1:B:292:PRO:HG3	1:B:630:TRP:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:MET:SD	1:B:729:THR:N	2.92	0.42
1:A:336:ASP:OD1	1:A:336:ASP:N	2.50	0.42
1:A:663:ILE:HD13	1:A:667:ILE:HG22	2.01	0.42
1:C:54:LEU:HA	1:C:269:PRO:HA	2.00	0.42
2:D:34:ARG:NE	2:D:107:CYS:SG	2.91	0.42
3:N:1:NAG:H4	3:N:2:NAG:H2	1.74	0.42
1:A:966:LYS:HB3	1:B:752:GLN:HB2	2.02	0.42
1:B:801:GLN:HE22	3:K:2:NAG:HN2	1.66	0.42
1:B:906:ILE:HD13	1:B:1046:LEU:HD21	2.02	0.42
1:C:78:ASP:N	1:C:78:ASP:OD1	2.41	0.42
1:C:453:PHE:H	1:C:488:PRO:HB3	1.84	0.42
1:C:525:LYS:HD2	1:C:527:SER:H	1.85	0.42
1:C:983:PRO:O	1:C:987:GLU:HG2	2.20	0.42
3:K:1:NAG:H5	3:K:2:NAG:O5	2.20	0.42
1:A:300:LEU:HD12	1:A:305:VAL:HG22	2.02	0.42
1:A:970:ILE:HG12	1:A:989:GLN:NE2	2.34	0.42
1:B:451:ARG:NH2	1:B:488:PRO:O	2.53	0.42
1:C:412:THR:OG1	2:E:54:ARG:NH2	2.53	0.42
1:A:321:GLU:O	1:A:536:VAL:HB	2.20	0.41
1:B:547:GLY:HA2	1:B:586:PRO:HA	2.02	0.41
1:C:151:GLU:HA	1:C:153:ARG:NH1	2.35	0.41
1:C:715:PHE:HA	1:C:1066:PRO:HA	2.02	0.41
1:C:805:ASP:OD1	1:C:805:ASP:N	2.48	0.41
1:A:200:SER:HB3	1:A:223:LEU:HD11	2.01	0.41
1:A:728:MET:N	1:A:771:GLN:OE1	2.43	0.41
1:B:196:PHE:O	1:B:225:ASP:HA	2.20	0.41
1:B:428:GLY:HA2	1:B:512:PHE:CE1	2.55	0.41
1:C:375:LYS:HA	1:C:381:PRO:HB3	2.01	0.41
1:C:794:PHE:HB2	1:C:799:PHE:HE2	1.85	0.41
2:D:5:LEU:HB3	2:D:99:CYS:SG	2.60	0.41
2:D:72:THR:HB	2:D:85:GLN:HB3	2.03	0.41
1:A:241:LEU:HD22	1:A:256:THR:HA	2.02	0.41
1:A:1012:ALA:HA	1:A:1015:ILE:HG22	2.01	0.41
1:A:1045:HIS:HA	1:A:1063:THR:HG22	2.02	0.41
1:B:969:ALA:HA	1:B:992:ARG:HH22	1.85	0.41
1:C:1139:GLN:HG3	1:C:1140:PRO:HD3	2.02	0.41
2:E:86:MET:CE	2:E:89:LEU:HD21	2.50	0.41
1:A:23:GLN:HA	1:A:77:PHE:CZ	2.55	0.41
1:A:801:GLN:O	1:A:814:PRO:HD2	2.19	0.41
1:B:400:ARG:HD3	1:B:492:TYR:CE1	2.56	0.41
1:C:97:ASN:HD21	1:C:100:ARG:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:THR:OG1	1:C:432:ALA:N	2.53	0.41
1:C:471:GLN:HE22	1:C:476:PRO:HA	1.84	0.41
1:A:33:THR:HA	1:A:58:PHE:CD1	2.54	0.41
1:A:113:GLN:HA	1:A:130:GLU:HG3	2.02	0.41
1:A:1064:TYR:HE1	1:A:1066:PRO:HG3	1.86	0.41
1:B:1123:CYS:HB2	1:B:1129:ILE:HD13	2.02	0.41
1:C:182:LYS:HG3	1:C:208:ARG:NH1	2.34	0.41
1:C:206:ILE:HD12	1:C:206:ILE:H	1.84	0.41
1:C:773:LYS:HB3	1:C:773:LYS:HE2	1.76	0.41
1:C:797:PHE:HD1	1:C:924:PHE:CD2	2.37	0.41
1:B:311:GLN:NE2	1:B:592:VAL:O	2.53	0.41
1:C:113:GLN:HA	1:C:130:GLU:HG3	2.03	0.41
1:C:126:ILE:HB	1:C:165:TYR:HB3	2.01	0.41
1:C:455:LYS:HD2	1:C:456:SER:H	1.86	0.41
1:C:555:LYS:HE2	1:C:555:LYS:HB2	1.89	0.41
3:P:1:NAG:H4	3:P:2:NAG:H2	1.73	0.41
1:A:197:LYS:HE2	1:A:197:LYS:HB2	1.92	0.41
1:A:449:LEU:HA	1:A:492:TYR:CE1	2.56	0.41
1:A:565:ASP:OD2	1:A:569:THR:OG1	2.39	0.41
1:B:154:VAL:HG23	1:B:155:TYR:HD1	1.86	0.41
1:B:505:TYR:O	1:B:507:VAL:HG23	2.20	0.41
1:B:794:PHE:O	1:B:797:PHE:HB2	2.19	0.41
1:C:611:GLY:N	1:C:644:ALA:O	2.49	0.41
1:A:476:PRO:HB2	1:A:478:ASN:OD1	2.21	0.41
1:A:827:ASP:N	1:A:827:ASP:OD1	2.53	0.41
1:B:659:CYS:SG	1:B:660:ASP:N	2.93	0.41
1:B:753:TYR:OH	1:B:991:ASP:OD1	2.20	0.41
1:B:859:PRO:HA	1:B:860:PRO:HD3	1.99	0.41
1:C:725:PRO:HD3	1:C:944:LYS:HE3	2.02	0.41
1:C:985:GLU:OE1	1:C:989:GLN:HG2	2.20	0.41
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.55	0.41
1:A:208:ARG:HD3	1:A:208:ARG:HA	1.88	0.41
1:A:418:TYR:HA	1:A:454:ARG:NH2	2.36	0.41
1:A:528:THR:HB	1:A:570:THR:HG21	2.02	0.41
1:A:821:ASN:O	1:A:824:THR:HG22	2.21	0.41
1:A:866:MET:H	1:A:866:MET:HG3	1.55	0.41
1:B:823:VAL:HG22	1:B:942:LEU:HD13	2.03	0.41
1:C:94:GLU:HB3	1:C:96:SER:O	2.21	0.41
1:C:122:THR:O	1:C:169:PRO:HD3	2.21	0.41
1:C:749:LEU:O	1:C:752:GLN:HG3	2.20	0.41
2:D:30:LEU:HD13	2:D:35:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:MET:SD	1:A:172:MET:N	2.93	0.40
1:A:471:GLN:HE22	1:A:476:PRO:HA	1.85	0.40
1:A:773:LYS:O	1:A:774:ASN:C	2.59	0.40
1:B:278:GLU:H	4:B:1303:NAG:H82	1.86	0.40
1:B:735:CYS:O	1:B:739:ILE:HG22	2.20	0.40
1:B:1079:CYS:HB2	1:B:1123:CYS:HB2	1.83	0.40
1:C:142:LYS:O	1:C:242:HIS:ND1	2.54	0.40
1:C:836:ASP:OD1	1:C:836:ASP:N	2.52	0.40
2:E:13:VAL:HG11	2:E:19:LEU:HG	2.03	0.40
1:A:529:ASN:ND2	1:A:536:VAL:O	2.54	0.40
1:A:1073:THR:O	1:A:1094:SER:N	2.54	0.40
1:B:400:ARG:HD3	1:B:492:TYR:CD1	2.55	0.40
1:B:822:LYS:HE3	1:B:935:LEU:O	2.21	0.40
1:C:292:PRO:HA	1:C:630:TRP:CZ2	2.56	0.40
2:D:76:ASP:OD2	2:D:76:ASP:N	2.54	0.40
1:A:879:ILE:HD12	1:A:879:ILE:HA	1.82	0.40
1:A:881:SER:HB3	1:A:884:THR:OG1	2.21	0.40
1:B:992:ARG:HG2	1:B:992:ARG:HH11	1.86	0.40
1:C:53:ASP:OD1	1:C:54:LEU:N	2.50	0.40
1:C:97:ASN:ND2	1:C:100:ARG:HD2	2.36	0.40
1:C:1023:ALA:HA	1:C:1026:MET:HG3	2.04	0.40
1:A:19:THR:HG23	1:A:75:LYS:HE2	2.03	0.40
1:A:50:SER:HA	1:A:273:LEU:HA	2.03	0.40
1:A:127:LYS:HG2	1:A:131:PHE:CZ	2.54	0.40
1:A:140:ASP:CG	1:A:153:ARG:HH22	2.24	0.40
1:B:32:PHE:HE2	1:B:212:ASP:HB2	1.85	0.40
1:B:617:VAL:HG13	1:B:621:ILE:HD11	2.04	0.40
1:B:866:MET:H	1:B:866:MET:HG3	1.57	0.40
1:C:967:PHE:HB2	1:C:993:LEU:HD23	2.04	0.40
1:C:1026:MET:HB3	1:C:1059:PHE:CZ	2.57	0.40
1:A:971:SER:OG	1:A:980:ARG:NH2	2.50	0.40
1:C:100:ARG:HG2	1:C:119:ASN:HB3	2.03	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	1086/1254 (87%)	1015 (94%)	67 (6%)	4 (0%)	34	71
1	B	1086/1254 (87%)	1004 (92%)	78 (7%)	4 (0%)	34	71
1	C	1086/1254 (87%)	1035 (95%)	47 (4%)	4 (0%)	34	71
2	D	126/126 (100%)	121 (96%)	5 (4%)	0	100	100
2	E	126/126 (100%)	124 (98%)	2 (2%)	0	100	100
All	All	3510/4014 (87%)	3299 (94%)	199 (6%)	12 (0%)	44	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	THR
1	C	531	VAL
1	A	480	VAL
1	A	528	THR
1	C	480	VAL
1	B	369	ALA
1	B	502	HIS
1	A	160	ASN
1	C	160	ASN
1	A	125	VAL
1	B	206	ILE
1	C	125	VAL

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	957/1096 (87%)	937 (98%)	20 (2%)	53	72
1	B	959/1096 (88%)	950 (99%)	9 (1%)	78	88
1	C	957/1096 (87%)	942 (98%)	15 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	106/104 (102%)	104 (98%)	2 (2%)	57 75
2	E	106/104 (102%)	106 (100%)	0	100 100
All	All	3085/3496 (88%)	3039 (98%)	46 (2%)	66 80

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	64	TRP
1	A	268	GLN
1	A	352	ARG
1	A	375	LYS
1	A	446	TYR
1	A	475	LYS
1	A	522	CYS
1	A	540	PHE
1	A	549	LEU
1	A	631	ARG
1	A	694	MET
1	A	714	ASN
1	A	728	MET
1	A	737	MET
1	A	834	TYR
1	A	855	LEU
1	A	866	MET
1	A	978	PHE
1	A	980	ARG
1	B	119	ASN
1	B	381	PRO
1	B	506	ARG
1	B	526	LYS
1	B	737	MET
1	B	798	ASN
1	B	866	MET
1	B	1035	LYS
1	B	1047	MET
1	C	21	ARG
1	C	89	TYR
1	C	172	MET
1	C	356	SER
1	C	375	LYS

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Mol	Chain	Res	Type
1	C	455	LYS
1	C	525	LYS
1	C	529	ASN
1	C	631	ARG
1	C	728	MET
1	C	760	LEU
1	C	966	LYS
1	C	1026	MET
1	C	1107	TYR
1	C	1135	TYR
2	D	33	TYR
2	D	62	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	419	ASN
1	A	610	GLN
1	A	910	GLN
1	B	236	GLN
1	B	801	GLN
1	B	904	ASN
1	C	419	ASN
1	C	752	GLN
2	E	2	GLN

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)

