Full wwPDB EM Validation Report

Nov 2, 2022 – 04:16 PM EDT

PDB ID	:	5KEL
EMDB ID	:	EMD-8240
Title	:	EBOV GP in complex with variable Fab domains of IgGs c2G4 and c13C6
Authors	:	Pallesen, J.; Murin, C.D.; de Val, N.; Cottrell, C.A.; Hastie, K.M.; Turner, H.L.; Fusco, M.L.; Flyak, A.I.; Zeitlin, L.; Crowe Jr., J.E.; Andersen, K.G.; Saphire, E.O.; Ward, A.B.
Deposited on	:	2016-06-09
Resolution	:	4.30 Å(reported)

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

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

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

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

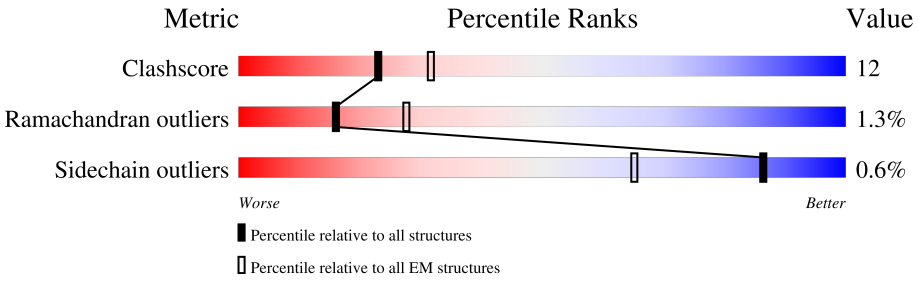
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 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	469	41% 9% 50%
1	E	469	41% 9% 50%
1	F	469	41% 9% 50%
2	B	143	60% 17% 21%
2	G	143	58% 19% 21%
2	I	143	60% 17% 21%
3	H	120	8% 90% 9%
3	P	120	8% 92% 8%

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Mol	Chain	Length	Quality of chain
3	Q	120	7% 90% 9%
4	L	107	94% 6%
4	T	107	94% 6%
4	U	107	94% 6%
5	C	121	19% 88% 10%
5	J	121	20% 88% 10%
5	M	121	18% 88% 10%
6	D	107	20% 92% 8%
6	N	107	20% 93% 7%
6	O	107	19% 93% 7%
7	K	2	50% 50% 50%
7	W	2	50% 50% 50%
7	a	2	50% 50% 50%
8	R	3	33% 33% 67%
8	X	3	33% 33% 67%
8	b	3	33% 100%
9	S	4	50% 25% 50% 25%
9	Y	4	50% 25% 50% 25%
9	c	4	50% 75% 25%
10	V	5	20% 60% 40%
10	Z	5	20% 60% 40%
10	d	5	20% 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	V	1	-	-	X	-
10	NAG	Z	1	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 19278 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 Ebola surface glycoprotein, GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		
1	E	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		
1	F	235	Total	C	N	O	S	0	0
			1828	1162	316	345	5		

- Molecule 2 is a protein called Ebola surface glycoprotein, GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	113	Total	C	N	O	S	0	0
			889	567	155	161	6		
2	G	113	Total	C	N	O	S	0	0
			889	567	155	161	6		
2	I	113	Total	C	N	O	S	0	0
			889	567	155	161	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	ILE	conflict	UNP Q05320
B	638	LEU	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	VAL	-	expression tag	UNP Q05320
B	641	ASP	-	expression tag	UNP Q05320
B	642	ASP	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	ASP	-	expression tag	UNP Q05320
G	544	THR	ILE	conflict	UNP Q05320
G	638	LEU	-	expression tag	UNP Q05320
G	639	GLU	-	expression tag	UNP Q05320
G	640	VAL	-	expression tag	UNP Q05320
G	641	ASP	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
G	642	ASP	-	expression tag	UNP Q05320
G	643	ASP	-	expression tag	UNP Q05320
G	644	ASP	-	expression tag	UNP Q05320
I	544	THR	ILE	conflict	UNP Q05320
I	638	LEU	-	expression tag	UNP Q05320
I	639	GLU	-	expression tag	UNP Q05320
I	640	VAL	-	expression tag	UNP Q05320
I	641	ASP	-	expression tag	UNP Q05320
I	642	ASP	-	expression tag	UNP Q05320
I	643	ASP	-	expression tag	UNP Q05320
I	644	ASP	-	expression tag	UNP Q05320

- Molecule 3 is a protein called c2G4 variable Fab domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			952	592	168	185	7		
3	P	120	Total	C	N	O	S	0	0
			952	592	168	185	7		
3	Q	120	Total	C	N	O	S	0	0
			952	592	168	185	7		

- Molecule 4 is a protein called c2G4 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			820	518	133	166	3		
4	T	107	Total	C	N	O	S	0	0
			820	518	133	166	3		
4	U	107	Total	C	N	O	S	0	0
			820	518	133	166	3		

- Molecule 5 is a protein called c13C6 variable Fab domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	121	Total	C	N	O	S	0	0
			930	593	154	180	3		
5	J	121	Total	C	N	O	S	0	0
			930	593	154	180	3		
5	M	121	Total	C	N	O	S	0	0
			930	593	154	180	3		

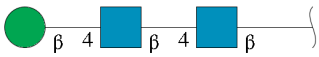
- Molecule 6 is a protein called c13C6 variable Fab domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	107	Total	C	N	O	S	0	0
			815	509	135	167	4		
6	N	107	Total	C	N	O	S	0	0
			815	509	135	167	4		
6	O	107	Total	C	N	O	S	0	0
			815	509	135	167	4		

- Molecule 7 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
7	K	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

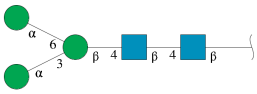


Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		
8	b	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

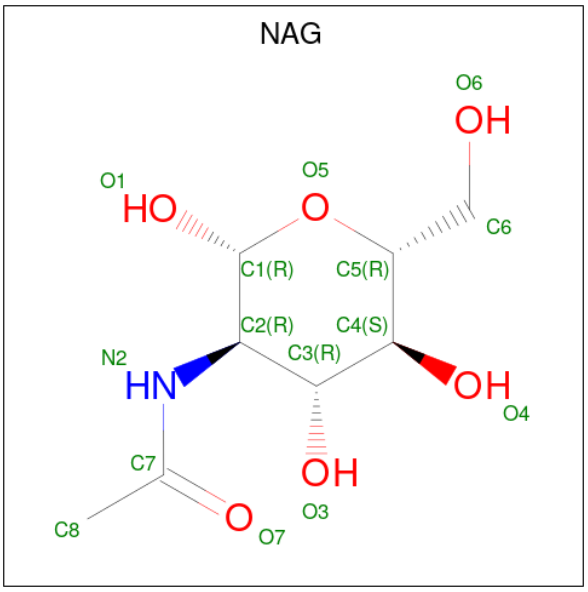
Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	4	Total	C	N	O	0	0
			50	28	2	20		
9	Y	4	Total	C	N	O	0	0
			50	28	2	20		
9	c	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	5	Total	C	N	O	0	0
			61	34	2	25		
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	d	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



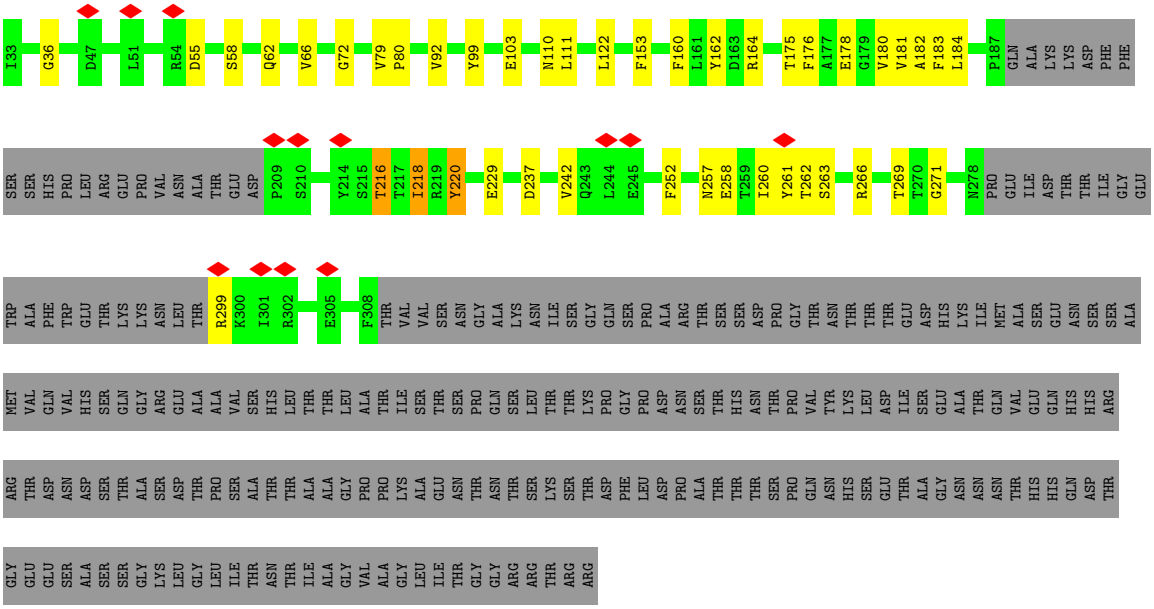
Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O 14 8 1 5	0
11	E	1	Total C N O 14 8 1 5	0
11	F	1	Total C N O 14 8 1 5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

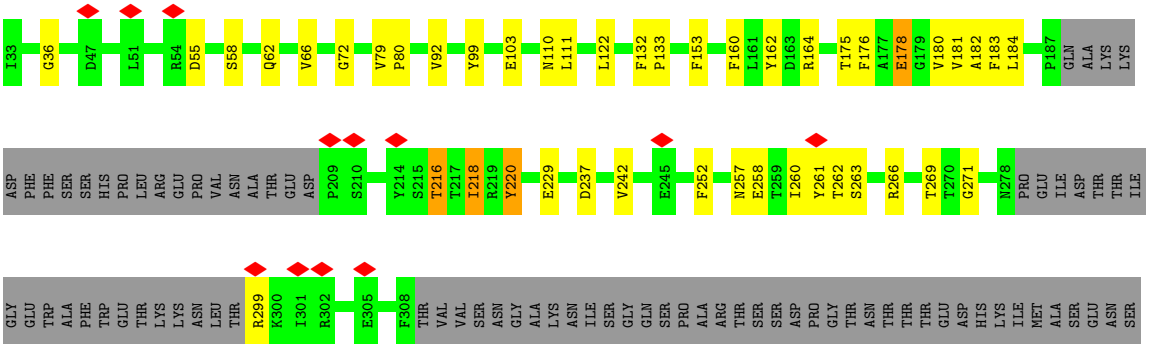
• Molecule 1: Ebola surface glycoprotein, GP1

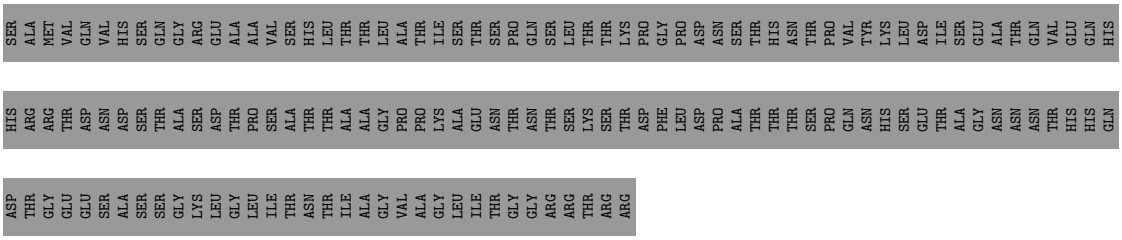
Chain A:



• Molecule 1: Ebola surface glycoprotein, GP1

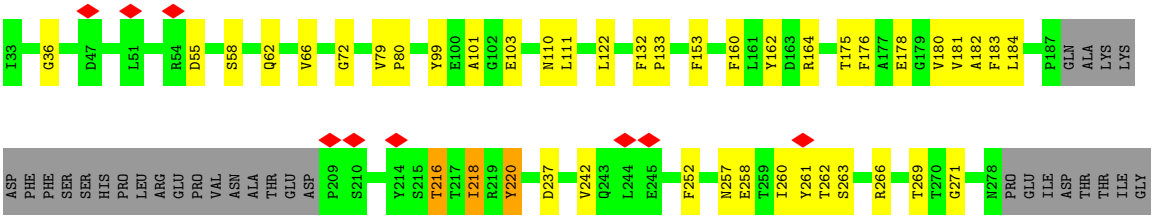
Chain E:

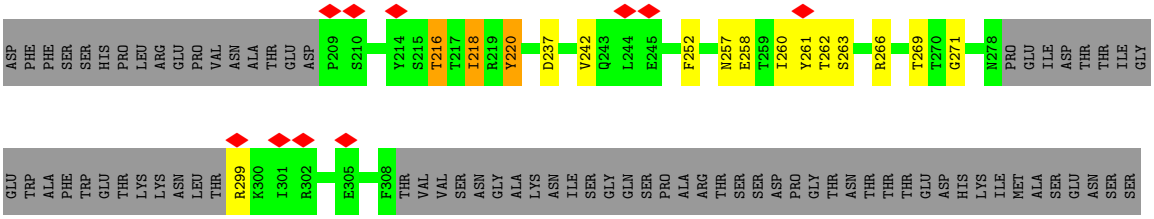


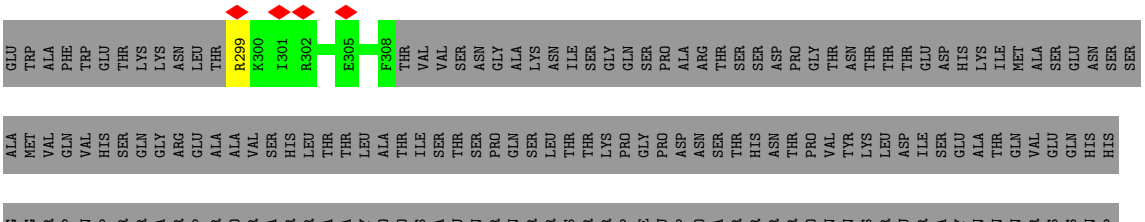


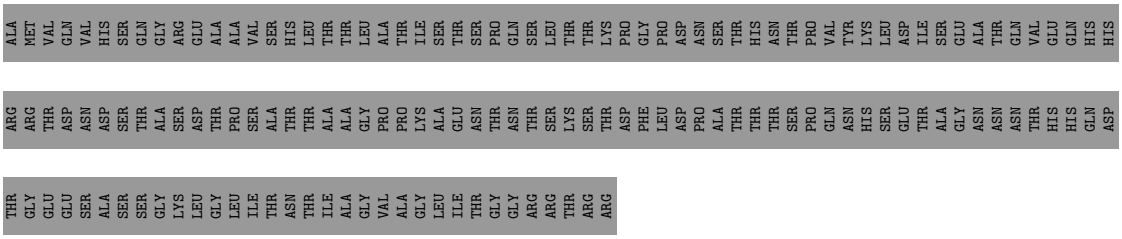
• Molecule 1: Ebola surface glycoprotein, GP1

Chain F:



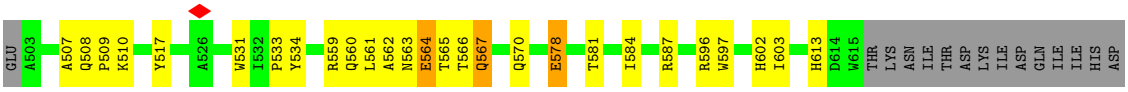






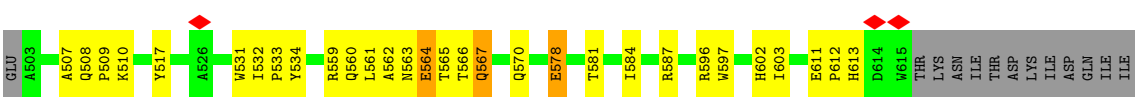
• Molecule 2: Ebola surface glycoprotein, GP2

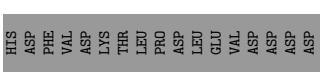
Chain B:



• Molecule 2: Ebola surface glycoprotein, GP2

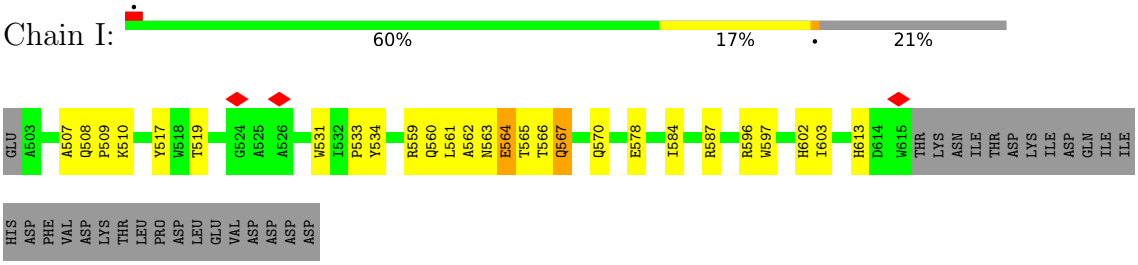
Chain G:





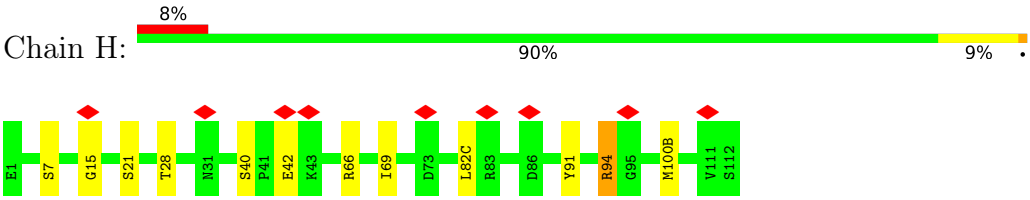
• Molecule 2: Ebola surface glycoprotein, GP2

Chain I:



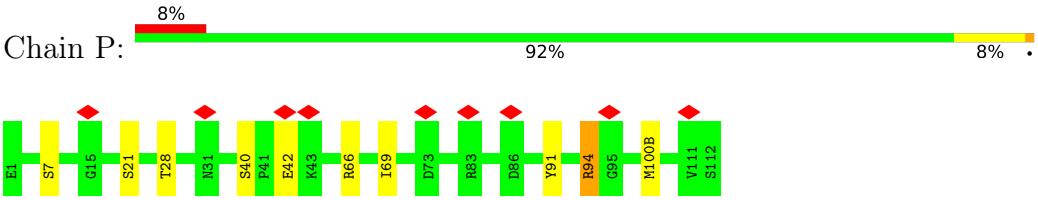
• Molecule 3: c2G4 variable Fab domain heavy chain

Chain H:



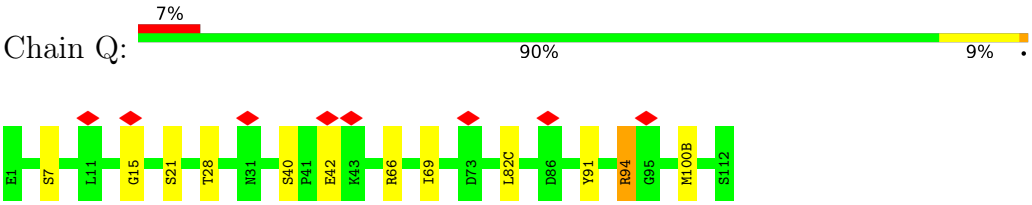
• Molecule 3: c2G4 variable Fab domain heavy chain

Chain P:



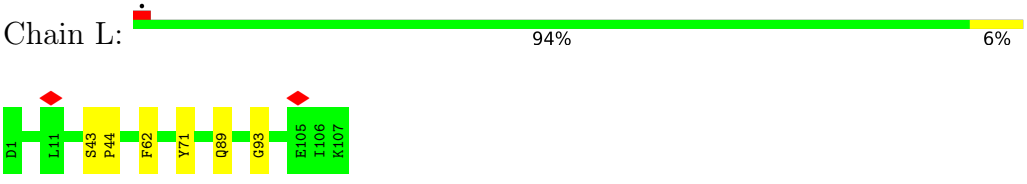
• Molecule 3: c2G4 variable Fab domain heavy chain

Chain Q:



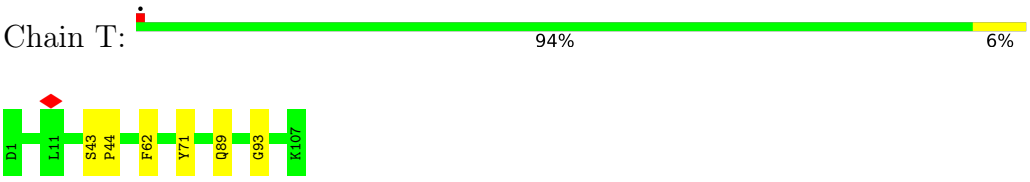
• Molecule 4: c2G4 variable Fab domain light chain

Chain L:



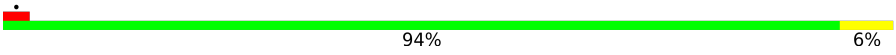
• Molecule 4: c2G4 variable Fab domain light chain

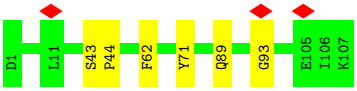
Chain T:



• Molecule 4: c2G4 variable Fab domain light chain

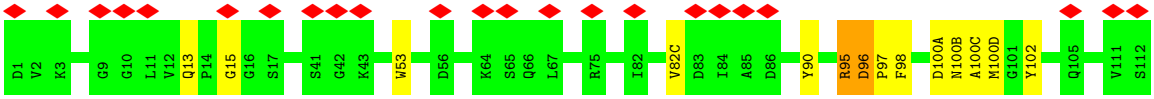
Chain U:





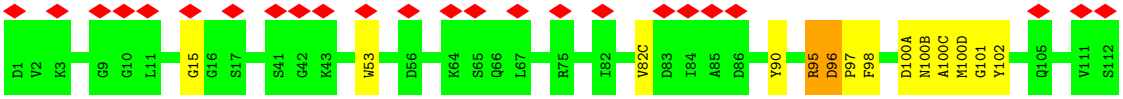
• Molecule 5: c13C6 variable Fab domain heavy chain

Chain C:



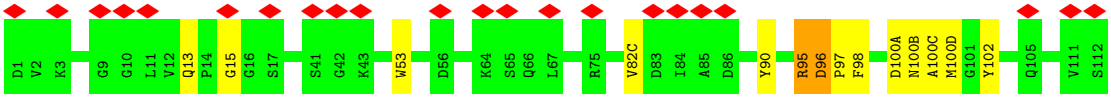
• Molecule 5: c13C6 variable Fab domain heavy chain

Chain J:



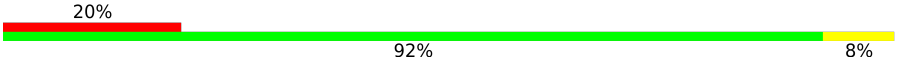
• Molecule 5: c13C6 variable Fab domain heavy chain

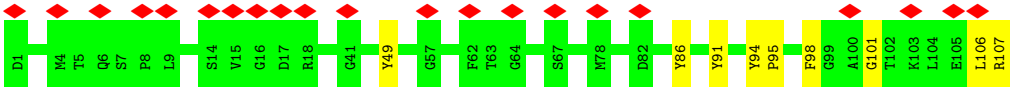
Chain M:



• Molecule 6: c13C6 variable Fab domain light chain

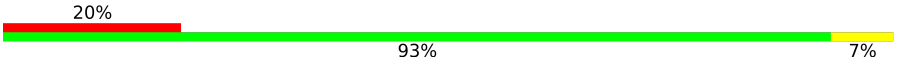
Chain D:

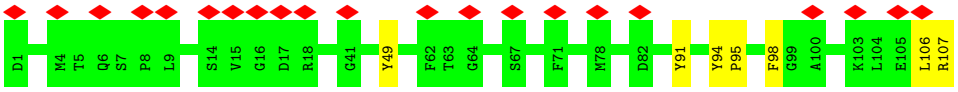




• Molecule 6: c13C6 variable Fab domain light chain

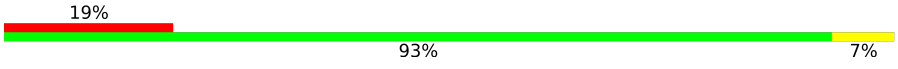
Chain N:

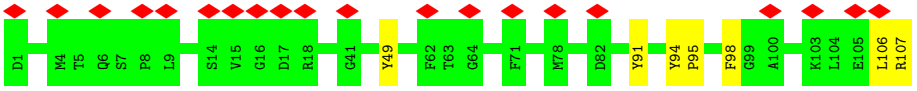




• Molecule 6: c13C6 variable Fab domain light chain

Chain O:





• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

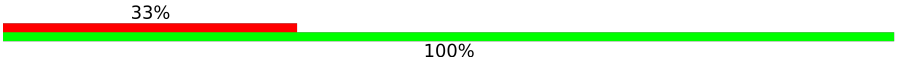
Chain R:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

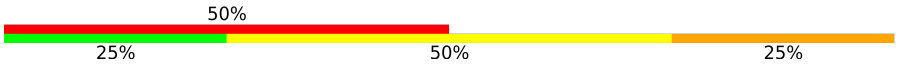
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



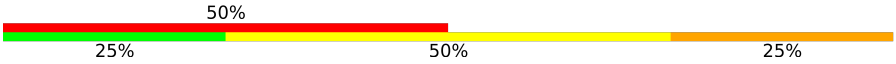
• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



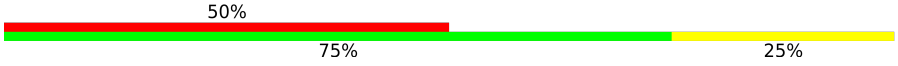
• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



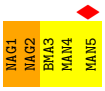
• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



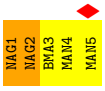
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



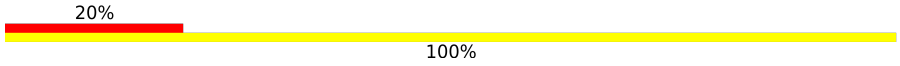
• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	86000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	319.63998, 319.63998, 319.63998	wwPDB
Map dimensions	244, 244, 244	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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, MAN, BMA

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	0.87	0/1868	0.93	4/2532 (0.2%)
1	E	0.87	0/1868	0.93	4/2532 (0.2%)
1	F	0.87	0/1868	0.93	4/2532 (0.2%)
2	B	0.84	1/913 (0.1%)	0.87	2/1246 (0.2%)
2	G	0.84	1/913 (0.1%)	0.87	2/1246 (0.2%)
2	I	0.84	2/913 (0.2%)	0.87	2/1246 (0.2%)
3	H	0.87	0/973	0.98	3/1311 (0.2%)
3	P	0.87	0/973	0.98	3/1311 (0.2%)
3	Q	0.87	0/973	0.98	3/1311 (0.2%)
4	L	0.78	0/839	0.88	0/1136
4	T	0.78	0/839	0.88	0/1136
4	U	0.78	0/839	0.88	0/1136
5	C	0.74	0/954	0.93	3/1292 (0.2%)
5	J	0.74	0/954	0.93	3/1292 (0.2%)
5	M	0.74	0/954	0.93	3/1292 (0.2%)
6	D	0.69	0/831	0.84	0/1127
6	N	0.69	0/831	0.84	0/1127
6	O	0.69	0/831	0.84	0/1127
All	All	0.82	4/19134 (0.0%)	0.91	36/25932 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	578	GLU	CG-CD	-5.45	1.43	1.51
2	G	578	GLU	CG-CD	-5.42	1.43	1.51
2	I	578	GLU	CG-CD	-5.39	1.43	1.51
2	I	578	GLU	CD-OE1	-5.01	1.20	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	164	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	164	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	E	164	ARG	NE-CZ-NH2	-7.01	116.79	120.30
5	M	102	TYR	CB-CG-CD1	-6.60	117.04	121.00
5	J	102	TYR	CB-CG-CD1	-6.59	117.04	121.00
1	E	99	TYR	CB-CG-CD2	-6.57	117.06	121.00
5	C	102	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	F	99	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	A	99	TYR	CB-CG-CD2	-6.55	117.07	121.00
3	H	66	ARG	NE-CZ-NH2	-6.47	117.07	120.30
3	Q	66	ARG	NE-CZ-NH2	-6.42	117.09	120.30
3	P	66	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	220	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	E	220	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	F	220	TYR	CB-CG-CD2	-6.24	117.25	121.00
2	G	534	TYR	CB-CG-CD1	-6.14	117.31	121.00
2	I	534	TYR	CB-CG-CD1	-6.13	117.32	121.00
2	B	534	TYR	CB-CG-CD1	-6.06	117.36	121.00
5	M	90	TYR	CB-CG-CD2	-5.88	117.47	121.00
5	C	90	TYR	CB-CG-CD2	-5.86	117.48	121.00
3	P	91	TYR	CB-CG-CD2	-5.86	117.48	121.00
5	J	90	TYR	CB-CG-CD2	-5.86	117.48	121.00
3	Q	91	TYR	CB-CG-CD2	-5.84	117.50	121.00
3	H	91	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	E	299	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	F	299	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	299	ARG	NE-CZ-NH2	-5.62	117.49	120.30
3	H	94	ARG	NE-CZ-NH1	-5.45	117.58	120.30
3	P	94	ARG	NE-CZ-NH1	-5.37	117.62	120.30
3	Q	94	ARG	NE-CZ-NH1	-5.33	117.63	120.30
5	C	95	ARG	NE-CZ-NH1	-5.31	117.64	120.30
5	J	95	ARG	NE-CZ-NH1	-5.30	117.65	120.30
5	M	95	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	B	587	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	G	587	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	I	587	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1828	0	1783	47	0
1	E	1828	0	1783	49	0
1	F	1828	0	1783	48	0
2	B	889	0	854	100	0
2	G	889	0	854	103	0
2	I	889	0	854	95	0
3	H	952	0	904	8	0
3	P	952	0	904	7	0
3	Q	952	0	904	8	0
4	L	820	0	789	4	0
4	T	820	0	789	4	0
4	U	820	0	789	4	0
5	C	930	0	894	19	0
5	J	930	0	894	18	0
5	M	930	0	894	19	0
6	D	815	0	791	6	0
6	N	815	0	791	5	0
6	O	815	0	791	5	0
7	K	28	0	25	6	0
7	W	28	0	25	6	0
7	a	28	0	25	0	0
8	R	39	0	34	2	0
8	X	39	0	34	2	0
8	b	39	0	34	0	0
9	S	50	0	43	4	0
9	Y	50	0	43	5	0
9	c	50	0	43	0	0
10	V	61	0	52	11	0
10	Z	61	0	52	10	0
10	d	61	0	52	0	0
11	A	14	0	13	0	0
11	E	14	0	13	0	0
11	F	14	0	13	0	0
All	All	19278	0	18546	445	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 12.