22 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	$\#\|Z\| > 2$
3	NAG	F	1	1,3	14,14,15	0.77	1 (7%)	17,19,21	0.71	1 (5%)
3	NAG	F	2	3	14,14,15	1.06	1 (7%)	17,19,21	1.26	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	H	1	1,3	14,14,15	0.47	0	17,19,21	1.34	2 (11%)
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	0.40	0
3	NAG	I	1	1,3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	I	2	3	14,14,15	0.62	1 (7%)	17,19,21	1.32	2 (11%)
3	NAG	J	1	1,3	14,14,15	1.61	1 (7%)	17,19,21	1.44	1 (5%)
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.68	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	K	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.35	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	M	1	1,3	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
3	NAG	M	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	N	1	1,3	14,14,15	0.17	0	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.59	0	17,19,21	0.50	0
3	NAG	O	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	O	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	P	1	1,3	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	P	2	3	14,14,15	0.50	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-5.52	1.34	1.43
3	F	2	NAG	O5-C1	3.82	1.49	1.43
3	K	2	NAG	O5-C1	2.95	1.48	1.43
3	O	1	NAG	O5-C1	-2.82	1.39	1.43
3	F	1	NAG	O5-C1	-2.66	1.39	1.43
3	K	1	NAG	O5-C1	-2.43	1.39	1.43
3	I	2	NAG	C1-C2	2.15	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C1-O5-C5	5.19	119.23	112.19
3	F	2	NAG	C1-O5-C5	4.81	118.72	112.19
3	J	1	NAG	C3-C4-C5	4.55	118.35	110.24
3	I	2	NAG	C2-N2-C7	4.22	128.91	122.90
3	M	1	NAG	C2-N2-C7	4.12	128.77	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	3.59	117.05	112.19
3	H	1	NAG	C3-C4-C5	3.00	115.59	110.24
3	J	2	NAG	C1-O5-C5	2.52	115.60	112.19
3	M	1	NAG	C1-C2-N2	2.37	114.53	110.49
3	O	1	NAG	C3-C4-C5	2.30	114.34	110.24
3	I	2	NAG	C1-C2-N2	2.17	114.20	110.49
3	K	1	NAG	C3-C4-C5	2.11	114.00	110.24
3	F	1	NAG	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	N	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C3-C2-N2-C7
3	O	1	NAG	C3-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7

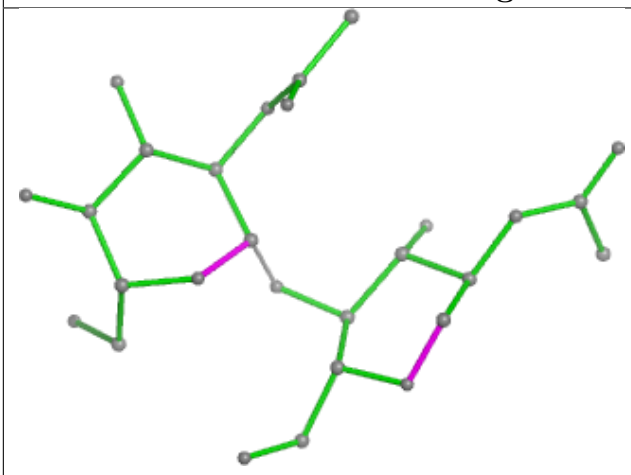
There are no ring outliers.

10 monomers are involved in 16 short contacts:

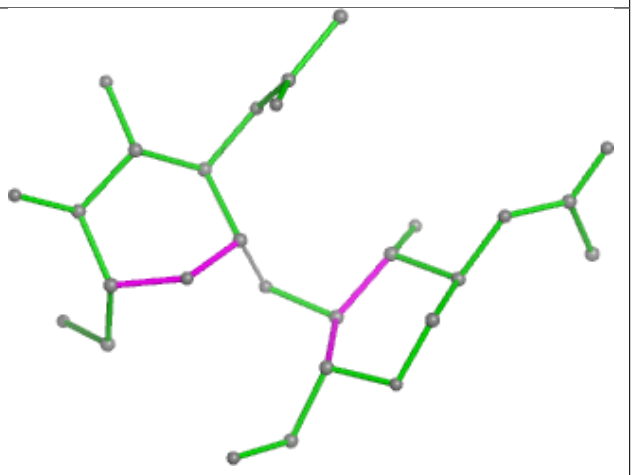
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	3	0
3	K	2	NAG	2	0
3	M	1	NAG	4	0
3	I	1	NAG	2	0
3	N	2	NAG	2	0
3	P	1	NAG	1	0
3	N	1	NAG	3	0
3	I	2	NAG	3	0
3	P	2	NAG	1	0
3	H	1	NAG	1	0