All (445) 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:G:507:ALA:C	2:G:509:PRO:HD2	1.39	1.42
2:I:507:ALA:C	2:I:509:PRO:HD2	1.39	1.41
2:B:507:ALA:C	2:B:509:PRO:HD2	1.39	1.40
2:B:531:TRP:CE2	2:I:567:GLN:OE1	1.76	1.38
2:B:567:GLN:OE1	2:G:531:TRP:CE2	1.76	1.37
2:G:567:GLN:OE1	2:I:531:TRP:CE2	1.76	1.34
2:B:567:GLN:OE1	2:G:531:TRP:CD2	1.81	1.34
2:G:567:GLN:OE1	2:I:531:TRP:CD2	1.81	1.33
2:B:531:TRP:CD2	2:I:567:GLN:OE1	1.81	1.32
2:G:507:ALA:O	2:G:509:PRO:HD2	1.14	1.29
2:I:507:ALA:O	2:I:509:PRO:HD2	1.13	1.29
2:B:507:ALA:C	2:B:509:PRO:CD	2.01	1.29
2:I:507:ALA:C	2:I:509:PRO:CD	2.01	1.28
2:G:507:ALA:C	2:G:509:PRO:CD	2.01	1.26
2:B:507:ALA:O	2:B:509:PRO:HD2	1.14	1.25
1:F:72:GLY:HA3	2:I:559:ARG:HH12	1.08	1.16
2:B:562:ALA:O	2:B:566:THR:HG23	1.45	1.16
2:B:570:GLN:HE21	2:G:533:PRO:CD	1.59	1.15
2:B:533:PRO:CD	2:I:570:GLN:HE21	1.59	1.15
2:I:562:ALA:O	2:I:566:THR:HG23	1.45	1.15
2:G:562:ALA:O	2:G:566:THR:HG23	1.45	1.14
2:G:570:GLN:HE21	2:I:533:PRO:CD	1.59	1.13
2:B:533:PRO:CG	2:I:570:GLN:HE21	1.62	1.12
5:J:95:ARG:HA	5:J:100(D):MET:HB3	1.29	1.11
2:B:507:ALA:HB1	10:V:1:NAG:O6	1.51	1.11
2:B:570:GLN:HE21	2:G:533:PRO:CG	1.62	1.11
2:G:570:GLN:HE21	2:I:533:PRO:CG	1.62	1.10
5:C:95:ARG:HA	5:C:100(D):MET:HB3	1.29	1.10
1:E:72:GLY:HA3	2:G:559:ARG:HH12	1.08	1.08
1:A:72:GLY:HA3	2:B:559:ARG:HH12	1.08	1.08
2:B:570:GLN:NE2	2:G:533:PRO:CG	2.18	1.07
2:G:570:GLN:NE2	2:I:533:PRO:CG	2.18	1.07
2:G:507:ALA:HB1	10:Z:1:NAG:O6	1.51	1.07
5:M:95:ARG:HA	5:M:100(D):MET:HB3	1.29	1.06
2:B:533:PRO:CG	2:I:570:GLN:NE2	2.18	1.06
1:E:110:ASN:OD1	1:E:175:THR:HG22	1.55	1.05
1:F:180:VAL:HB	2:I:566:THR:HG21	1.05	1.05
10:Z:1:NAG:H62	10:Z:2:NAG:C7	1.86	1.05
1:A:110:ASN:OD1	1:A:175:THR:HG22	1.55	1.04
10:V:1:NAG:H62	10:V:2:NAG:C7	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ASN:OD1	1:F:175:THR:HG22	1.55	1.04
1:E:180:VAL:HB	2:G:566:THR:HG21	1.05	1.03
1:A:180:VAL:HB	2:B:566:THR:HG21	1.05	1.02
2:B:531:TRP:CD2	2:I:567:GLN:CD	2.32	1.02
2:B:567:GLN:CD	2:G:531:TRP:CD2	2.32	1.01
2:G:567:GLN:CD	2:I:531:TRP:CD2	2.33	1.00
1:F:180:VAL:HB	2:I:566:THR:CG2	1.92	0.98
1:E:180:VAL:HB	2:G:566:THR:CG2	1.92	0.98
1:A:180:VAL:HB	2:B:566:THR:CG2	1.92	0.98
2:B:507:ALA:O	2:B:509:PRO:CD	2.09	0.97
2:G:507:ALA:O	2:G:509:PRO:CD	2.09	0.97
5:M:97:PRO:CG	5:M:100(C):ALA:HB1	1.96	0.96
5:C:97:PRO:CG	5:C:100(C):ALA:HB1	1.96	0.96
5:J:97:PRO:HG2	5:J:100(C):ALA:HB1	1.49	0.94
5:C:97:PRO:HG2	5:C:100(C):ALA:HB1	1.49	0.94
5:J:97:PRO:CG	5:J:100(C):ALA:HB1	1.96	0.94
2:B:531:TRP:CG	2:I:567:GLN:CD	2.41	0.94
1:A:72:GLY:HA3	2:B:559:ARG:NH1	1.83	0.93
2:G:567:GLN:CD	2:I:531:TRP:CG	2.41	0.93
1:F:72:GLY:HA3	2:I:559:ARG:NH1	1.83	0.93
2:B:567:GLN:CD	2:G:531:TRP:CG	2.41	0.93
5:M:97:PRO:HG2	5:M:100(C):ALA:HB1	1.49	0.93
2:B:533:PRO:HD3	2:I:570:GLN:HE21	1.34	0.93
9:Y:1:NAG:H62	9:Y:2:NAG:C7	1.98	0.93
9:S:1:NAG:H62	9:S:2:NAG:C7	1.98	0.92
1:E:72:GLY:HA3	2:G:559:ARG:NH1	1.83	0.92
2:B:531:TRP:HB3	2:I:567:GLN:NE2	1.85	0.92
2:G:567:GLN:NE2	2:I:531:TRP:HB3	1.85	0.92
2:G:570:GLN:HE21	2:I:533:PRO:HD3	1.34	0.92
2:B:570:GLN:HE21	2:G:533:PRO:HD3	1.34	0.91
2:B:567:GLN:NE2	2:G:531:TRP:HB3	1.85	0.91
2:G:507:ALA:C	2:G:509:PRO:HD3	1.90	0.90
2:I:507:ALA:C	2:I:509:PRO:HD3	1.90	0.90
2:I:507:ALA:O	2:I:509:PRO:CD	2.09	0.90
2:B:507:ALA:C	2:B:509:PRO:HD3	1.90	0.90
2:G:570:GLN:NE2	2:I:533:PRO:HG2	1.88	0.89
2:G:567:GLN:NE2	2:I:531:TRP:CG	2.41	0.89
2:B:567:GLN:NE2	2:G:531:TRP:CG	2.41	0.87
2:B:531:TRP:CG	2:I:567:GLN:NE2	2.41	0.87
2:B:570:GLN:NE2	2:G:533:PRO:HG2	1.88	0.87
2:B:560:GLN:NE2	2:B:564:GLU:OE1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:508:GLN:N	2:I:509:PRO:CD	2.36	0.86
2:I:560:GLN:NE2	2:I:564:GLU:OE1	2.08	0.86
2:G:560:GLN:NE2	2:G:564:GLU:OE1	2.08	0.86
1:F:182:ALA:HB2	2:I:562:ALA:HA	1.58	0.86
1:E:180:VAL:CB	2:G:566:THR:HG21	2.01	0.85
5:J:97:PRO:HD2	5:J:100(C):ALA:O	1.76	0.85
2:B:533:PRO:HG2	2:I:570:GLN:NE2	1.88	0.85
1:A:182:ALA:HB2	2:B:562:ALA:HA	1.58	0.85
5:M:97:PRO:HD2	5:M:100(C):ALA:O	1.76	0.85
2:G:508:GLN:N	2:G:509:PRO:CD	2.36	0.84
2:B:507:ALA:CB	10:V:1:NAG:O6	2.26	0.84
5:C:97:PRO:HD2	5:C:100(C):ALA:O	1.76	0.84
1:E:182:ALA:HB2	2:G:562:ALA:HA	1.58	0.84
2:B:508:GLN:N	2:B:509:PRO:CD	2.36	0.83
2:G:507:ALA:CB	10:Z:1:NAG:O6	2.26	0.83
2:I:564:GLU:N	2:I:564:GLU:OE2	2.11	0.83
2:B:564:GLU:N	2:B:564:GLU:OE2	2.11	0.82
2:G:564:GLU:N	2:G:564:GLU:OE2	2.11	0.82
1:F:55:ASP:OD1	1:F:55:ASP:O	1.99	0.80
1:E:55:ASP:OD1	1:E:55:ASP:O	1.99	0.80
2:B:570:GLN:NE2	2:G:533:PRO:CD	2.42	0.80
1:F:180:VAL:CB	2:I:566:THR:HG21	2.01	0.80
1:A:55:ASP:OD1	1:A:55:ASP:O	1.99	0.79
2:I:567:GLN:NE2	2:I:567:GLN:O	2.15	0.79
1:A:260:ILE:HG22	1:A:261:TYR:CD1	2.18	0.79
1:F:260:ILE:HG22	1:F:261:TYR:CD1	2.18	0.79
2:B:567:GLN:NE2	2:B:567:GLN:O	2.15	0.79
1:E:260:ILE:HG22	1:E:261:TYR:CD1	2.18	0.79
2:B:531:TRP:CZ2	2:I:567:GLN:OE1	2.36	0.78
2:B:533:PRO:CD	2:I:570:GLN:NE2	2.42	0.78
1:A:180:VAL:CB	2:B:566:THR:HG21	2.01	0.78
2:B:531:TRP:CD2	2:I:567:GLN:NE2	2.52	0.78
2:G:567:GLN:NE2	2:G:567:GLN:O	2.16	0.78
2:B:567:GLN:NE2	2:G:531:TRP:CD2	2.52	0.77
2:B:508:GLN:N	2:B:509:PRO:HD3	1.99	0.77
2:G:567:GLN:NE2	2:I:531:TRP:CD2	2.52	0.77
2:B:567:GLN:OE1	2:G:531:TRP:CZ2	2.37	0.76
3:P:69:ILE:HD12	3:P:69:ILE:C	2.06	0.76
1:A:257:ASN:OD1	1:A:260:ILE:HG13	1.85	0.76
3:H:69:ILE:HD12	3:H:69:ILE:C	2.06	0.76
5:C:100(D):MET:O	6:D:91:TYR:OH	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:69:ILE:C	3:Q:69:ILE:HD12	2.06	0.76
2:G:567:GLN:OE1	2:I:531:TRP:CZ2	2.37	0.76
2:G:508:GLN:N	2:G:509:PRO:HD3	1.99	0.76
2:G:570:GLN:NE2	2:I:533:PRO:CD	2.42	0.76
5:M:100(D):MET:O	6:O:91:TYR:OH	2.03	0.76
2:I:508:GLN:N	2:I:509:PRO:HD3	1.99	0.76
1:E:257:ASN:OD1	1:E:260:ILE:HG13	1.86	0.76
1:F:257:ASN:OD1	1:F:260:ILE:HG13	1.86	0.76
5:J:100(D):MET:O	6:N:91:TYR:OH	2.03	0.75
2:B:567:GLN:NE2	2:G:531:TRP:CB	2.50	0.75
3:Q:69:ILE:HD12	3:Q:69:ILE:O	1.87	0.75
2:G:567:GLN:NE2	2:I:531:TRP:CB	2.50	0.75
2:B:531:TRP:CB	2:I:567:GLN:NE2	2.50	0.74
3:H:69:ILE:HD12	3:H:69:ILE:O	1.87	0.74
3:P:69:ILE:HD12	3:P:69:ILE:O	1.87	0.74
1:F:72:GLY:CA	2:I:559:ARG:HH12	1.95	0.73
2:B:507:ALA:CB	2:B:509:PRO:HD3	2.18	0.73
2:G:567:GLN:OE1	2:I:531:TRP:CE3	2.42	0.73
2:G:507:ALA:CB	2:G:509:PRO:HD3	2.18	0.72
2:I:507:ALA:CB	2:I:509:PRO:HD3	2.18	0.72
1:E:72:GLY:CA	2:G:559:ARG:HH12	1.95	0.72
1:E:181:VAL:H	2:G:566:THR:HG22	1.55	0.72
1:A:72:GLY:CA	2:B:559:ARG:HH12	1.95	0.72
2:B:567:GLN:OE1	2:G:531:TRP:CE3	2.42	0.72
1:F:181:VAL:H	2:I:566:THR:HG22	1.55	0.71
2:B:531:TRP:CE3	2:I:567:GLN:OE1	2.42	0.71
1:A:181:VAL:H	2:B:566:THR:HG22	1.55	0.70
5:C:97:PRO:CD	5:C:100(C):ALA:HB1	2.21	0.70
5:J:97:PRO:CD	5:J:100(C):ALA:HB1	2.21	0.69
5:M:97:PRO:CD	5:M:100(C):ALA:HB1	2.21	0.69
1:F:237:ASP:OD1	1:F:261:TYR:OH	2.12	0.68
10:Z:1:NAG:H62	10:Z:2:NAG:C8	2.24	0.68
1:E:237:ASP:OD1	1:E:261:TYR:OH	2.12	0.67
1:E:182:ALA:HB2	2:G:562:ALA:CA	2.25	0.67
1:F:182:ALA:HB2	2:I:562:ALA:CA	2.25	0.67
1:A:237:ASP:OD1	1:A:261:TYR:OH	2.12	0.67
2:B:533:PRO:HG2	2:I:570:GLN:HE22	1.60	0.66
10:V:1:NAG:H62	10:V:2:NAG:C8	2.24	0.66
1:A:182:ALA:HB2	2:B:562:ALA:CA	2.25	0.66
2:G:507:ALA:HB1	10:Z:1:NAG:HO6	1.61	0.65
2:G:570:GLN:HE22	2:I:533:PRO:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLY:CA	2:G:559:ARG:NH1	2.58	0.64
2:B:570:GLN:NE2	2:G:533:PRO:HG3	2.12	0.64
1:F:72:GLY:CA	2:I:559:ARG:NH1	2.58	0.64
1:F:110:ASN:OD1	1:F:175:THR:CG2	2.40	0.64
1:A:183:PHE:HD1	2:B:565:THR:HG21	1.63	0.64
2:I:507:ALA:CB	2:I:509:PRO:CD	2.76	0.64
1:A:110:ASN:OD1	1:A:175:THR:CG2	2.40	0.63
2:B:570:GLN:HE22	2:G:533:PRO:HG2	1.60	0.63
2:I:570:GLN:OE1	2:I:570:GLN:HA	1.98	0.63
2:G:507:ALA:CB	2:G:509:PRO:CD	2.76	0.63
1:E:183:PHE:HD1	2:G:565:THR:HG21	1.63	0.63
2:B:507:ALA:CB	2:B:509:PRO:CD	2.76	0.63
10:V:1:NAG:H62	10:V:2:NAG:O7	1.98	0.63
10:Z:1:NAG:H62	10:Z:2:NAG:O7	1.98	0.63
2:B:570:GLN:OE1	2:B:570:GLN:HA	1.98	0.63
2:G:570:GLN:NE2	2:I:533:PRO:HG3	2.12	0.63
9:S:2:NAG:H61	9:S:3:BMA:H2	1.81	0.63
1:A:72:GLY:CA	2:B:559:ARG:NH1	2.58	0.62
7:K:2:NAG:H82	7:K:2:NAG:H3	1.80	0.62
7:W:2:NAG:H82	7:W:2:NAG:H3	1.80	0.62
2:G:570:GLN:OE1	2:G:570:GLN:HA	1.98	0.62
1:F:183:PHE:HD1	2:I:565:THR:HG21	1.63	0.62
1:E:110:ASN:OD1	1:E:175:THR:CG2	2.40	0.62
9:Y:2:NAG:H61	9:Y:3:BMA:H2	1.81	0.61
1:E:216:THR:HG23	1:E:216:THR:O	2.00	0.61
1:F:258:GLU:O	1:F:262:THR:OG1	2.19	0.61
1:F:216:THR:HG23	1:F:216:THR:O	2.00	0.61
8:X:2:NAG:O7	8:X:2:NAG:H3	2.01	0.61
7:W:2:NAG:H3	7:W:2:NAG:C8	2.31	0.61
8:R:2:NAG:O7	8:R:2:NAG:H3	2.01	0.61
7:K:2:NAG:H3	7:K:2:NAG:C8	2.31	0.60
2:B:533:PRO:HG3	2:I:570:GLN:NE2	2.12	0.60
5:C:100(C):ALA:HB2	6:D:49:TYR:CE1	2.37	0.60
1:A:258:GLU:O	1:A:262:THR:OG1	2.19	0.60
5:C:97:PRO:HB2	5:C:100(C):ALA:CB	2.32	0.60
5:M:97:PRO:HB2	5:M:100(C):ALA:CB	2.32	0.60
2:G:507:ALA:HB1	2:G:509:PRO:HD3	1.84	0.60
2:I:507:ALA:HB1	2:I:509:PRO:HD3	1.84	0.60
5:M:100(C):ALA:HB2	6:O:49:TYR:CE1	2.37	0.60
1:F:257:ASN:OD1	1:F:260:ILE:CG1	2.50	0.59
1:A:257:ASN:OD1	1:A:260:ILE:CG1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ASN:OD1	1:E:260:ILE:CG1	2.50	0.59
1:E:258:GLU:O	1:E:262:THR:OG1	2.19	0.59
2:I:507:ALA:HB3	2:I:509:PRO:CG	2.33	0.59
2:G:507:ALA:HB3	2:G:509:PRO:CG	2.33	0.59
5:J:100(C):ALA:HB2	6:N:49:TYR:CE1	2.37	0.59
1:A:216:THR:HG23	1:A:216:THR:O	2.00	0.58
5:M:97:PRO:HD2	5:M:100(C):ALA:HB1	1.85	0.58
1:F:183:PHE:CD1	2:I:565:THR:HG21	2.38	0.58
1:F:184:LEU:HD12	1:F:184:LEU:C	2.23	0.58
1:E:183:PHE:CD1	2:G:565:THR:HG21	2.38	0.58
5:J:97:PRO:HB2	5:J:100(C):ALA:CB	2.32	0.58
5:C:97:PRO:HD2	5:C:100(C):ALA:HB1	1.85	0.58
5:J:97:PRO:HD2	5:J:100(C):ALA:HB1	1.85	0.58
2:B:507:ALA:HB3	2:B:509:PRO:CG	2.33	0.58
5:M:53:TRP:CE3	5:M:53:TRP:HA	2.39	0.58
1:A:183:PHE:CD1	2:B:565:THR:HG21	2.38	0.58
1:A:184:LEU:HD12	1:A:184:LEU:C	2.23	0.58
2:B:531:TRP:O	2:I:570:GLN:CG	2.52	0.58
2:G:570:GLN:CG	2:I:531:TRP:O	2.52	0.58
1:F:162:TYR:CZ	1:F:176:PHE:HB3	2.39	0.58
1:E:162:TYR:CZ	1:E:176:PHE:HB3	2.39	0.58
7:W:1:NAG:H61	7:W:2:NAG:C1	2.34	0.58
1:A:162:TYR:CZ	1:A:176:PHE:HB3	2.39	0.58
1:E:184:LEU:C	1:E:184:LEU:HD12	2.23	0.58
1:E:184:LEU:HD12	1:E:184:LEU:O	2.05	0.57
5:J:53:TRP:HA	5:J:53:TRP:CE3	2.39	0.57
1:F:184:LEU:HD12	1:F:184:LEU:O	2.05	0.57
2:B:507:ALA:HB1	2:B:509:PRO:HD3	1.84	0.57
2:B:570:GLN:CG	2:G:531:TRP:O	2.52	0.57
7:K:1:NAG:H61	7:K:2:NAG:C1	2.34	0.57