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

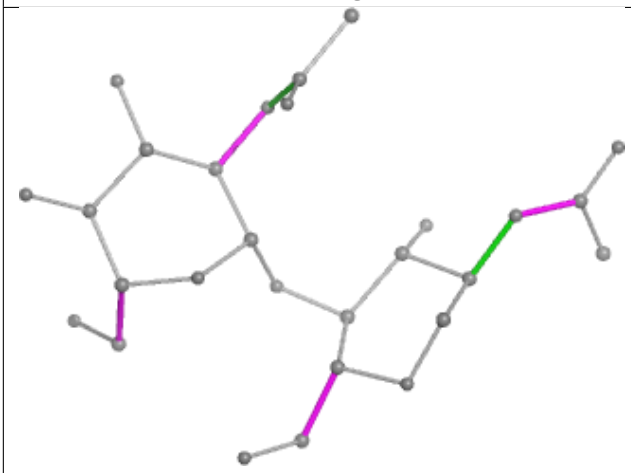
Oligosaccharide Chain F



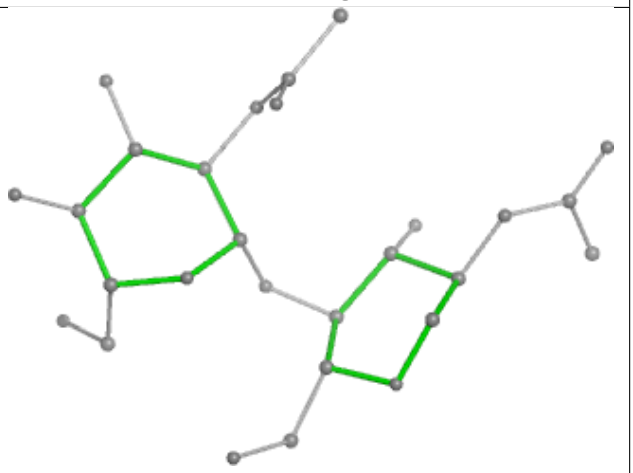
Bond lengths



Bond angles

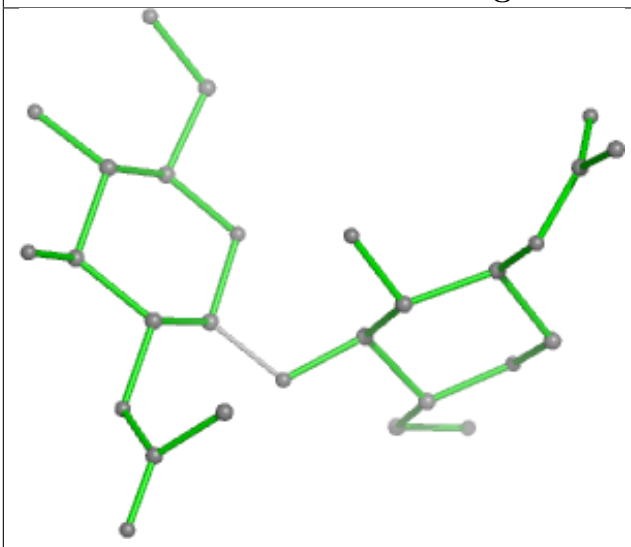


Torsions

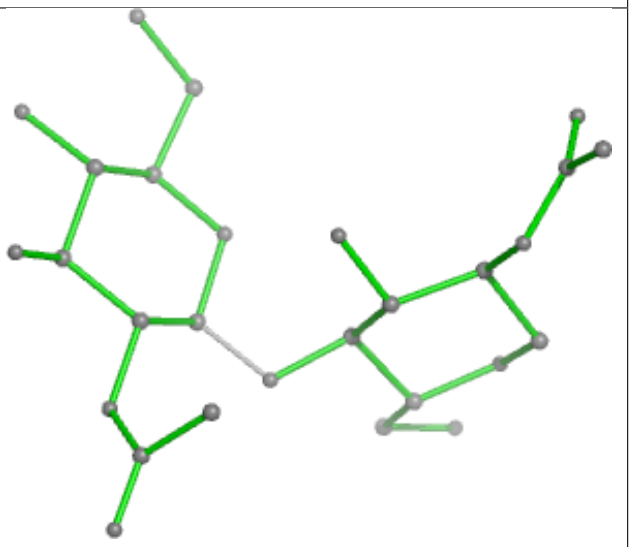


Rings

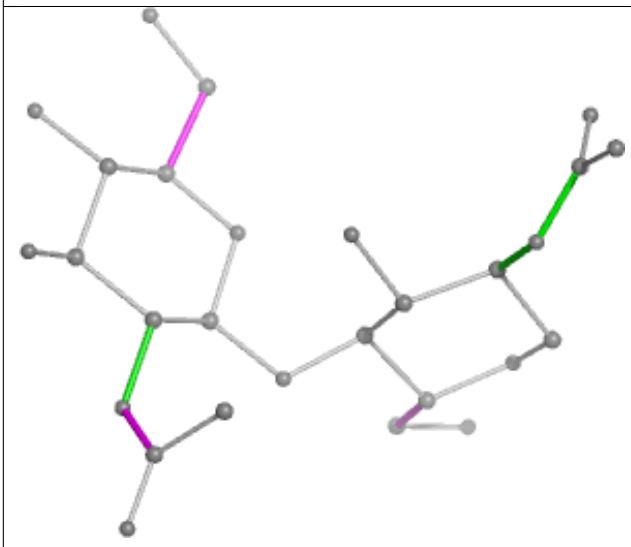
Oligosaccharide Chain G



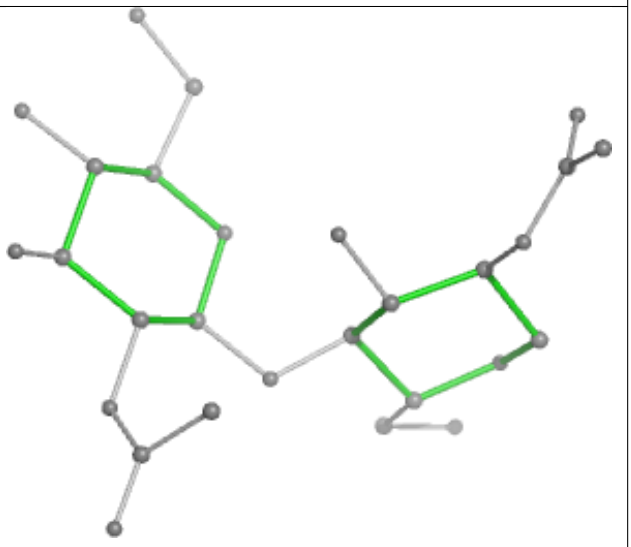
Bond lengths



Bond angles

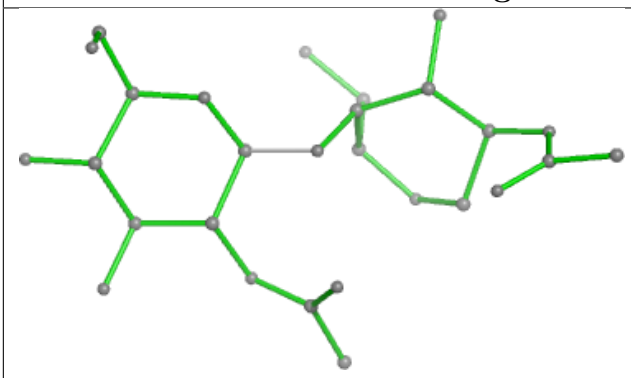


Torsions

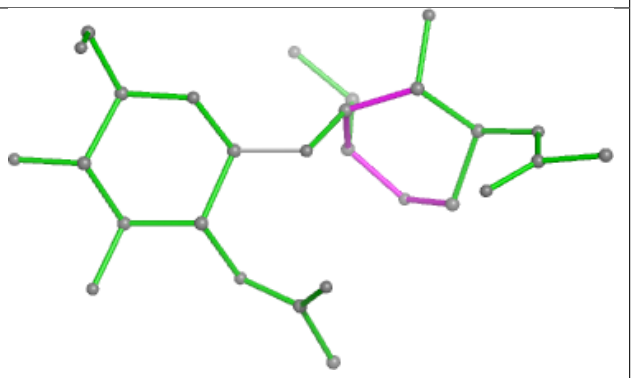


Rings

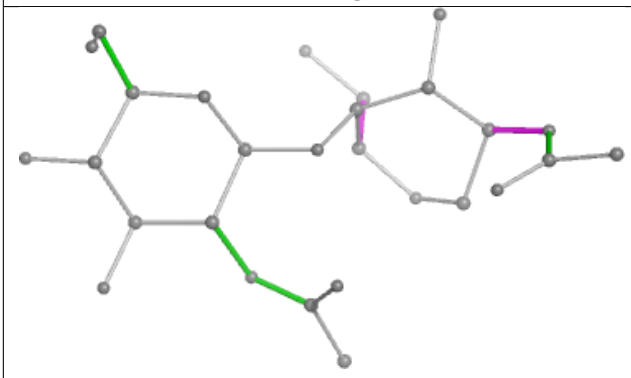
Oligosaccharide Chain H



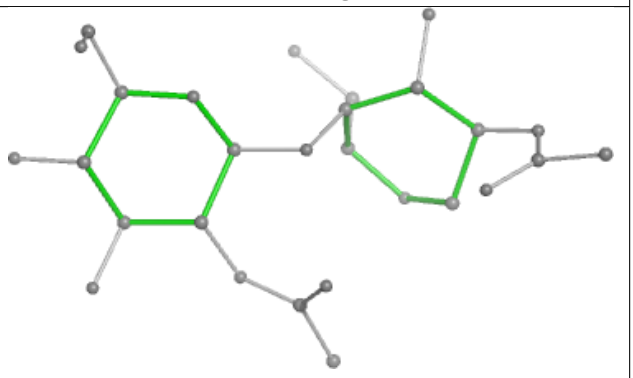
Bond lengths



Bond angles

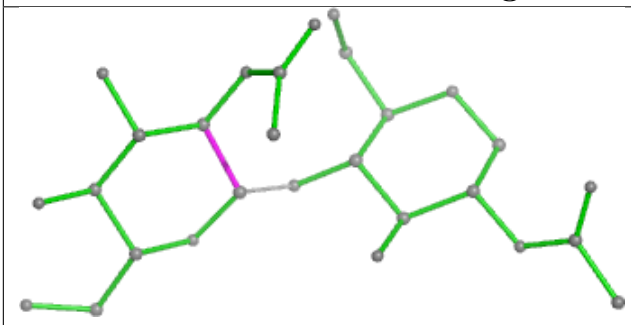


Torsions

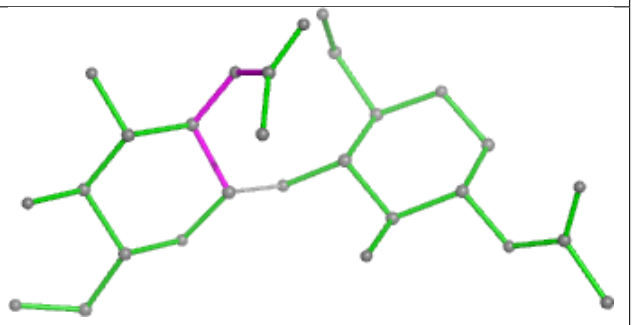


Rings

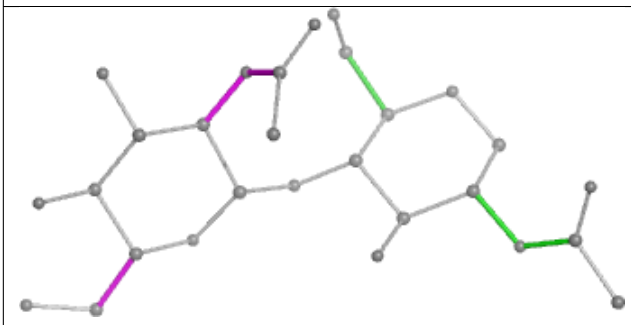
Oligosaccharide Chain I



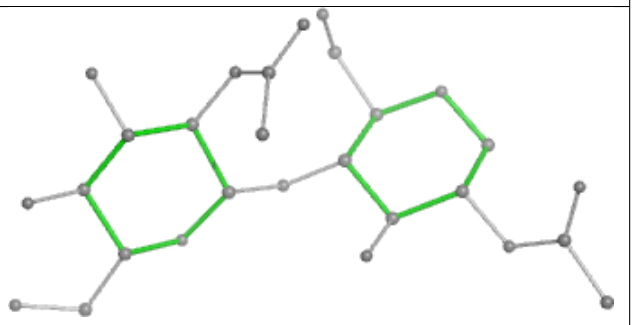
Bond lengths



Bond angles

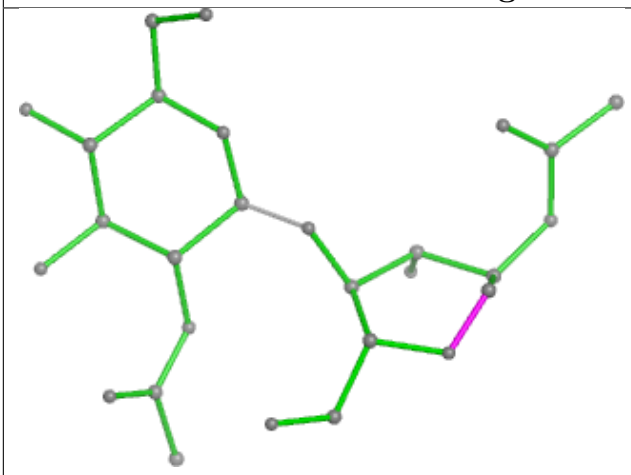


Torsions

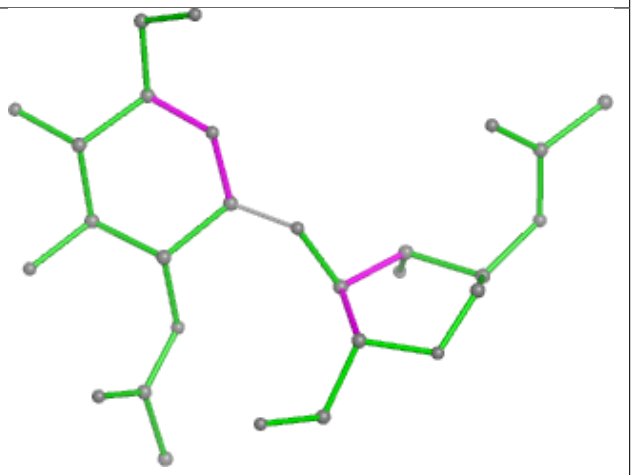


Rings

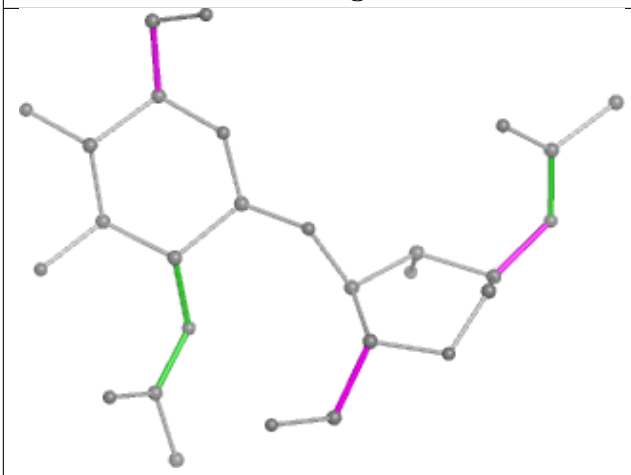
Oligosaccharide Chain J



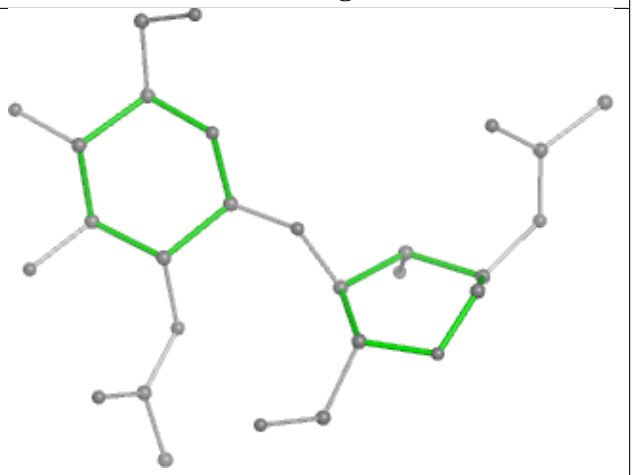
Bond lengths



Bond angles

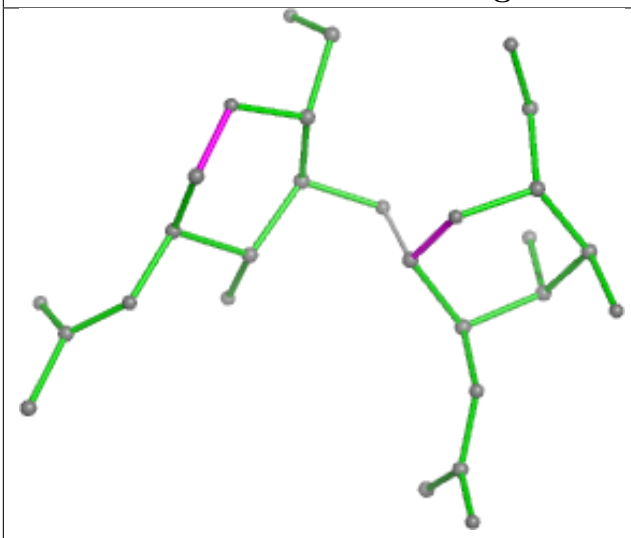


Torsions

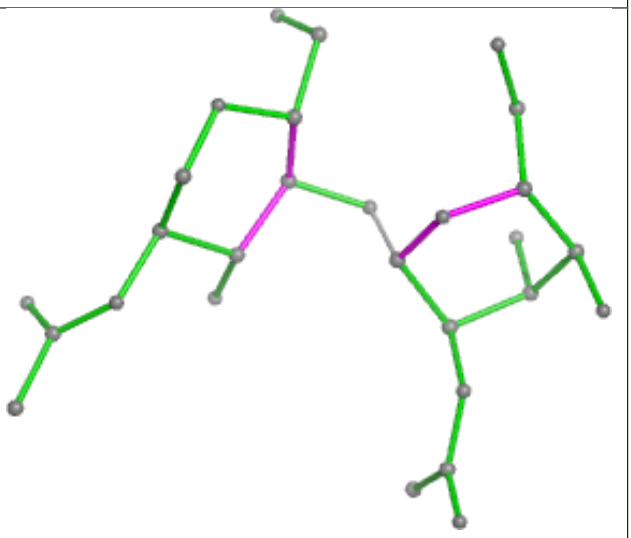


Rings

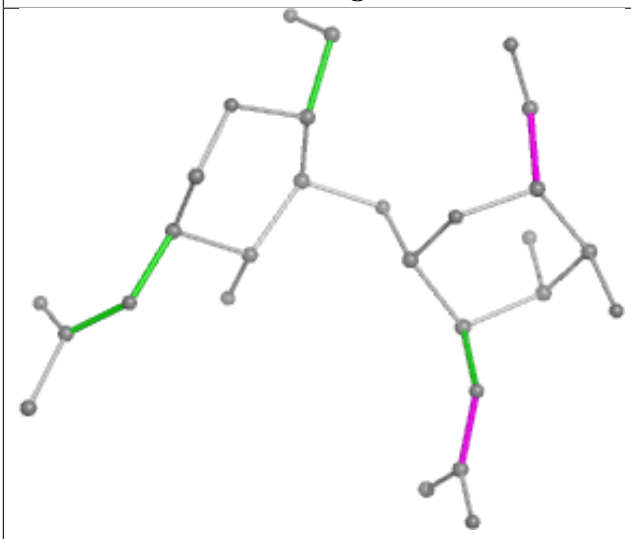
Oligosaccharide Chain K



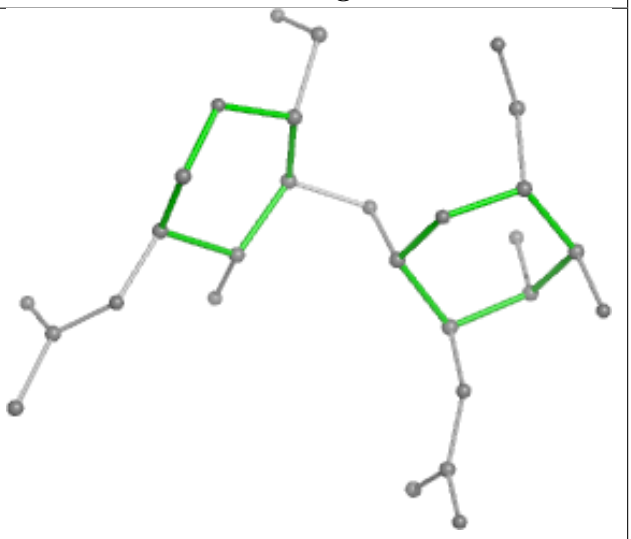
Bond lengths



Bond angles

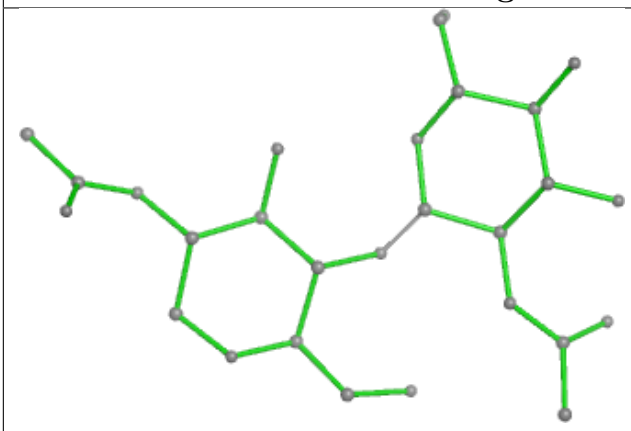


Torsions

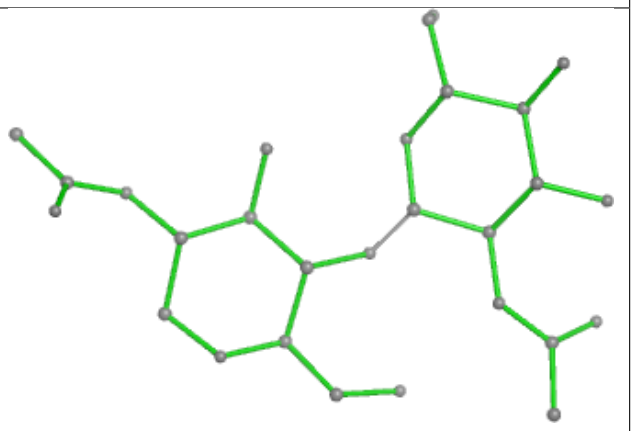


Rings

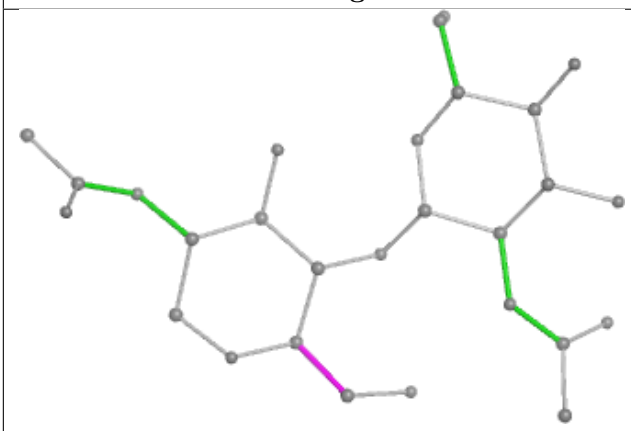
Oligosaccharide Chain L



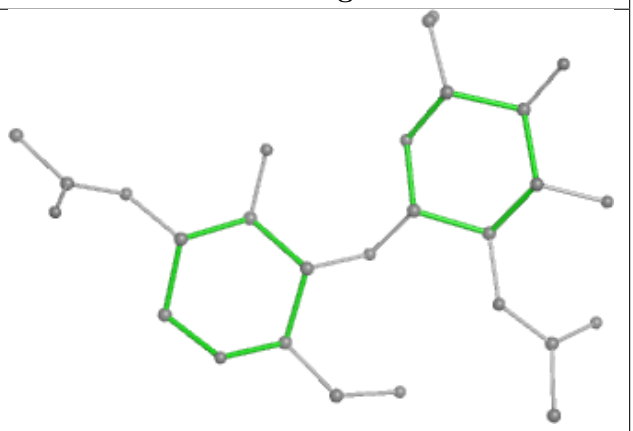
Bond lengths



Bond angles

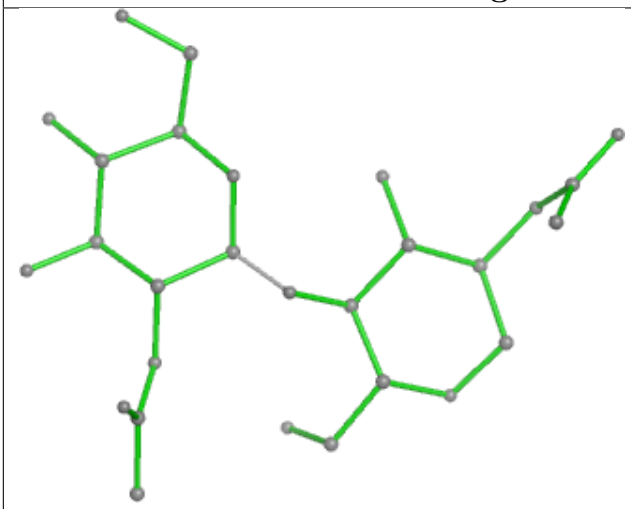


Torsions

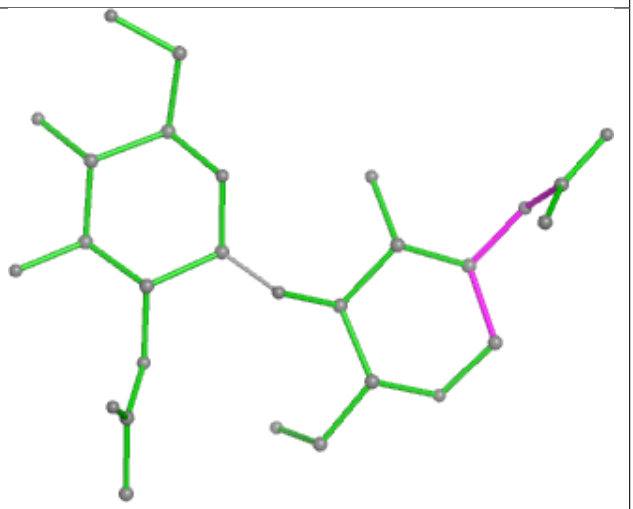


Rings

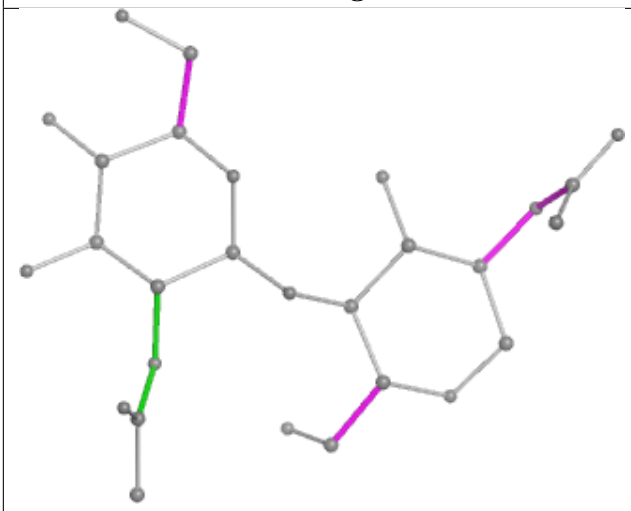
Oligosaccharide Chain M



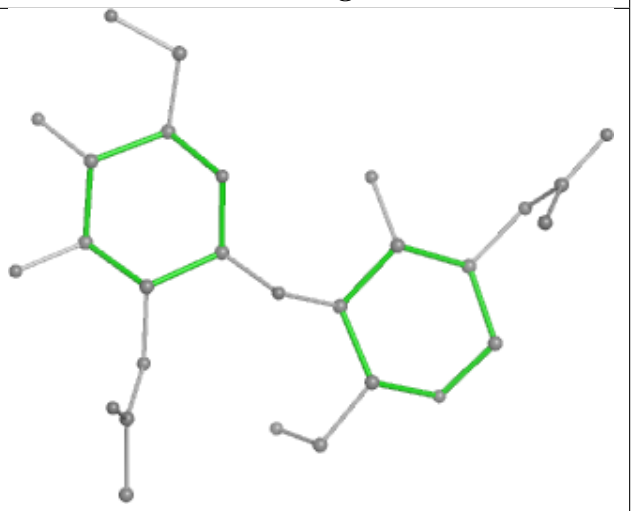
Bond lengths



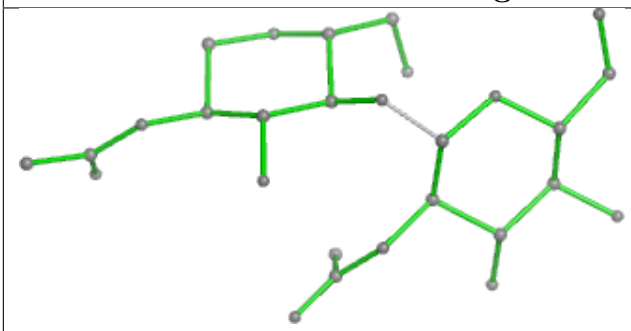
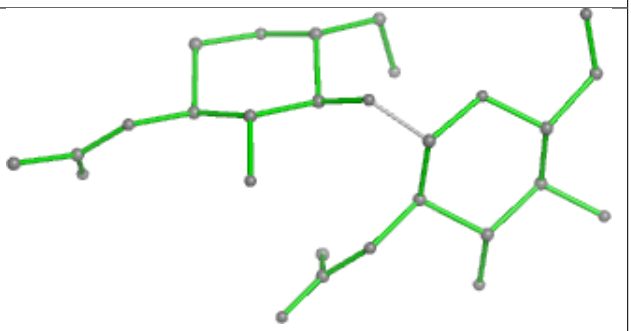
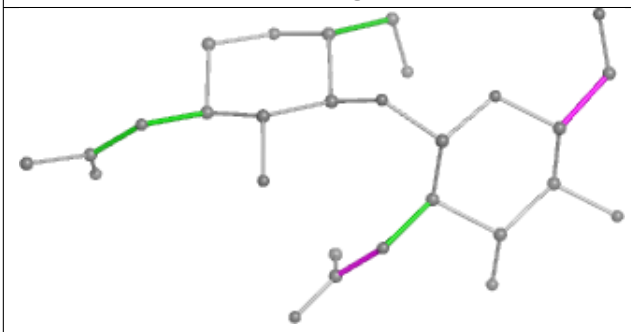
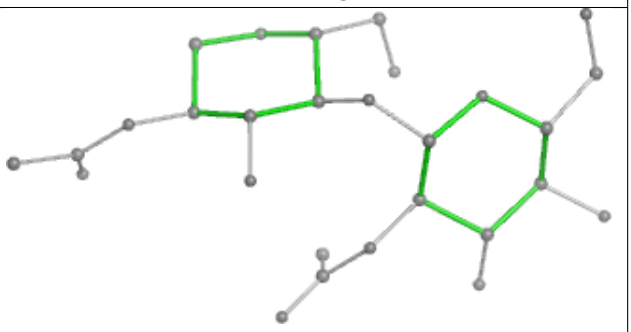
Bond angles