5:C:53:TRP:HA	5:C:53:TRP:CE3	2.39	0.56
1:A:184:LEU:HD12	1:A:184:LEU:O	2.05	0.56
1:F:182:ALA:HB2	2:I:562:ALA:CB	2.36	0.55
2:B:533:PRO:HD3	2:I:570:GLN:NE2	2.14	0.55
1:A:182:ALA:HB2	2:B:562:ALA:CB	2.36	0.55
1:E:182:ALA:HB2	2:G:562:ALA:CB	2.36	0.54
2:B:507:ALA:HB3	2:B:509:PRO:HG3	1.90	0.54
1:F:252:PHE:CD1	1:F:252:PHE:C	2.81	0.54
2:B:507:ALA:HB1	10:V:1:NAG:HO6	1.64	0.54
2:G:507:ALA:HB3	2:G:509:PRO:HG3	1.90	0.54
2:B:570:GLN:NE2	2:G:533:PRO:HD3	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:PHE:CD1	1:E:252:PHE:C	2.81	0.53
1:A:252:PHE:C	1:A:252:PHE:CD1	2.81	0.53
2:B:531:TRP:CD1	2:I:567:GLN:CD	2.82	0.53
2:B:567:GLN:CD	2:G:531:TRP:CD1	2.82	0.53
2:I:507:ALA:HB3	2:I:509:PRO:HG3	1.90	0.53
7:W:1:NAG:H61	7:W:2:NAG:C7	2.39	0.53
2:I:507:ALA:CA	2:I:509:PRO:CD	2.87	0.53
7:K:1:NAG:H61	7:K:2:NAG:C7	2.39	0.53
3:H:28:THR:HG23	3:H:28:THR:O	2.09	0.52
2:G:567:GLN:CD	2:I:531:TRP:CD1	2.82	0.52
1:A:266:ARG:O	1:A:266:ARG:HG2	2.10	0.52
1:E:266:ARG:HG2	1:E:266:ARG:O	2.10	0.52
1:E:229:GLU:HG2	7:W:1:NAG:C7	2.40	0.52
1:A:229:GLU:HG2	7:K:1:NAG:C7	2.40	0.52
1:E:36:GLY:CA	2:G:561:LEU:HD21	2.40	0.52
1:F:36:GLY:CA	2:I:561:LEU:HD21	2.40	0.51
3:P:28:THR:O	3:P:28:THR:HG23	2.09	0.51
5:J:100(A):ASP:O	5:J:100(B):ASN:HB2	2.11	0.51
2:B:531:TRP:O	2:I:570:GLN:HG2	2.11	0.51
2:G:567:GLN:NE2	2:I:531:TRP:CE3	2.77	0.51
3:Q:28:THR:HG23	3:Q:28:THR:O	2.09	0.51
1:A:36:GLY:CA	2:B:561:LEU:HD21	2.40	0.51
2:G:507:ALA:CA	2:G:509:PRO:CD	2.87	0.51
2:B:570:GLN:HG2	2:G:531:TRP:O	2.11	0.51
2:G:570:GLN:HG2	2:I:531:TRP:O	2.11	0.51
1:F:266:ARG:O	1:F:266:ARG:HG2	2.10	0.51
2:B:531:TRP:CE3	2:I:567:GLN:NE2	2.77	0.50
2:B:507:ALA:HB3	2:B:509:PRO:CD	2.41	0.50
2:I:507:ALA:HB3	2:I:509:PRO:CD	2.41	0.50
5:M:100(A):ASP:O	5:M:100(B):ASN:HB2	2.11	0.50
2:G:570:GLN:NE2	2:I:533:PRO:HD3	2.14	0.50
5:C:100(A):ASP:O	5:C:100(B):ASN:HB2	2.11	0.50
3:P:40:SER:OG	3:P:42:GLU:OE1	2.30	0.50
1:F:252:PHE:CD1	1:F:252:PHE:O	2.65	0.50
1:A:252:PHE:CD1	1:A:252:PHE:O	2.65	0.50
3:H:40:SER:OG	3:H:42:GLU:OE1	2.30	0.50
3:Q:40:SER:OG	3:Q:42:GLU:OE1	2.30	0.50
2:B:507:ALA:CA	2:B:509:PRO:CD	2.87	0.49
2:B:563:ASN:OD1	10:V:1:NAG:N2	2.46	0.49
1:E:252:PHE:CD1	1:E:252:PHE:O	2.65	0.49
2:G:507:ALA:HB3	2:G:509:PRO:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:563:ASN:OD1	10:Z:1:NAG:N2	2.46	0.49
2:B:567:GLN:NE2	2:G:531:TRP:CE3	2.77	0.49
2:I:510:LYS:HD3	2:I:510:LYS:N	2.28	0.49
7:K:1:NAG:H62	7:K:2:NAG:O7	2.12	0.49
10:V:1:NAG:C6	10:V:2:NAG:C8	2.91	0.49
7:W:1:NAG:H62	7:W:2:NAG:O7	2.12	0.49
2:B:510:LYS:HD3	2:B:510:LYS:N	2.28	0.48
2:G:510:LYS:HD3	2:G:510:LYS:N	2.28	0.48
1:F:36:GLY:HA3	2:I:561:LEU:HD21	1.95	0.48
5:C:53:TRP:HA	5:C:53:TRP:HE3	1.79	0.48
5:J:95:ARG:CA	5:J:100(D):MET:HB3	2.21	0.48
4:U:62:PHE:N	4:U:62:PHE:CD1	2.81	0.48
2:G:570:GLN:HG3	2:I:531:TRP:O	2.13	0.48
8:R:1:NAG:O6	8:R:2:NAG:H83	2.14	0.48
2:B:531:TRP:O	2:I:570:GLN:HG3	2.13	0.48
10:Z:1:NAG:C6	10:Z:2:NAG:C8	2.91	0.48
4:L:62:PHE:N	4:L:62:PHE:CD1	2.81	0.48
5:J:53:TRP:HA	5:J:53:TRP:HE3	1.79	0.48
1:A:36:GLY:HA3	2:B:561:LEU:HD21	1.95	0.48
1:E:36:GLY:HA3	2:G:561:LEU:HD21	1.95	0.47
2:B:570:GLN:HG3	2:G:531:TRP:O	2.13	0.47
3:H:7:SER:OG	3:H:21:SER:OG	2.32	0.47
2:B:602:HIS:HE2	2:G:613:HIS:HD1	1.62	0.47
2:G:602:HIS:HE2	2:I:613:HIS:HD1	1.62	0.47
4:T:62:PHE:N	4:T:62:PHE:CD1	2.81	0.47
5:J:97:PRO:CB	5:J:100(C):ALA:HB1	2.43	0.47
2:B:563:ASN:HB3	2:B:564:GLU:OE2	2.15	0.47
2:G:563:ASN:HB3	2:G:564:GLU:OE2	2.15	0.47
8:X:1:NAG:O6	8:X:2:NAG:H83	2.14	0.47
3:P:69:ILE:C	3:P:69:ILE:CD1	2.74	0.47
2:G:508:GLN:HB3	10:Z:2:NAG:H81	1.98	0.46
2:I:563:ASN:HB3	2:I:564:GLU:OE2	2.15	0.46
2:B:508:GLN:HB3	10:V:2:NAG:H81	1.98	0.46
3:P:7:SER:OG	3:P:21:SER:OG	2.32	0.46
2:B:613:HIS:HD1	2:I:602:HIS:HE2	1.62	0.46
5:C:13:GLN:OE1	5:C:13:GLN:N	2.45	0.46
5:C:97:PRO:CB	5:C:100(C):ALA:HB1	2.43	0.46
5:M:97:PRO:CB	5:M:100(C):ALA:HB1	2.43	0.46
6:O:98:PHE:CD1	6:O:98:PHE:N	2.84	0.46
2:I:560:GLN:HG3	2:I:564:GLU:OE1	2.16	0.45
1:A:72:GLY:C	2:B:559:ARG:NH1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:98:PHE:CD1	6:D:98:PHE:N	2.84	0.45
1:F:72:GLY:C	2:I:559:ARG:NH1	2.70	0.45
4:L:89:GLN:OE1	4:L:89:GLN:N	2.50	0.45
6:O:106:LEU:O	6:O:107:ARG:HB3	2.17	0.45
1:A:269:THR:OG1	1:A:271:GLY:O	2.35	0.45
1:E:220:TYR:CD2	1:E:220:TYR:N	2.85	0.45
4:T:89:GLN:N	4:T:89:GLN:OE1	2.50	0.45
5:J:97:PRO:CB	5:J:100(C):ALA:CB	2.95	0.45
6:N:98:PHE:CD1	6:N:98:PHE:N	2.84	0.45
3:P:100(B):MET:HG3	3:P:100(B):MET:O	2.16	0.45
3:Q:7:SER:OG	3:Q:21:SER:OG	2.32	0.45
1:A:220:TYR:N	1:A:220:TYR:CD2	2.85	0.45
1:E:72:GLY:C	2:G:559:ARG:NH1	2.70	0.45
2:I:508:GLN:O	2:I:508:GLN:HG3	2.16	0.45
4:U:89:GLN:N	4:U:89:GLN:OE1	2.50	0.45
1:F:220:TYR:CD2	1:F:220:TYR:N	2.85	0.45
1:E:269:THR:OG1	1:E:271:GLY:O	2.35	0.44
5:M:53:TRP:HA	5:M:53:TRP:HE3	1.79	0.44
2:B:560:GLN:HG3	2:B:564:GLU:OE1	2.16	0.44
5:C:97:PRO:CB	5:C:100(C):ALA:CB	2.95	0.44
2:G:560:GLN:HG3	2:G:564:GLU:OE1	2.16	0.44
3:Q:100(B):MET:O	3:Q:100(B):MET:HG3	2.16	0.44
1:A:176:PHE:O	1:A:176:PHE:CD1	2.71	0.44
5:C:95:ARG:CA	5:C:100(D):MET:HB3	2.21	0.44
6:D:106:LEU:O	6:D:107:ARG:HB3	2.16	0.44
1:F:176:PHE:O	1:F:176:PHE:CD1	2.71	0.44
1:A:66:VAL:O	1:A:66:VAL:HG23	2.17	0.44
1:E:176:PHE:O	1:E:176:PHE:CD1	2.71	0.44
1:F:66:VAL:O	1:F:66:VAL:HG23	2.17	0.44
1:F:262:THR:OG1	1:F:263:SER:N	2.51	0.44
5:M:13:GLN:OE1	5:M:13:GLN:N	2.45	0.44
5:J:100(D):MET:HA	5:J:101:GLY:HA3	1.29	0.44
3:H:100(B):MET:O	3:H:100(B):MET:HG3	2.16	0.44
1:F:269:THR:OG1	1:F:271:GLY:O	2.35	0.44
2:B:507:ALA:CB	10:V:1:NAG:HO6	2.27	0.44
5:M:97:PRO:CB	5:M:100(C):ALA:CB	2.95	0.44
2:G:508:GLN:O	2:G:508:GLN:HG3	2.16	0.44
6:N:106:LEU:O	6:N:107:ARG:HB3	2.17	0.43
1:E:66:VAL:HG23	1:E:66:VAL:O	2.17	0.43
1:A:262:THR:OG1	1:A:263:SER:N	2.51	0.43
2:B:508:GLN:O	2:B:508:GLN:HG3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:71:TYR:CD1	4:U:71:TYR:N	2.87	0.43
1:E:262:THR:OG1	1:E:263:SER:N	2.51	0.43
4:L:71:TYR:CD1	4:L:71:TYR:N	2.87	0.43
2:G:507:ALA:CA	2:G:509:PRO:HD3	2.47	0.43
1:A:111:LEU:HD23	1:A:111:LEU:C	2.39	0.43
4:T:71:TYR:CD1	4:T:71:TYR:N	2.87	0.43
1:F:216:THR:O	1:F:216:THR:CG2	2.67	0.43
2:I:507:ALA:CA	2:I:509:PRO:HD3	2.47	0.43
6:N:94:TYR:HA	6:N:95:PRO:C	2.40	0.42
1:F:111:LEU:C	1:F:111:LEU:HD23	2.39	0.42
1:E:55:ASP:OD1	1:E:55:ASP:C	2.58	0.42
1:E:58:SER:N	1:E:62:GLN:OE1	2.53	0.42
1:E:178:GLU:H	1:E:178:GLU:HG3	1.59	0.42
1:E:132:PHE:HA	1:E:133:PRO:HD3	1.86	0.42
1:E:216:THR:O	1:E:216:THR:CG2	2.67	0.42
9:S:2:NAG:H61	9:S:3:BMA:C1	2.49	0.42
1:A:58:SER:N	1:A:62:GLN:OE1	2.53	0.42
5:M:95:ARG:CA	5:M:100(D):MET:HB3	2.21	0.42
6:O:94:TYR:HA	6:O:95:PRO:C	2.40	0.42
1:E:111:LEU:C	1:E:111:LEU:HD23	2.39	0.42
2:I:567:GLN:NE2	2:I:567:GLN:C	2.73	0.42
9:Y:2:NAG:H61	9:Y:3:BMA:C2	2.49	0.42
3:H:69:ILE:C	3:H:69:ILE:CD1	2.74	0.42
1:E:103:GLU:HA	2:G:517:TYR:HA	2.01	0.42
1:A:55:ASP:OD1	1:A:55:ASP:C	2.58	0.42
1:A:218:ILE:O	1:A:218:ILE:HG22	2.20	0.42
6:D:94:TYR:HA	6:D:95:PRO:C	2.40	0.42
1:E:218:ILE:O	1:E:218:ILE:HG22	2.20	0.42
1:F:58:SER:N	1:F:62:GLN:OE1	2.53	0.42
2:G:567:GLN:NE2	2:G:567:GLN:C	2.73	0.42
9:Y:2:NAG:H61	9:Y:3:BMA:C1	2.49	0.42
2:B:578:GLU:OE1	2:B:581:THR:N	2.49	0.42
1:F:132:PHE:HA	1:F:133:PRO:HD3	1.86	0.42
2:B:596:ARG:HB2	2:B:597:TRP:CE3	2.55	0.41
2:G:596:ARG:HB2	2:G:597:TRP:CE3	2.55	0.41
3:Q:69:ILE:C	3:Q:69:ILE:CD1	2.74	0.41
1:A:103:GLU:HA	2:B:517:TYR:HA	2.01	0.41
2:B:567:GLN:NE2	2:B:567:GLN:C	2.73	0.41
5:M:15:GLY:N	5:M:82(C):VAL:O	2.54	0.41
3:H:15:GLY:N	3:H:82(C):LEU:O	2.53	0.41
1:E:79:VAL:HB	1:E:80:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:GLY:N	3:Q:82(C):LEU:O	2.53	0.41
1:A:160:PHE:HB3	1:A:176:PHE:HB2	2.02	0.41
4:T:43:SER:HB3	4:T:44:PRO:HD2	2.02	0.41
1:F:103:GLU:HA	2:I:517:TYR:HA	2.01	0.41
5:M:96:ASP:HB3	5:M:97:PRO:CD	2.51	0.41
1:A:79:VAL:HB	1:A:80:PRO:HD3	2.02	0.41
1:F:218:ILE:O	1:F:218:ILE:HG22	2.20	0.41
2:I:596:ARG:HB2	2:I:597:TRP:CE3	2.55	0.41
5:M:97:PRO:HG2	5:M:100(C):ALA:CB	2.36	0.41
9:S:2:NAG:H61	9:S:3:BMA:C2	2.49	0.41
9:Y:1:NAG:H62	9:Y:2:NAG:C8	2.50	0.41
4:L:43:SER:HB3	4:L:44:PRO:HD2	2.02	0.41
1:A:92:VAL:O	1:A:92:VAL:HG23	2.20	0.41
5:C:15:GLY:N	5:C:82(C):VAL:O	2.54	0.41
5:J:15:GLY:N	5:J:82(C):VAL:O	2.54	0.41
5:J:96:ASP:HB3	5:J:97:PRO:CD	2.51	0.41
1:F:79:VAL:HB	1:F:80:PRO:HD3	2.02	0.41
1:F:260:ILE:HG22	1:F:261:TYR:CE1	2.56	0.41
4:U:43:SER:HB3	4:U:44:PRO:HD2	2.02	0.41
2:B:508:GLN:HB3	10:V:2:NAG:C8	2.51	0.41
1:E:36:GLY:HA3	2:G:561:LEU:CD2	2.51	0.41
1:F:36:GLY:HA3	2:I:561:LEU:CD2	2.51	0.41
5:C:96:ASP:HB3	5:C:97:PRO:CD	2.51	0.40
2:G:611:GLU:HA	2:G:612:PRO:HD3	1.96	0.40
6:D:86:TYR:O	6:D:101:GLY:HA2	2.22	0.40
1:E:92:VAL:O	1:E:92:VAL:HG23	2.20	0.40
2:G:532:ILE:HA	2:G:533:PRO:HD3	1.91	0.40
1:E:160:PHE:HB3	1:E:176:PHE:HB2	2.02	0.40
2:G:508:GLN:HB3	10:Z:2:NAG:C8	2.51	0.40
2:G:578:GLU:OE1	2:G:581:THR:N	2.49	0.40
1:F:101:ALA:HB1	2:I:519:THR:HA	2.04	0.40
1:F:160:PHE:HB3	1:F:176:PHE:HB2	2.02	0.40
1:A:216:THR:O	1:A:216:THR:CG2	2.67	0.40
1:A:260:ILE:HG22	1:A:261:TYR:CE1	2.56	0.40
5:C:53:TRP:O	5:C:53:TRP:CD2	2.75	0.40
1:F:55:ASP:OD1	1:F:55:ASP:C	2.58	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	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	6	38
1	E	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	6	38
1	F	229/469 (49%)	216 (94%)	8 (4%)	5 (2%)	6	38
2	B	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	8	42
2	G	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	8	42
2	I	111/143 (78%)	103 (93%)	6 (5%)	2 (2%)	8	42
3	H	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	P	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
3	Q	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
4	L	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	15	54
4	T	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	15	54
4	U	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	15	54
5	C	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	9	43
5	J	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	9	43
5	M	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	9	43
6	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
6	N	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
6	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
All	All	2361/3201 (74%)	2250 (95%)	81 (3%)	30 (1%)	16	48