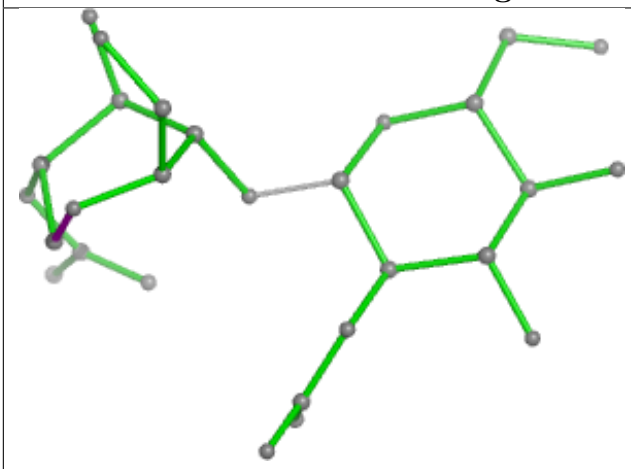
Torsions



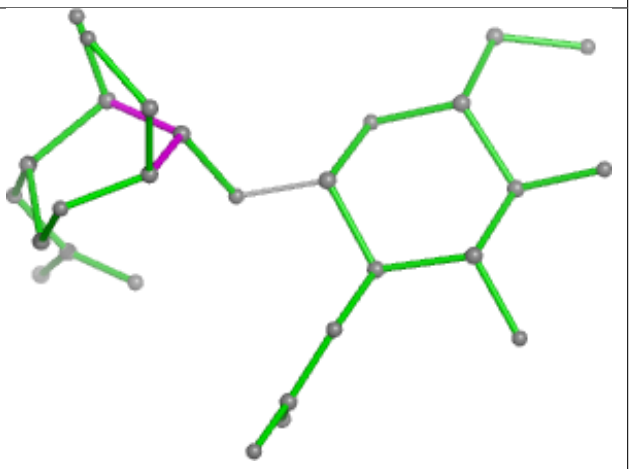
Rings

Oligosaccharide Chain N	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

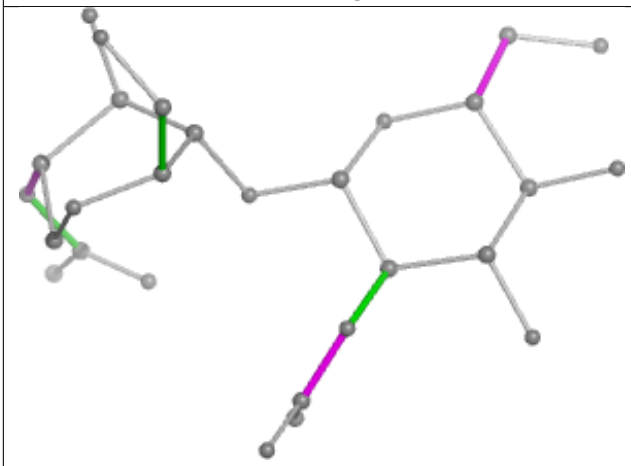
Oligosaccharide Chain O



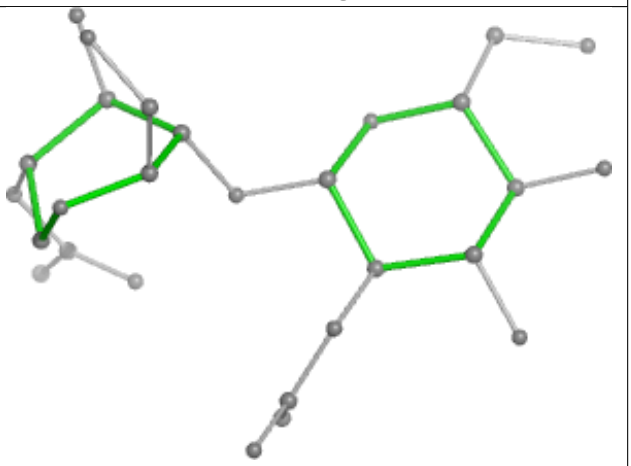
Bond lengths



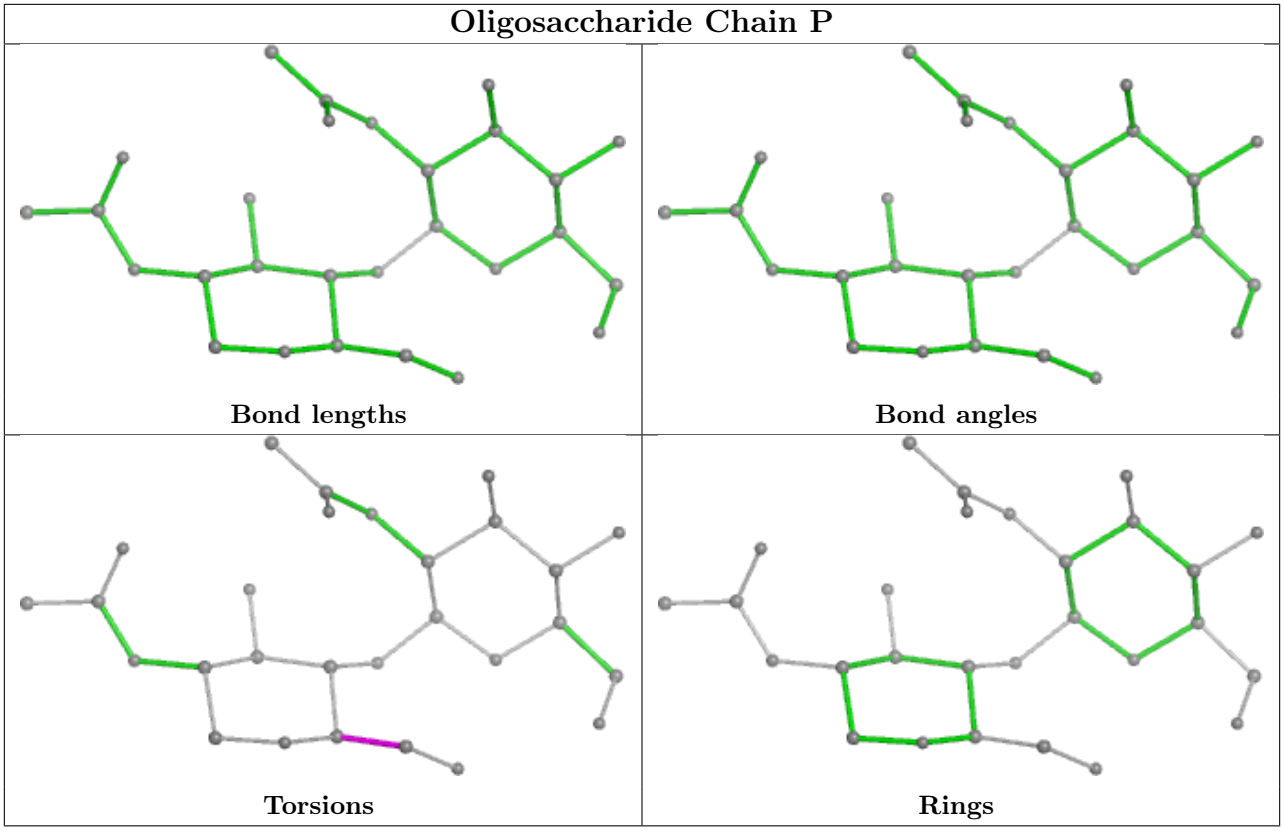
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

15 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	C	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1302	1	14,14,15	0.39	0	17,19,21	0.57	0
4	NAG	A	1303	-	14,14,15	0.45	0	17,19,21	0.69	0
4	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.34	0
4	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.37	0
4	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	A	1302	1	14,14,15	0.41	0	17,19,21	1.28	2 (11%)
4	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1308	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.49	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	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1302	NAG	C2-N2-C7	4.34	129.09	122.90
4	A	1302	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	C	1301	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	B	1304	NAG	C1-C2-N2-C7
4	C	1302	NAG	O5-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1305	NAG	C3-C2-N2-C7
4	A	1302	NAG	C3-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	NAG	1	0
4	B	1301	NAG	1	0
4	A	1302	NAG	2	0
4	B	1303	NAG	3	0
4	C	1306	NAG	2	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.

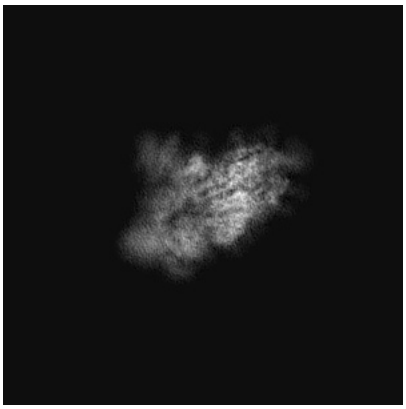
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17296. These allow visual inspection of the internal detail of the map and identification of artifacts.

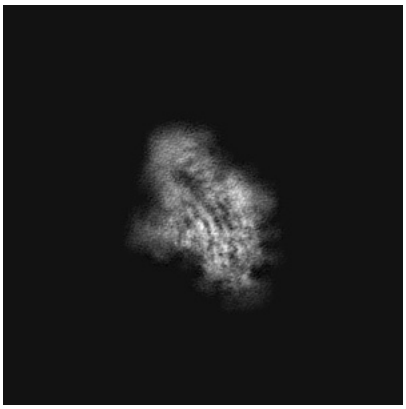
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

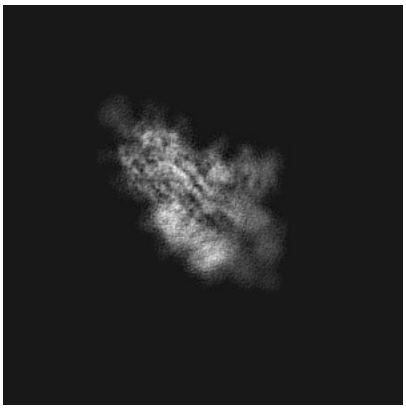
6.1.1 Primary map



X

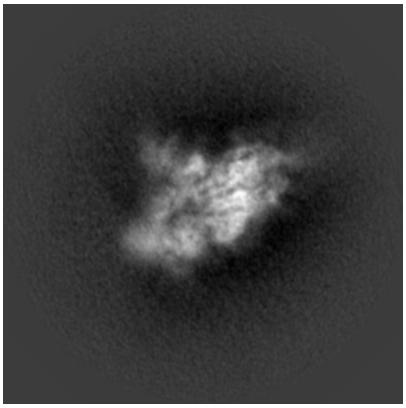


Y

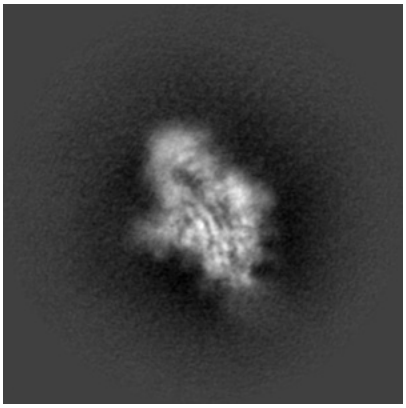


Z

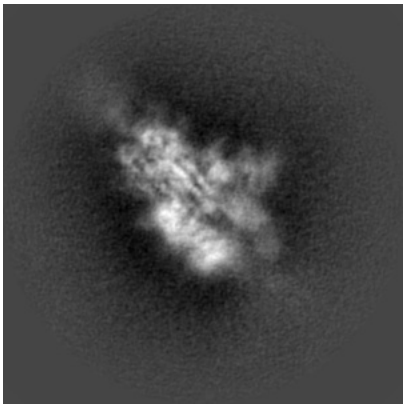
6.1.2 Raw map



X



Y

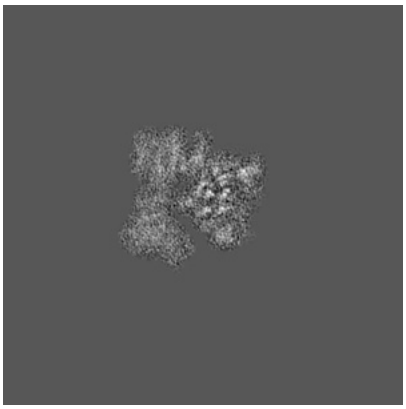


Z

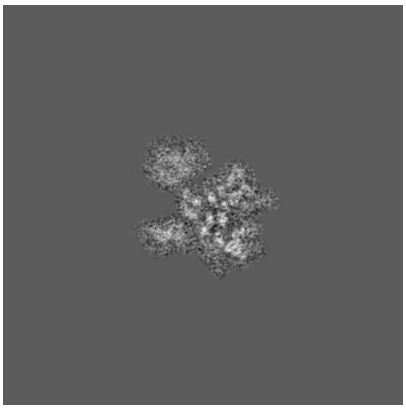
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