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	THR
1	A	242	VAL
1	E	216	THR
1	E	242	VAL

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Mol	Chain	Res	Type
1	F	216	THR
1	F	242	VAL
1	A	153	PHE
1	E	153	PHE
1	F	153	PHE
1	A	122	LEU
1	A	218	ILE
5	C	98	PHE
1	E	122	LEU
1	E	218	ILE
5	J	98	PHE
1	F	122	LEU
1	F	218	ILE
5	M	98	PHE
2	B	584	ILE
4	L	93	GLY
5	C	96	ASP
2	G	584	ILE
4	T	93	GLY
5	J	96	ASP
2	I	584	ILE
4	U	93	GLY
5	M	96	ASP
2	B	603	ILE
2	G	603	ILE
2	I	603	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/399 (49%)	196 (100%)	1 (0%)	88 93
1	E	197/399 (49%)	196 (100%)	1 (0%)	88 93
1	F	197/399 (49%)	196 (100%)	1 (0%)	88 93
2	B	92/122 (75%)	90 (98%)	2 (2%)	52 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	92/122 (75%)	90 (98%)	2 (2%)	52 71
2	I	92/122 (75%)	90 (98%)	2 (2%)	52 71
3	H	101/101 (100%)	100 (99%)	1 (1%)	76 86
3	P	101/101 (100%)	100 (99%)	1 (1%)	76 86
3	Q	101/101 (100%)	100 (99%)	1 (1%)	76 86
4	L	91/91 (100%)	91 (100%)	0	100 100
4	T	91/91 (100%)	91 (100%)	0	100 100
4	U	91/91 (100%)	91 (100%)	0	100 100
5	C	99/99 (100%)	99 (100%)	0	100 100
5	J	99/99 (100%)	99 (100%)	0	100 100
5	M	99/99 (100%)	99 (100%)	0	100 100
6	D	92/92 (100%)	92 (100%)	0	100 100
6	N	92/92 (100%)	92 (100%)	0	100 100
6	O	92/92 (100%)	92 (100%)	0	100 100
All	All	2016/2712 (74%)	2004 (99%)	12 (1%)	86 92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
2	B	564	GLU
2	B	567	GLN
3	H	94	ARG
1	E	178	GLU
2	G	564	GLU
2	G	567	GLN
3	P	94	ARG
1	F	178	GLU
2	I	564	GLU
2	I	567	GLN
3	Q	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	567	GLN

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Mol	Chain	Res	Type
2	B	570	GLN
2	G	567	GLN
2	G	570	GLN
5	J	100(B)	ASN
2	I	567	GLN
2	I	570	GLN
5	M	100(B)	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