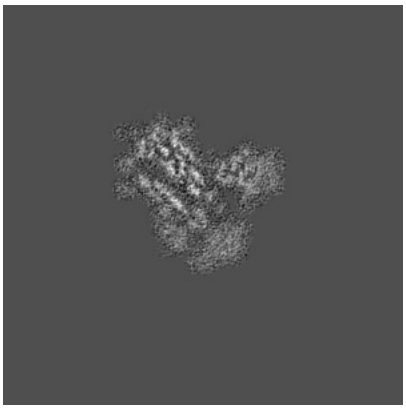
6.2.1 Primary map



X Index: 150

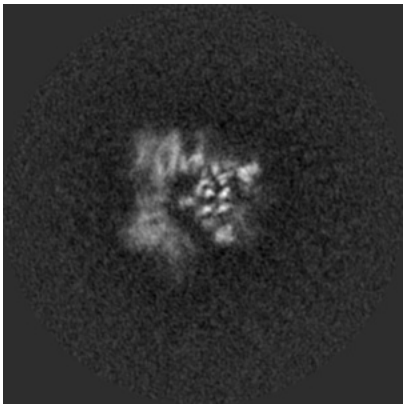


Y Index: 150

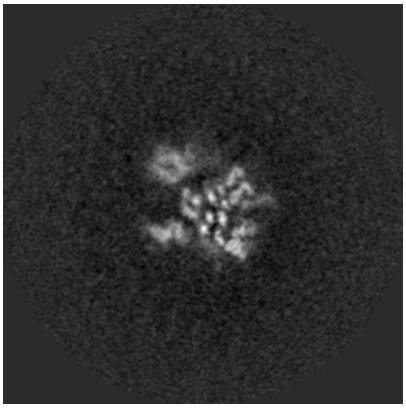


Z Index: 150

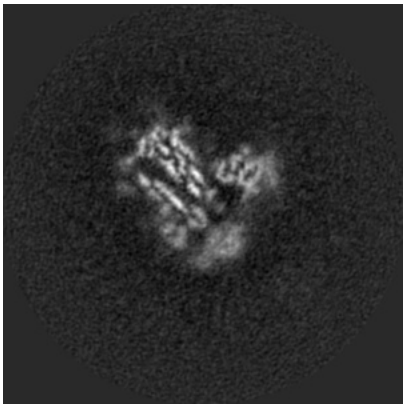
6.2.2 Raw map



X Index: 150



Y Index: 150

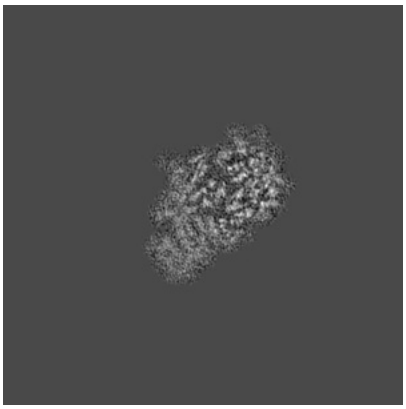


Z Index: 150

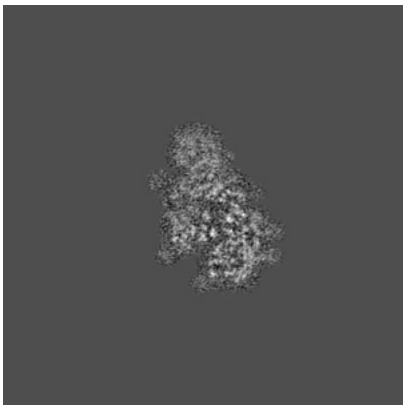
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

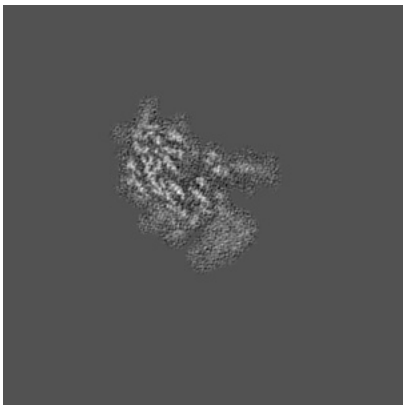
6.3.1 Primary map



X Index: 128

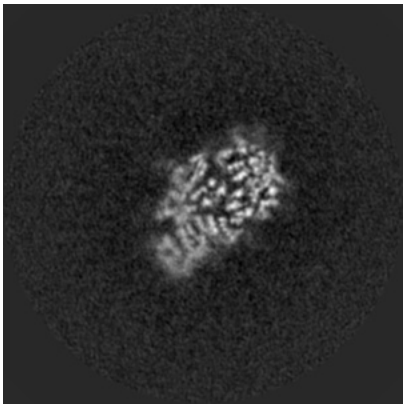


Y Index: 176

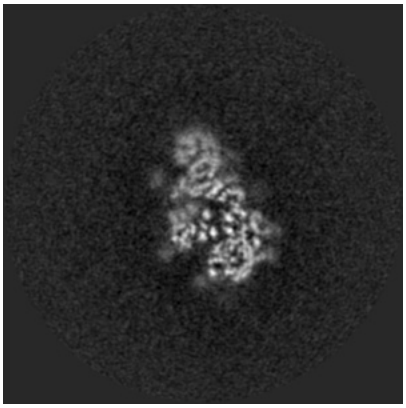


Z Index: 159

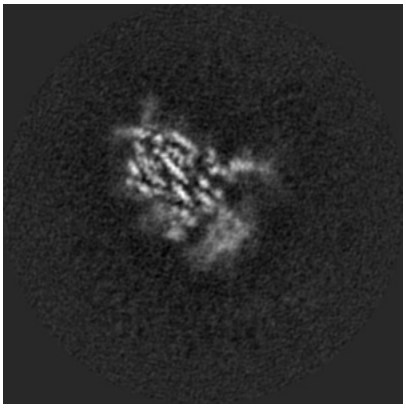
6.3.2 Raw map



X Index: 128



Y Index: 176

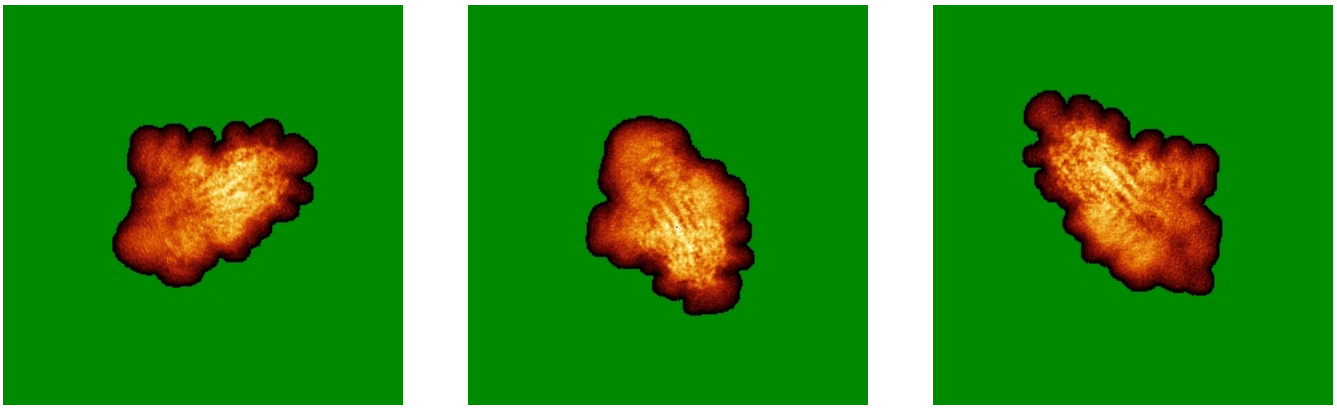


Z Index: 157

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

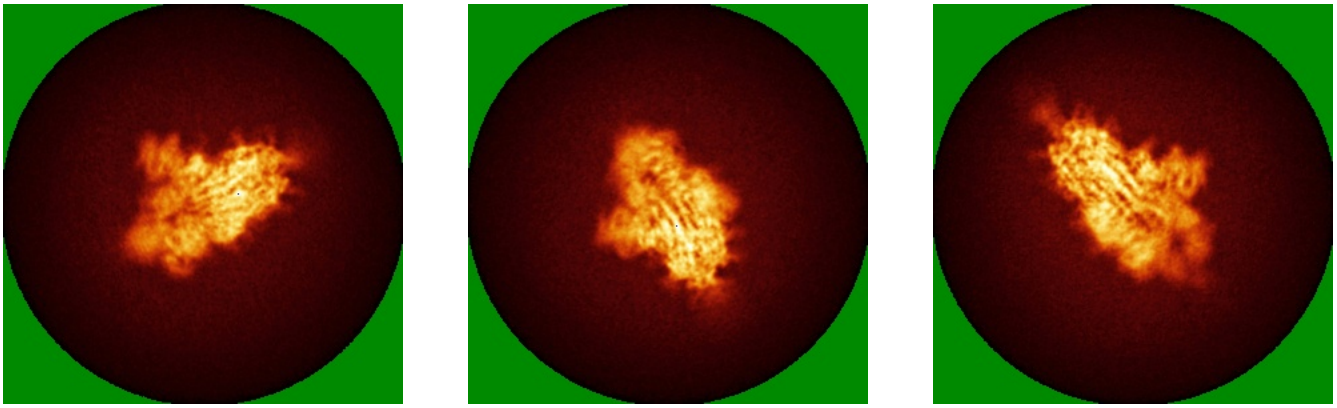
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

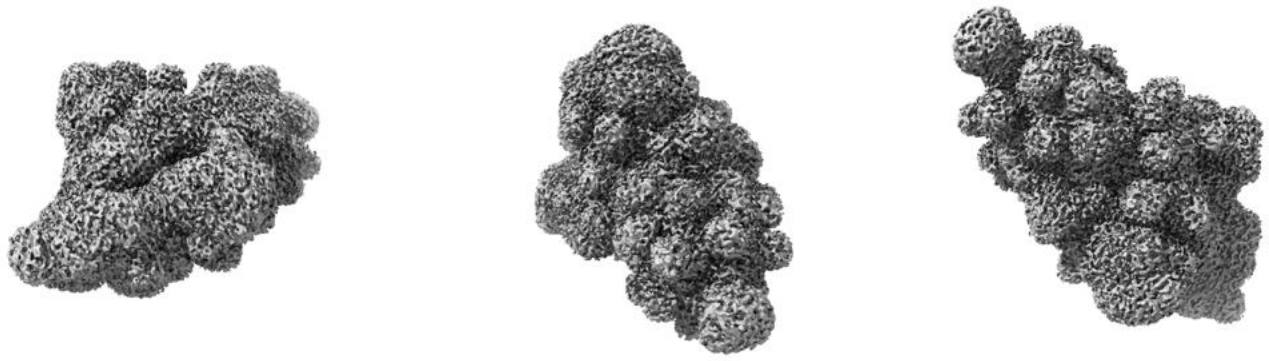


X Y Z

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 0.004. 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.