42 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	$\#\|Z\| > 2$
7	NAG	K	1	7,1	14,14,15	0.69	0	17,19,21	2.31	2 (11%)
7	NAG	K	2	7	14,14,15	0.27	0	17,19,21	0.58	0
8	NAG	R	1	8,1	14,14,15	0.50	0	17,19,21	0.72	0
8	NAG	R	2	8	14,14,15	0.30	0	17,19,21	0.60	0
8	BMA	R	3	8	11,11,12	0.23	0	15,15,17	0.71	0
9	NAG	S	1	9,1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
9	NAG	S	2	9	14,14,15	0.27	0	17,19,21	0.66	0
9	BMA	S	3	9	11,11,12	0.24	0	15,15,17	0.70	0
9	MAN	S	4	9	11,11,12	0.22	0	15,15,17	0.58	0
10	NAG	V	1	10,2	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
10	NAG	V	2	10	14,14,15	0.32	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BMA	V	3	10	11,11,12	0.24	0	15,15,17	0.94	1 (6%)
10	MAN	V	4	10	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
10	MAN	V	5	10	11,11,12	0.27	0	15,15,17	1.07	3 (20%)
7	NAG	W	1	7,1	14,14,15	0.68	0	17,19,21	2.31	2 (11%)
7	NAG	W	2	7	14,14,15	0.27	0	17,19,21	0.58	0
8	NAG	X	1	8,1	14,14,15	0.50	0	17,19,21	0.73	0
8	NAG	X	2	8	14,14,15	0.30	0	17,19,21	0.60	0
8	BMA	X	3	8	11,11,12	0.24	0	15,15,17	0.71	0
9	NAG	Y	1	9,1	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
9	NAG	Y	2	9	14,14,15	0.27	0	17,19,21	0.66	0
9	BMA	Y	3	9	11,11,12	0.24	0	15,15,17	0.70	0
9	MAN	Y	4	9	11,11,12	0.22	0	15,15,17	0.58	0
10	NAG	Z	1	10,2	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
10	NAG	Z	2	10	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
10	BMA	Z	3	10	11,11,12	0.24	0	15,15,17	0.93	1 (6%)
10	MAN	Z	4	10	11,11,12	0.25	0	15,15,17	1.05	1 (6%)
10	MAN	Z	5	10	11,11,12	0.26	0	15,15,17	1.07	3 (20%)
7	NAG	a	1	7,1	14,14,15	0.68	0	17,19,21	2.31	2 (11%)
7	NAG	a	2	7	14,14,15	0.27	0	17,19,21	0.58	0
8	NAG	b	1	8,1	14,14,15	0.50	0	17,19,21	0.72	0
8	NAG	b	2	8	14,14,15	0.30	0	17,19,21	0.59	0
8	BMA	b	3	8	11,11,12	0.24	0	15,15,17	0.71	0
9	NAG	c	1	9,1	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
9	NAG	c	2	9	14,14,15	0.27	0	17,19,21	0.66	0
9	BMA	c	3	9	11,11,12	0.24	0	15,15,17	0.70	0
9	MAN	c	4	9	11,11,12	0.22	0	15,15,17	0.58	0
10	NAG	d	1	10,2	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
10	NAG	d	2	10	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
10	BMA	d	3	10	11,11,12	0.24	0	15,15,17	0.94	1 (6%)
10	MAN	d	4	10	11,11,12	0.25	0	15,15,17	1.05	1 (6%)
10	MAN	d	5	10	11,11,12	0.26	0	15,15,17	1.07	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	K	2	7	-	3/6/23/26	0/1/1/1
8	NAG	R	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	2/2/19/22	0/1/1/1
9	NAG	S	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	0/2/19/22	0/1/1/1
9	MAN	S	4	9	-	0/2/19/22	0/1/1/1
10	NAG	V	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	V	2	10	-	1/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
10	MAN	V	4	10	-	0/2/19/22	0/1/1/1
10	MAN	V	5	10	-	0/2/19/22	0/1/1/1
7	NAG	W	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	W	2	7	-	3/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	0/2/19/22	0/1/1/1
10	NAG	Z	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
7	NAG	a	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	a	2	7	-	3/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	2/2/19/22	0/1/1/1
9	NAG	c	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	c	2	9	-	0/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	1/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	MAN	d	5	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	1	NAG	C1-O5-C5	7.47	122.32	112.19
7	K	1	NAG	C1-O5-C5	7.47	122.31	112.19
7	a	1	NAG	C1-O5-C5	7.46	122.30	112.19
7	K	1	NAG	O5-C1-C2	-5.00	103.39	111.29
7	W	1	NAG	O5-C1-C2	-4.99	103.41	111.29
7	a	1	NAG	O5-C1-C2	-4.98	103.43	111.29
10	d	3	BMA	C1-C2-C3	2.68	112.96	109.67
10	V	3	BMA	C1-C2-C3	2.68	112.96	109.67
10	d	2	NAG	O5-C1-C2	-2.66	107.09	111.29
10	V	2	NAG	O5-C1-C2	-2.65	107.11	111.29
10	Z	3	BMA	C1-C2-C3	2.64	112.92	109.67
10	Z	2	NAG	O5-C1-C2	-2.63	107.14	111.29
9	Y	1	NAG	C1-O5-C5	2.59	115.71	112.19
9	c	1	NAG	C1-O5-C5	2.59	115.70	112.19
9	S	1	NAG	C1-O5-C5	2.59	115.69	112.19
10	Z	1	NAG	C1-O5-C5	2.54	115.63	112.19
10	V	1	NAG	C1-O5-C5	2.52	115.60	112.19
10	d	1	NAG	C1-O5-C5	2.52	115.60	112.19
10	d	5	MAN	C1-O5-C5	-2.49	108.81	112.19
10	Z	5	MAN	C1-O5-C5	-2.48	108.84	112.19
10	V	5	MAN	C1-O5-C5	-2.47	108.84	112.19
10	V	4	MAN	O2-C2-C3	-2.14	105.86	110.14
10	Z	4	MAN	O2-C2-C3	-2.13	105.88	110.14
10	d	4	MAN	O2-C2-C3	-2.12	105.88	110.14
10	Z	5	MAN	O5-C5-C6	2.08	110.46	107.20
10	V	5	MAN	O5-C5-C6	2.07	110.45	107.20
10	d	5	MAN	O5-C5-C6	2.07	110.44	107.20
10	Z	5	MAN	O6-C6-C5	-2.04	104.29	111.29
10	d	5	MAN	O6-C6-C5	-2.04	104.31	111.29
10	V	5	MAN	O6-C6-C5	-2.03	104.31	111.29

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C3-C2-N2-C7
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
7	W	1	NAG	C3-C2-N2-C7
7	W	2	NAG	C8-C7-N2-C2
7	W	2	NAG	O7-C7-N2-C2
7	a	1	NAG	C3-C2-N2-C7
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
7	K	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C8-C7-N2-C2
7	W	1	NAG	C8-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	K	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	K	2	NAG	C1-C2-N2-C7
7	W	2	NAG	C1-C2-N2-C7
7	a	2	NAG	C1-C2-N2-C7
8	R	1	NAG	C1-C2-N2-C7
8	X	1	NAG	C1-C2-N2-C7
8	b	1	NAG	C1-C2-N2-C7
7	K	1	NAG	O7-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2
8	R	3	BMA	O5-C5-C6-O6
8	X	3	BMA	O5-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
10	d	2	NAG	O5-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
10	Z	2	NAG	O5-C5-C6-O6
8	R	2	NAG	C3-C2-N2-C7
8	X	2	NAG	C3-C2-N2-C7
8	b	2	NAG	C3-C2-N2-C7
7	K	1	NAG	C1-C2-N2-C7
7	W	1	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
8	R	3	BMA	C4-C5-C6-O6
8	X	3	BMA	C4-C5-C6-O6
8	b	3	BMA	C4-C5-C6-O6
8	X	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	R	2	NAG	C4-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6

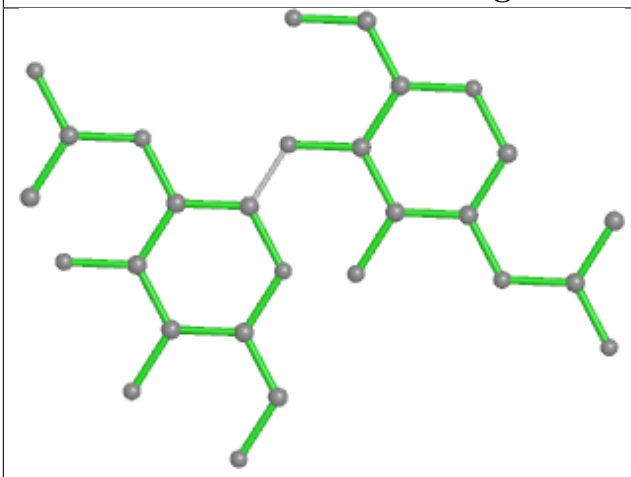
There are no ring outliers.

18 monomers are involved in 46 short contacts:

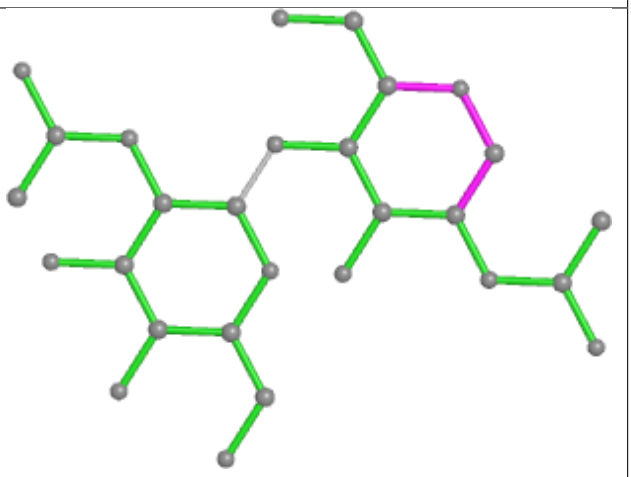
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Y	3	BMA	3	0
9	Y	1	NAG	2	0
8	X	2	NAG	2	0
8	R	2	NAG	2	0
7	W	1	NAG	4	0
9	S	2	NAG	4	0
7	K	1	NAG	4	0
8	R	1	NAG	1	0
10	V	1	NAG	9	0
9	S	1	NAG	1	0
10	Z	2	NAG	6	0
7	K	2	NAG	5	0
9	Y	2	NAG	5	0
7	W	2	NAG	5	0
9	S	3	BMA	3	0
10	Z	1	NAG	8	0
8	X	1	NAG	1	0
10	V	2	NAG	6	0

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

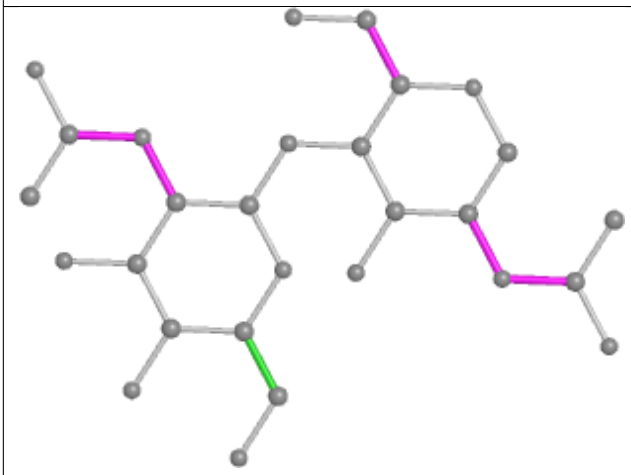
Oligosaccharide Chain K



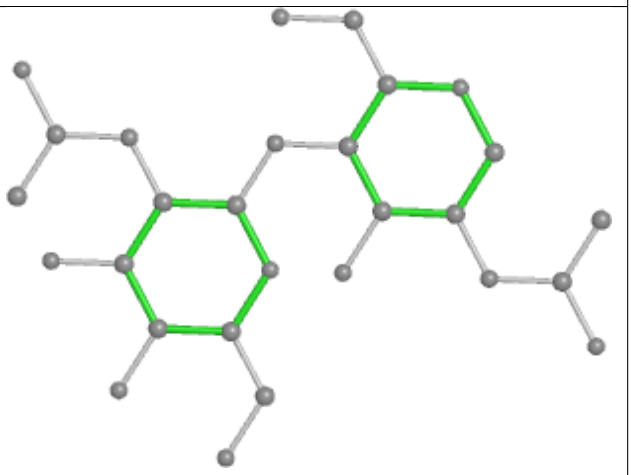
Bond lengths



Bond angles

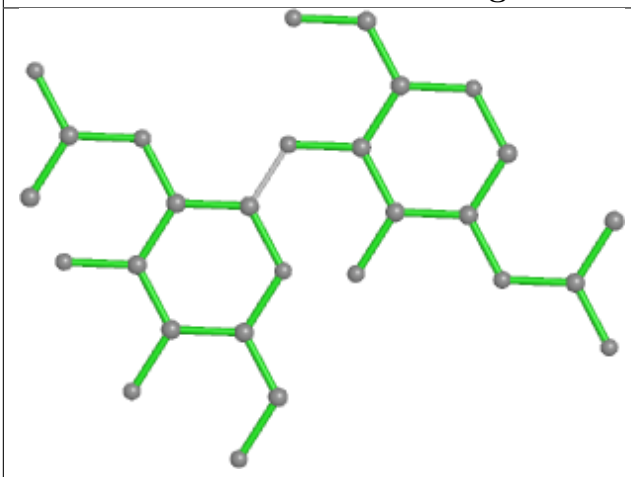


Torsions

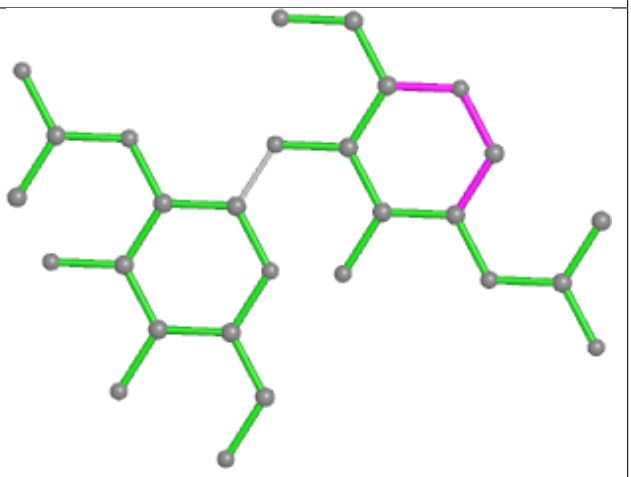


Rings

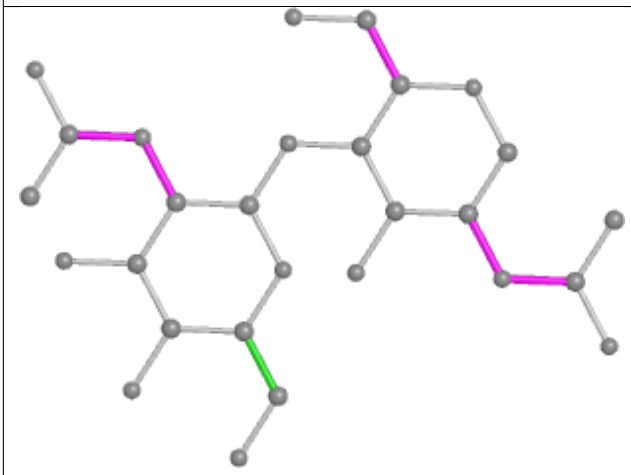
Oligosaccharide Chain W



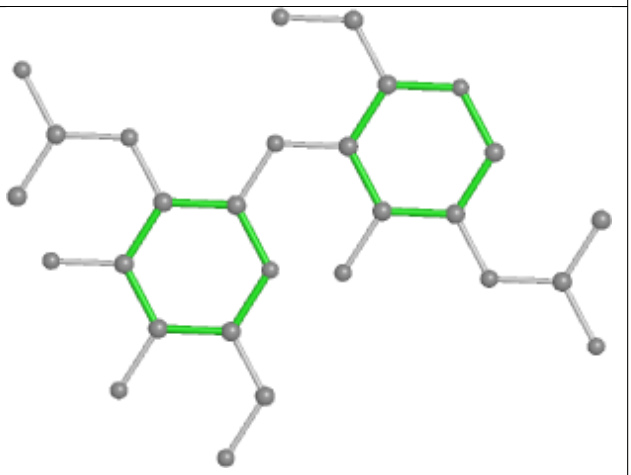
Bond lengths



Bond angles

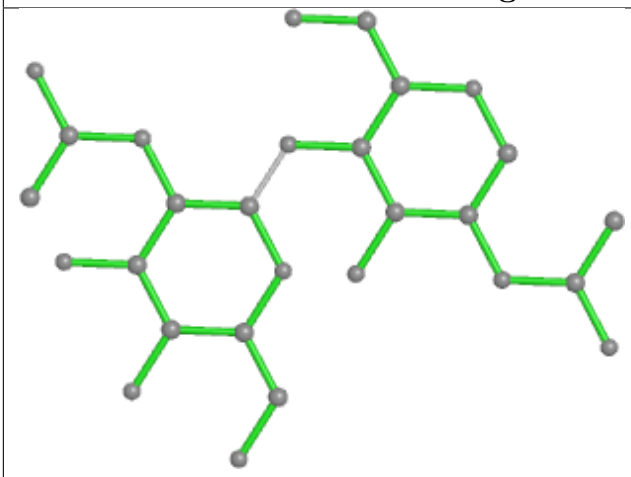


Torsions

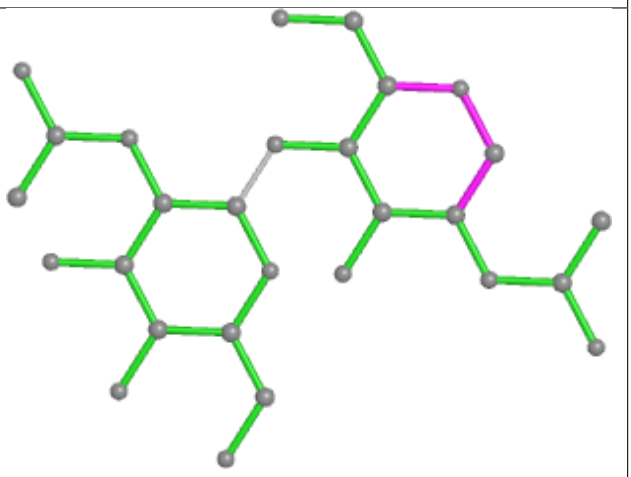


Rings

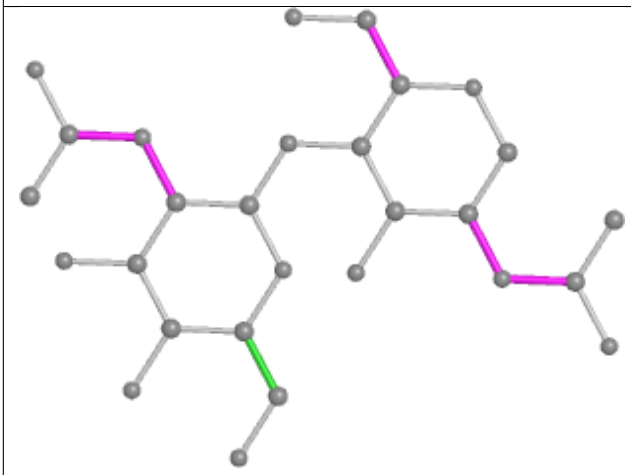
Oligosaccharide Chain a



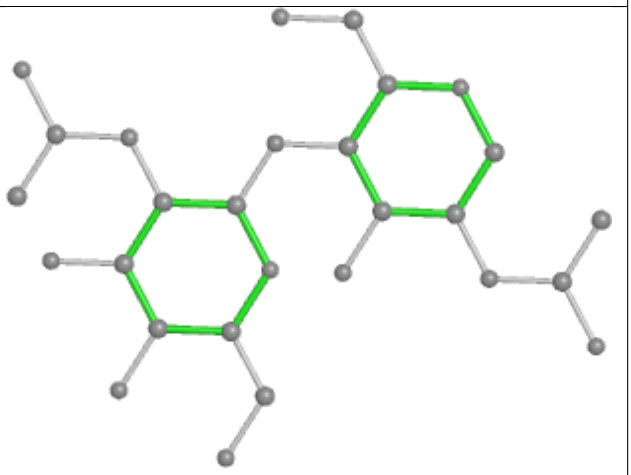
Bond lengths



Bond angles

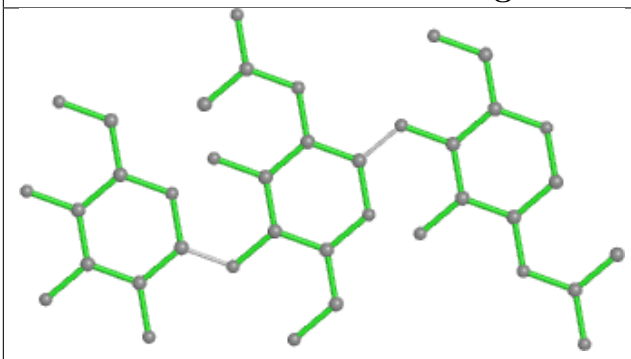


Torsions

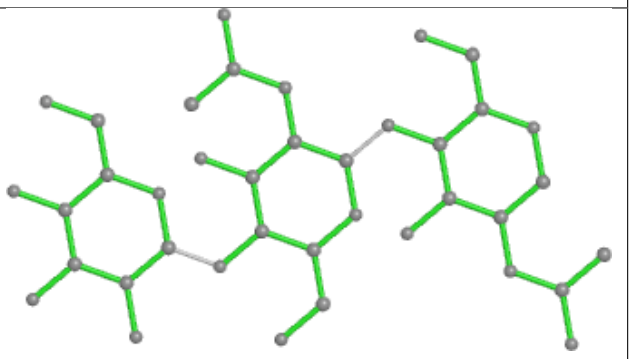


Rings

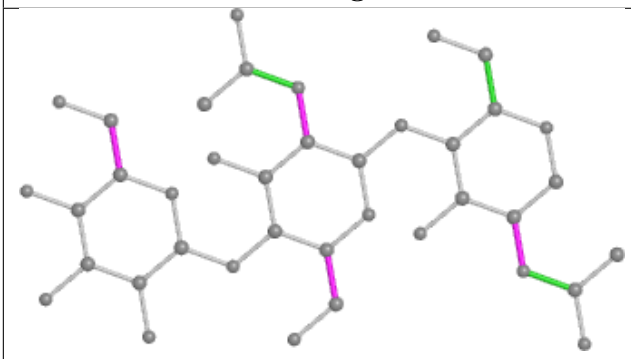
Oligosaccharide Chain R



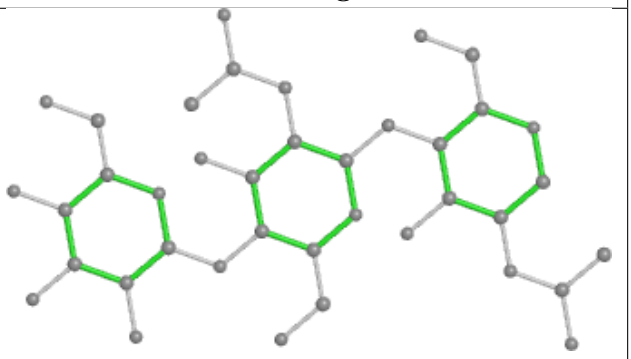
Bond lengths



Bond angles

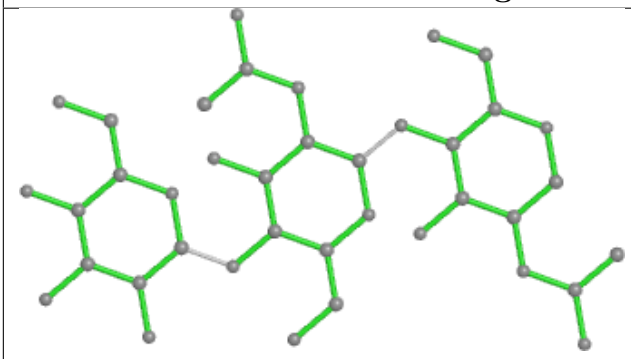


Torsions

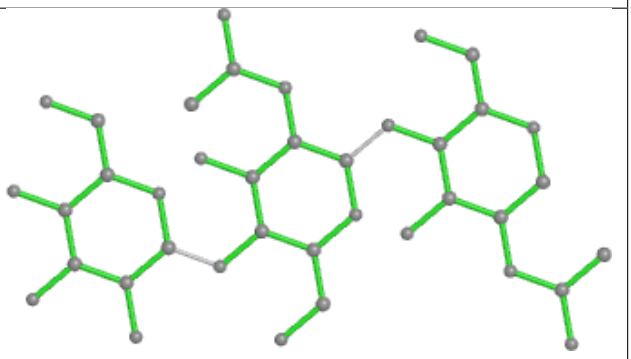


Rings

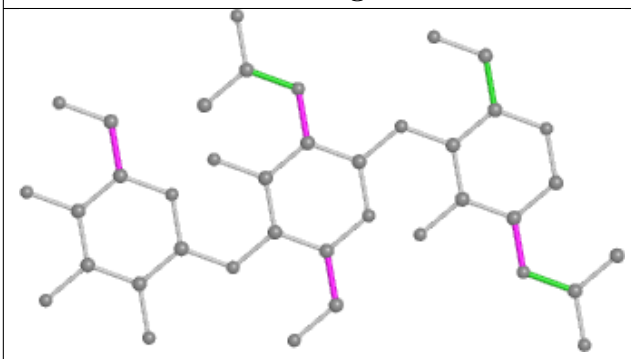
Oligosaccharide Chain X



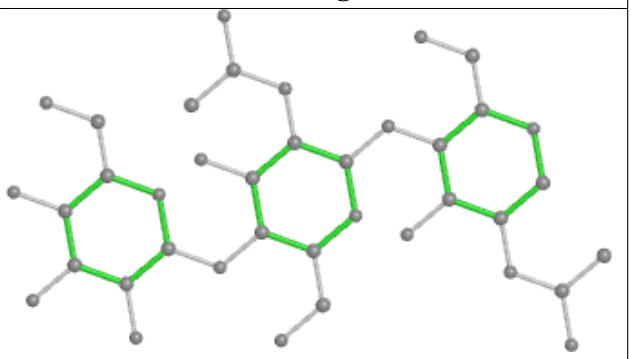
Bond lengths



Bond angles

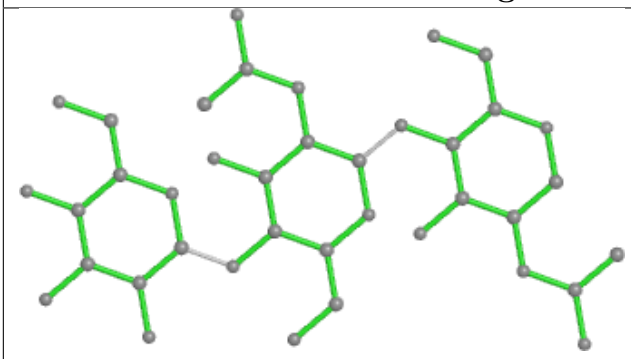


Torsions

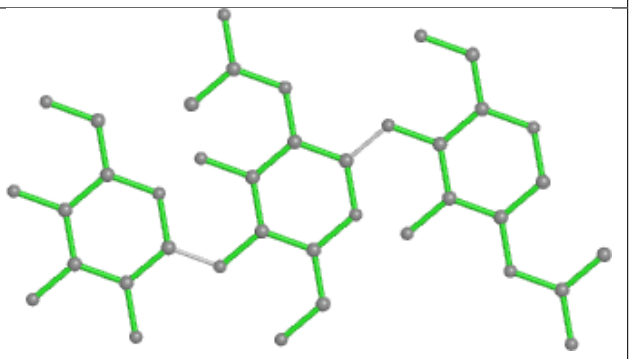


Rings

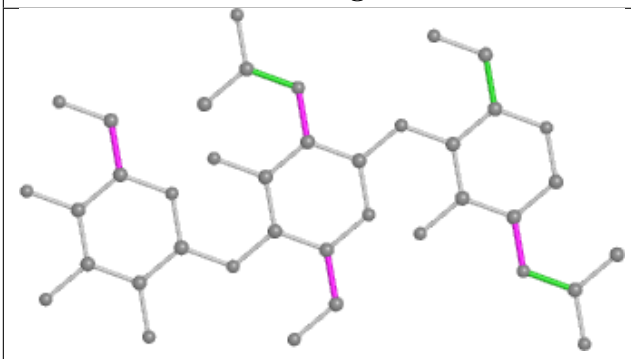