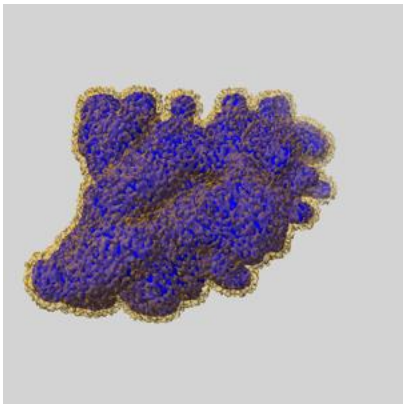
6.6 Mask visualisation

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

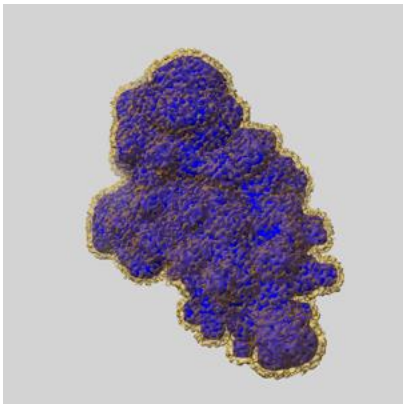
A mask typically either:

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

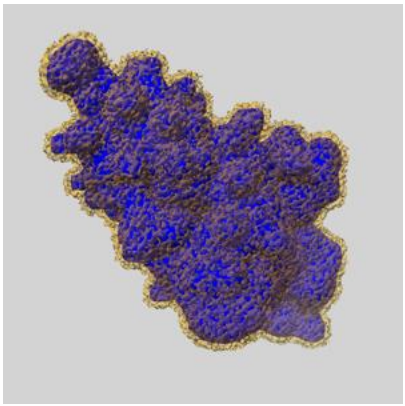
6.6.1 emd_17296_msk_1.map



X



Y

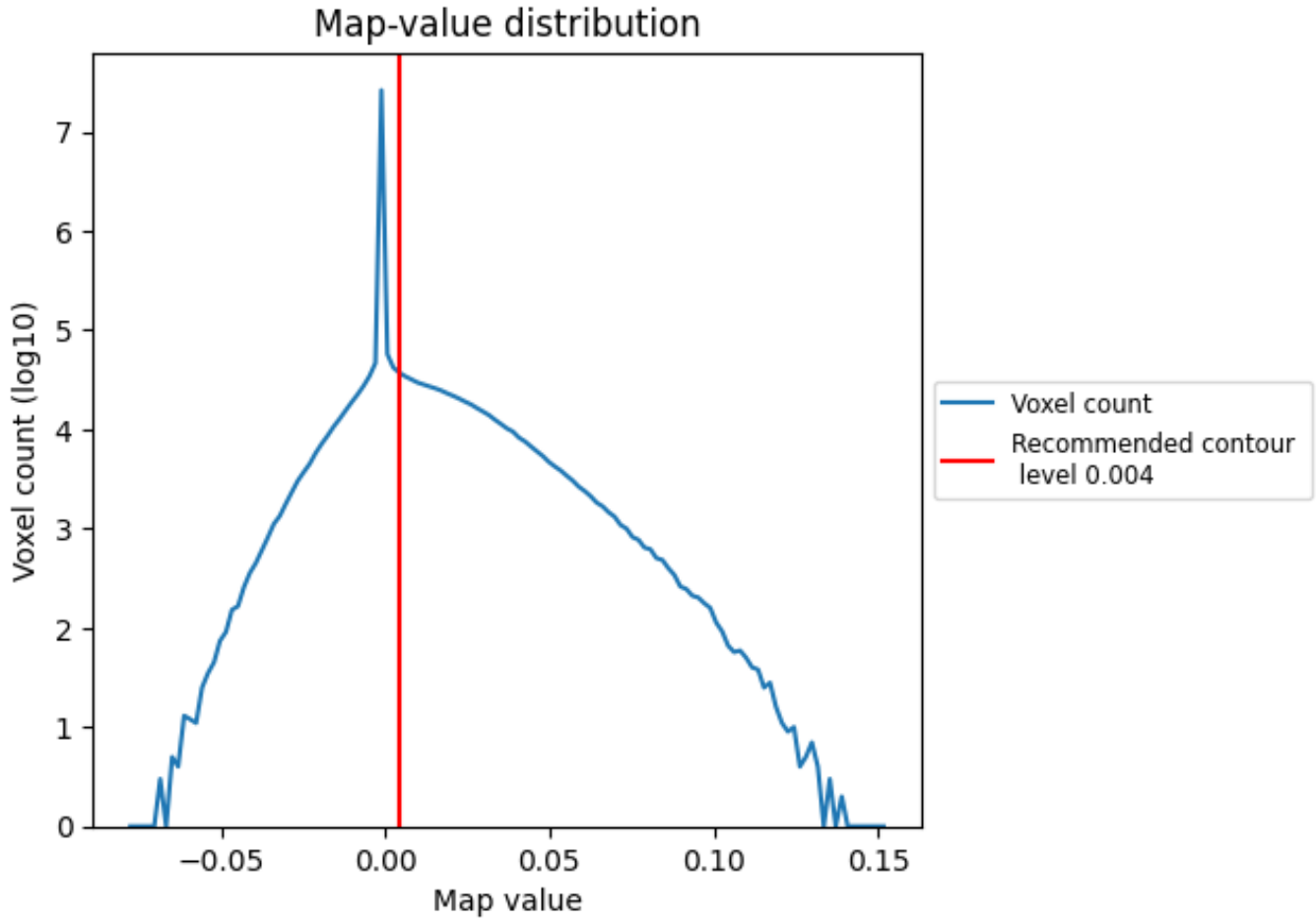


Z

7 Map analysis

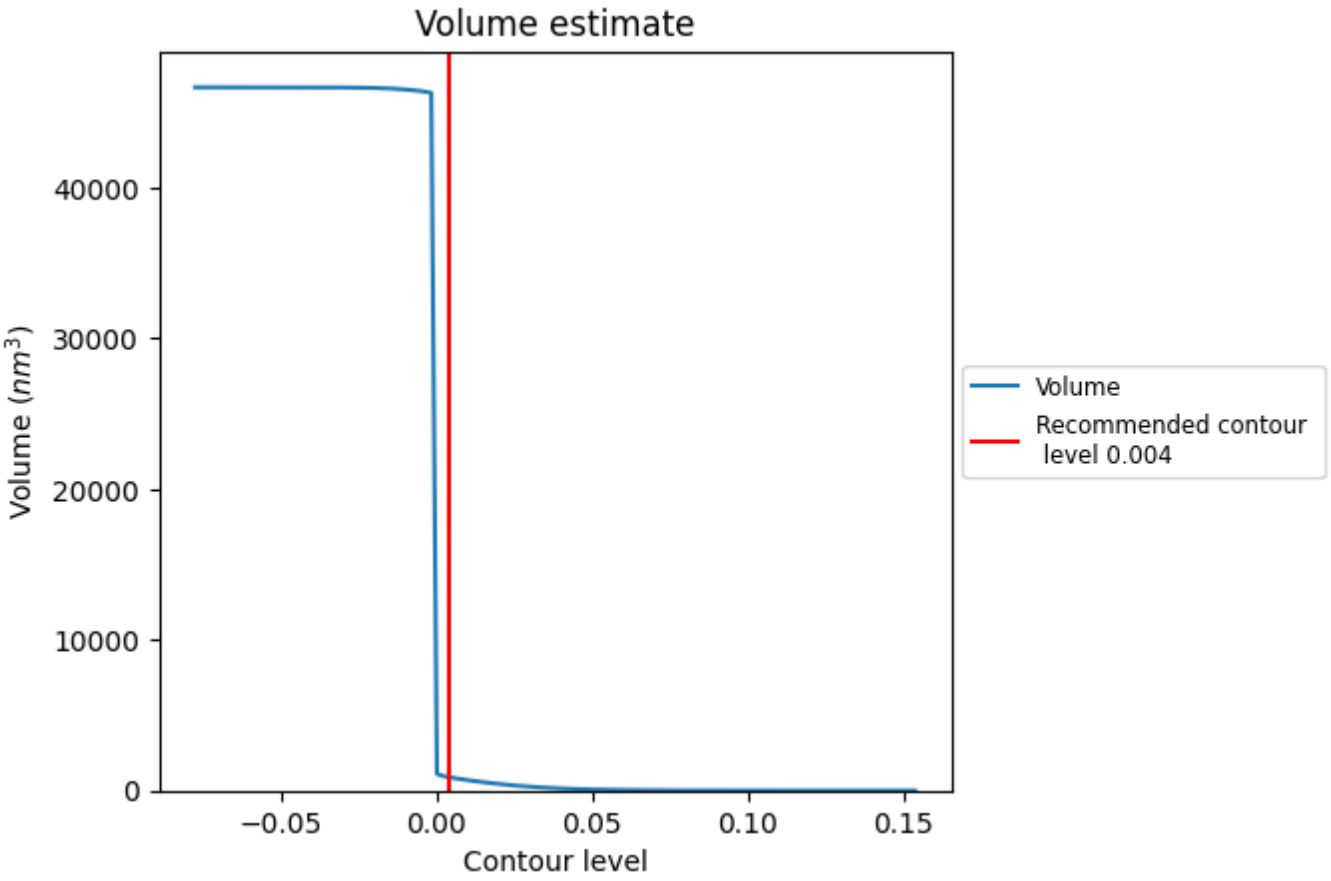
This section contains the results of statistical analysis of the map.

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.

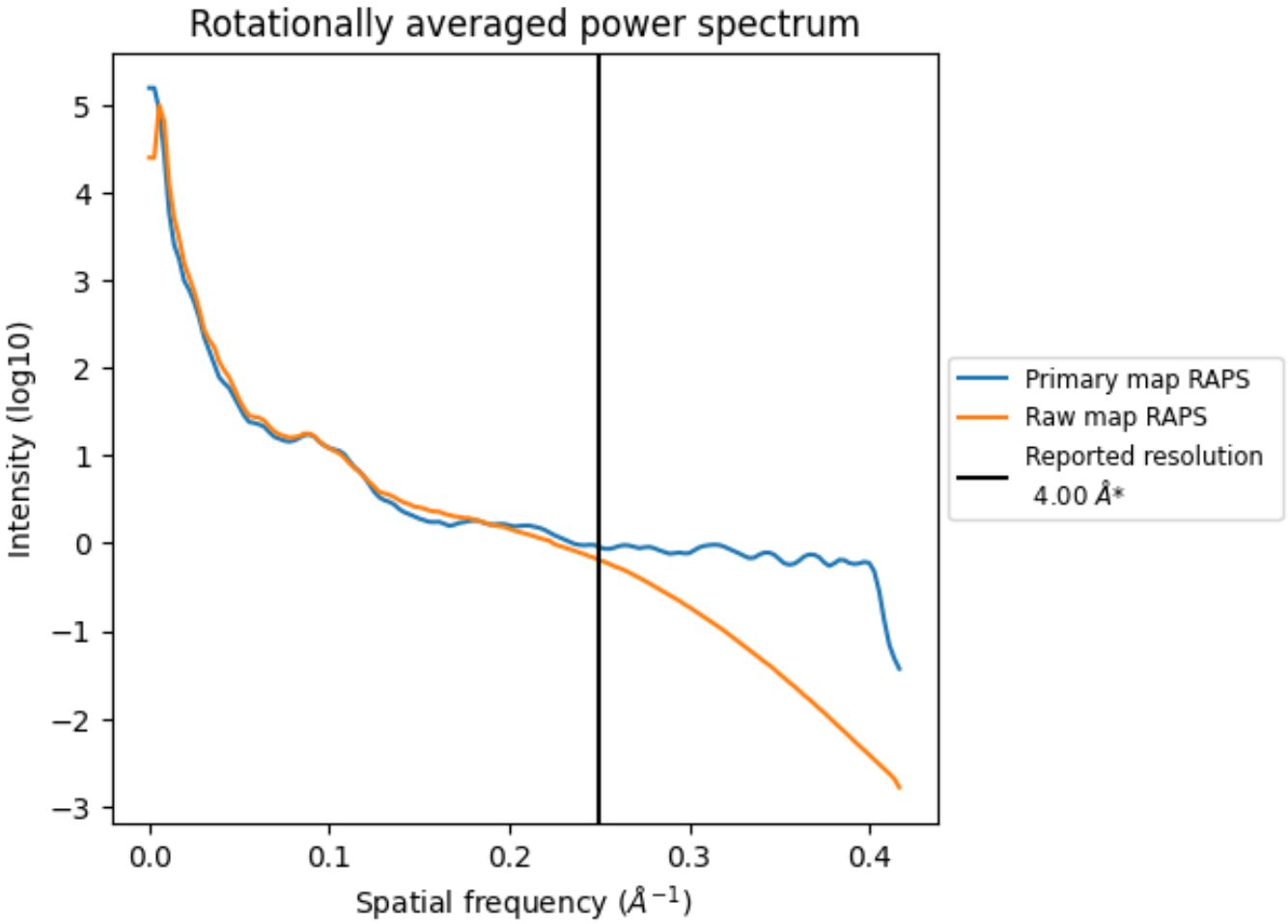
7.2 Volume estimate



The volume at the recommended contour level is 884 nm^3; this corresponds to an approximate mass of 798 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)

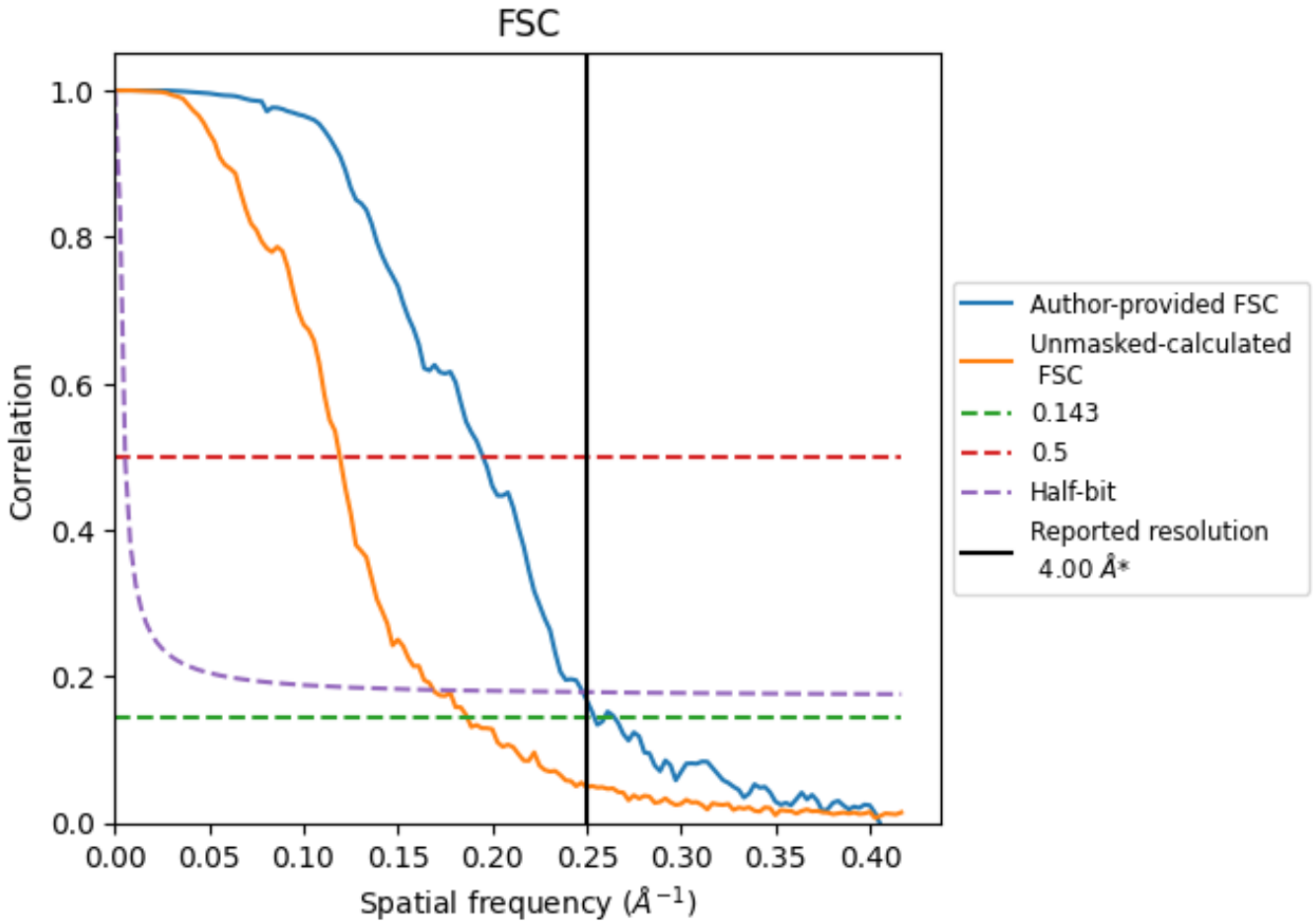


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

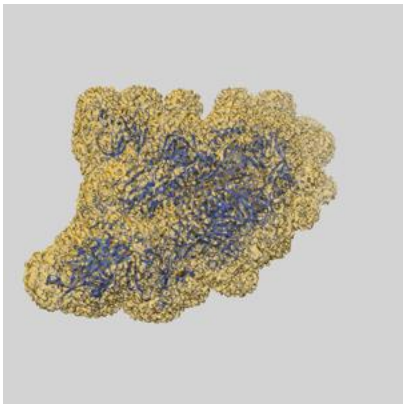
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	5.13	4.03
Unmasked-calculated*	5.35	8.38	5.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.35 differs from the reported value 4.0 by more than 10 %

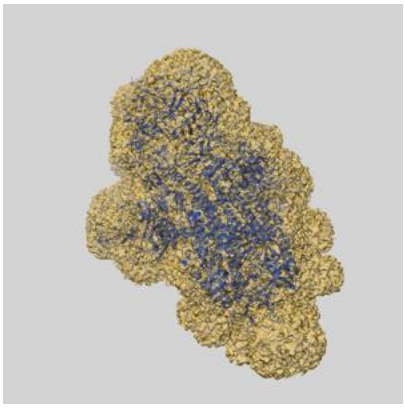
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17296 and PDB model 8OYU. Per-residue inclusion information can be found in section 3 on page 12.

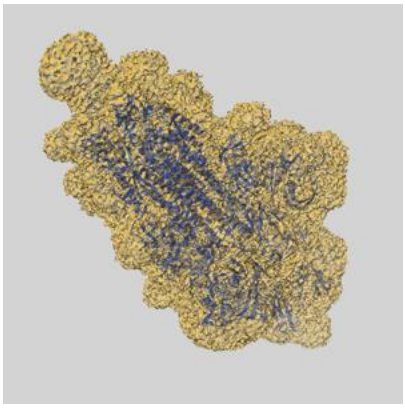
9.1 Map-model overlay



X



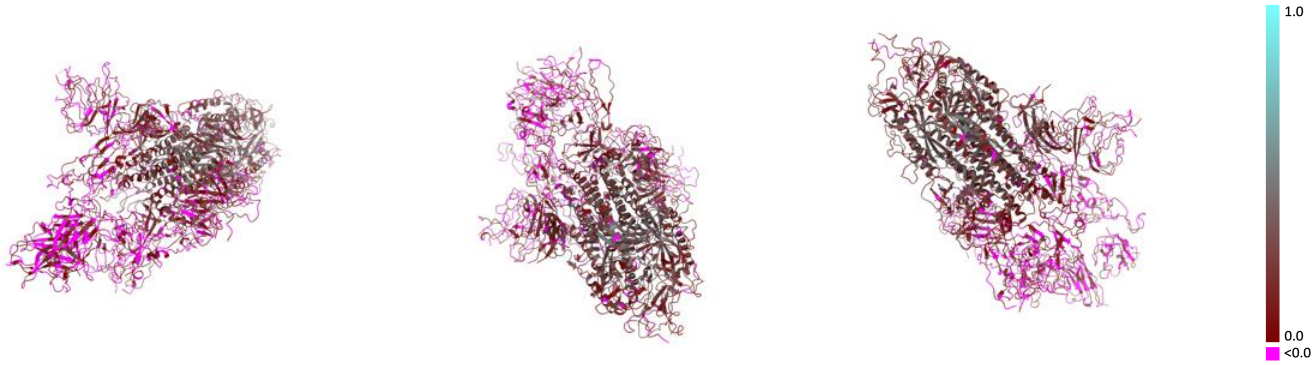
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

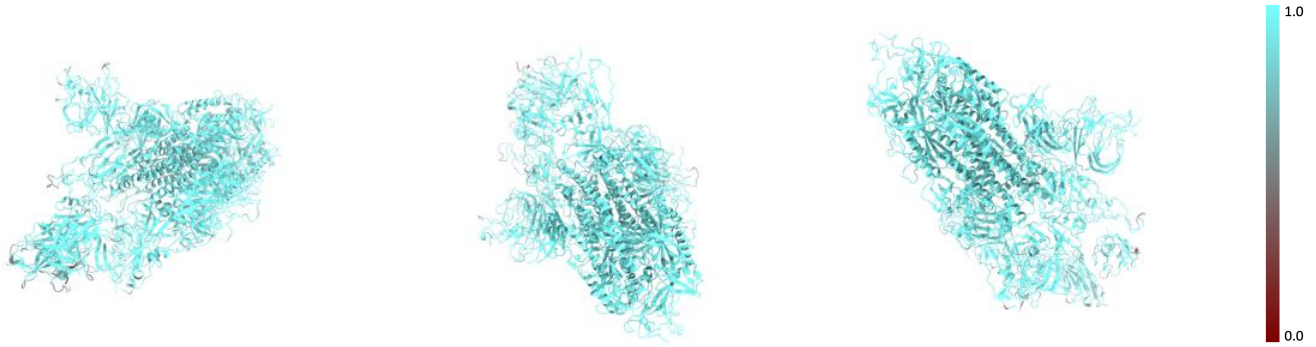
9.2 Q-score mapped to coordinate model (i)



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.

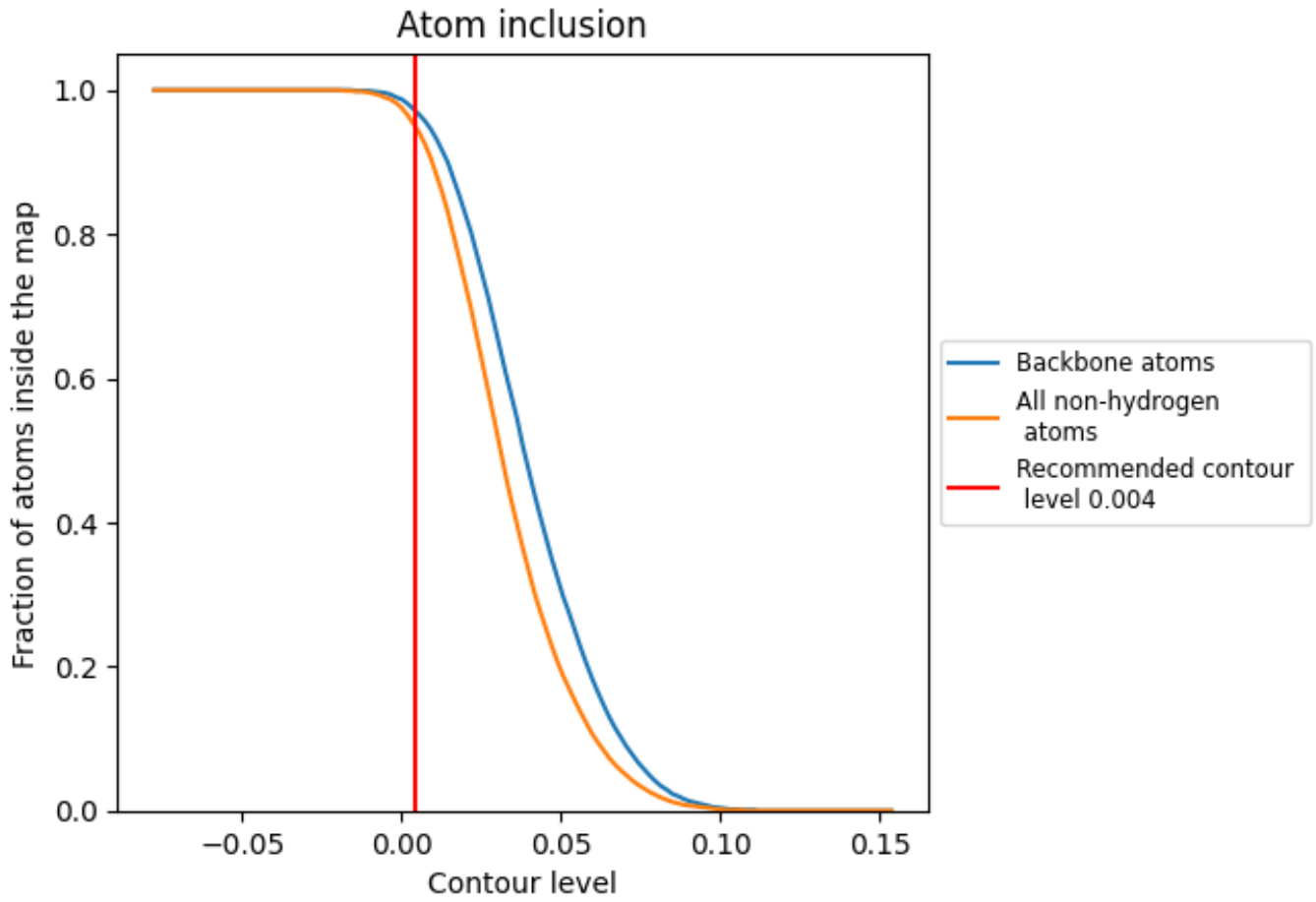
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9510	0.1450
A	0.9540	0.1390
B	0.9620	0.1720
C	0.9520	0.1510
D	0.8650	0.0140
E	0.8880	0.0220
F	0.9640	0.1750
G	0.9640	0.1050
H	0.9290	0.2990
I	1.0000	0.2050
J	0.8930	0.2300
K	0.9290	0.0910
L	1.0000	0.2740
M	1.0000	0.1750
N	0.9640	0.1980
O	0.9640	0.1220
P	1.0000	0.2960