Oligosaccharide Chain b



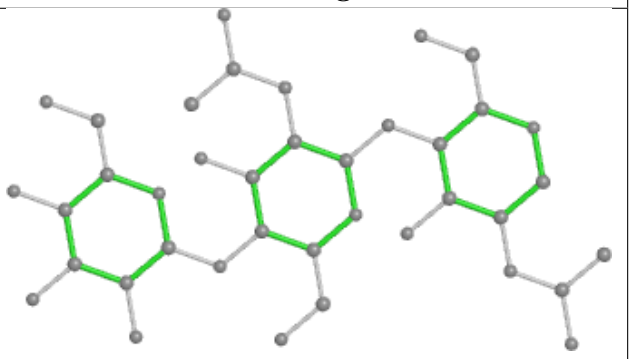
Bond lengths



Bond angles

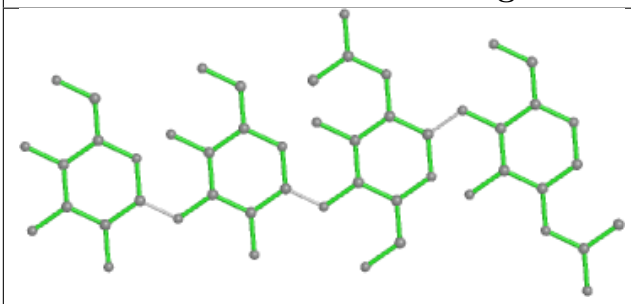


Torsions

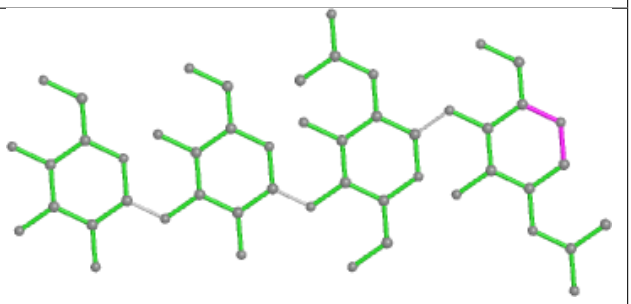


Rings

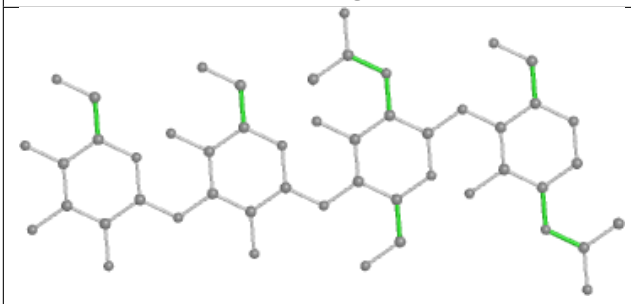
Oligosaccharide Chain S



Bond lengths



Bond angles



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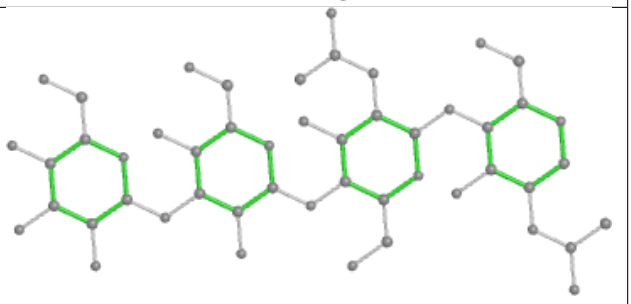
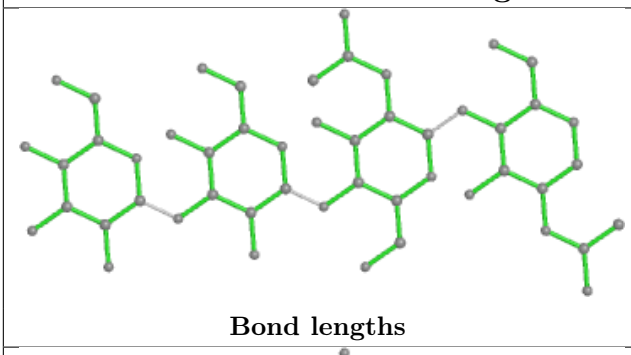
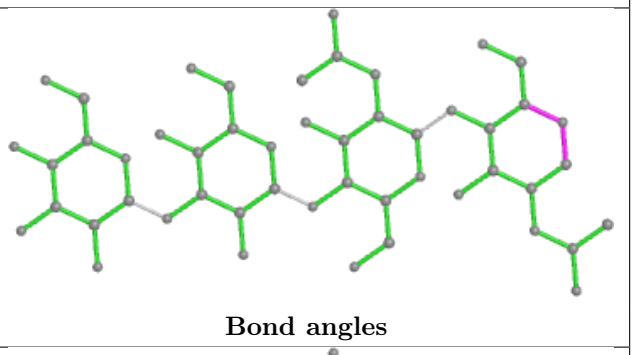


Rings

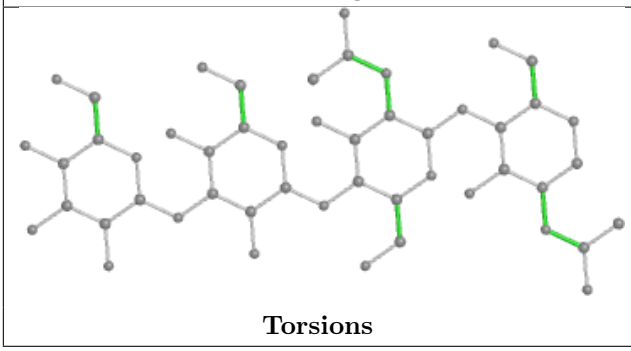
Oligosaccharide Chain Y



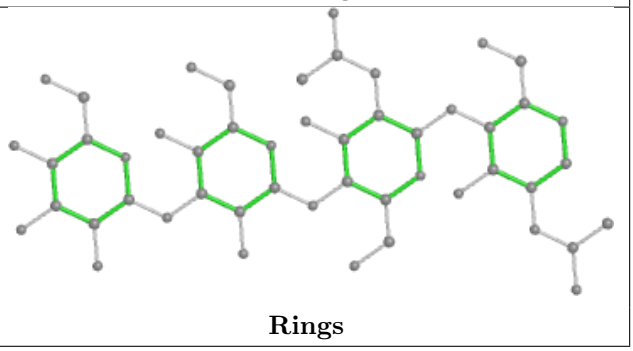
Bond lengths



Bond angles

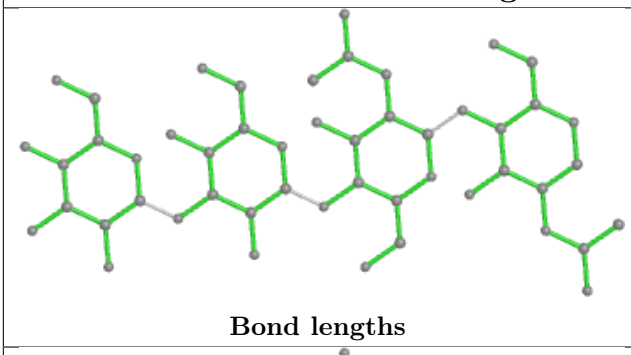


Torsions

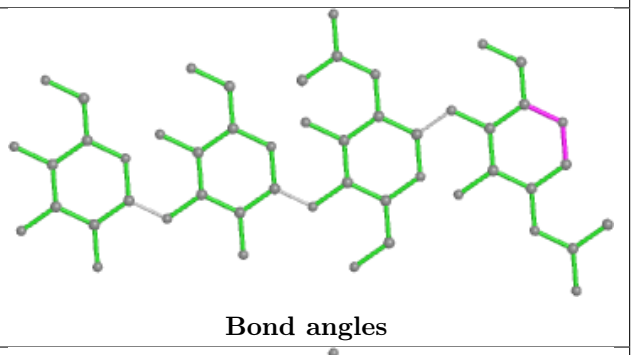


Rings

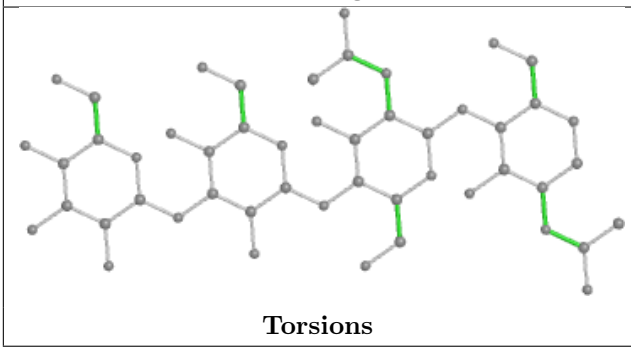
Oligosaccharide Chain c



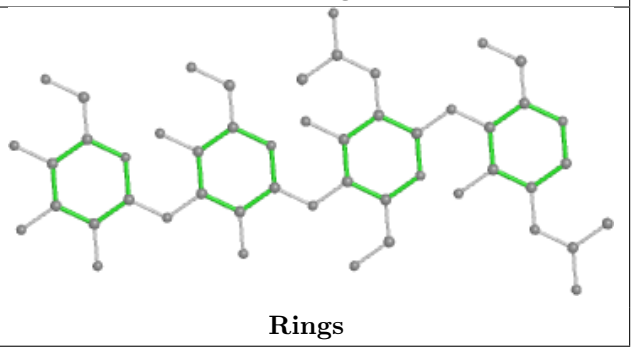
Bond lengths



Bond angles

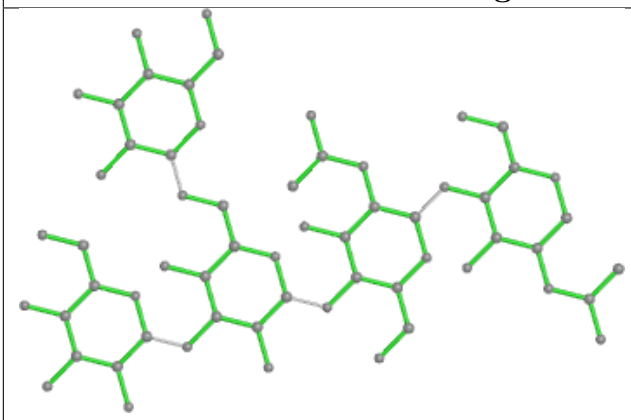


Torsions

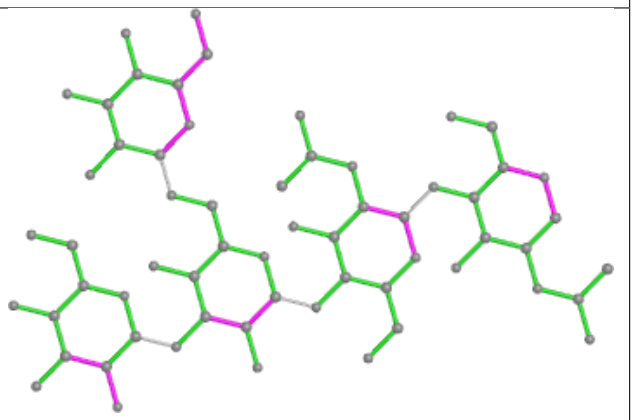


Rings

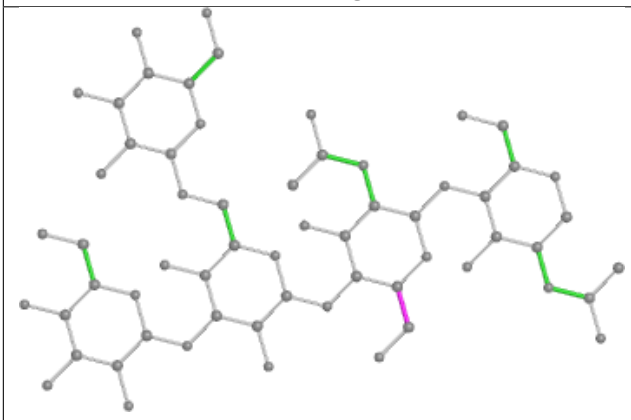
Oligosaccharide Chain V



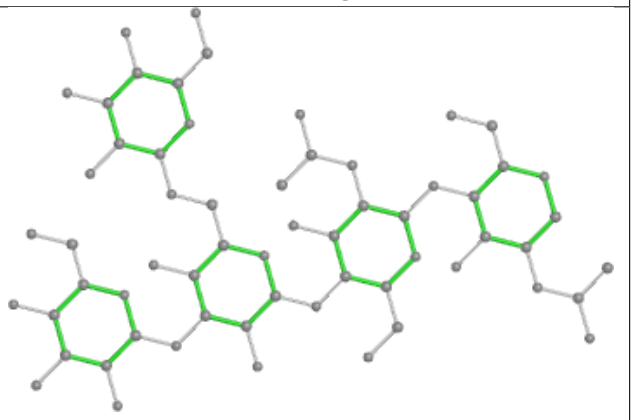
Bond lengths



Bond angles

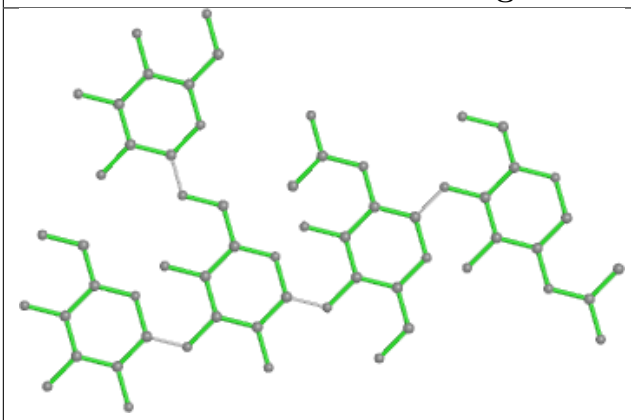


Torsions

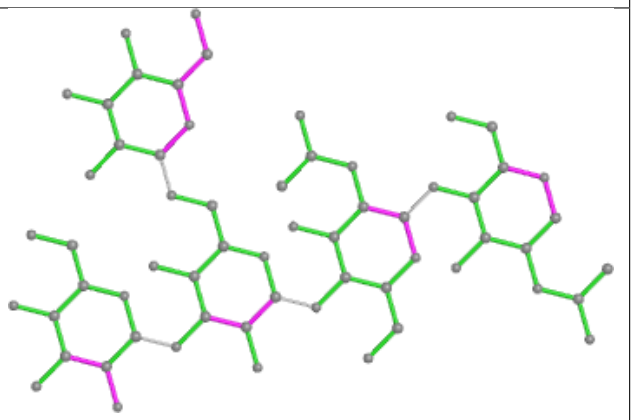


Rings

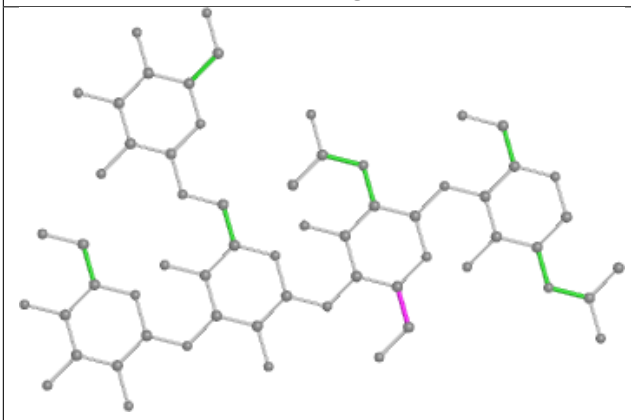
Oligosaccharide Chain Z



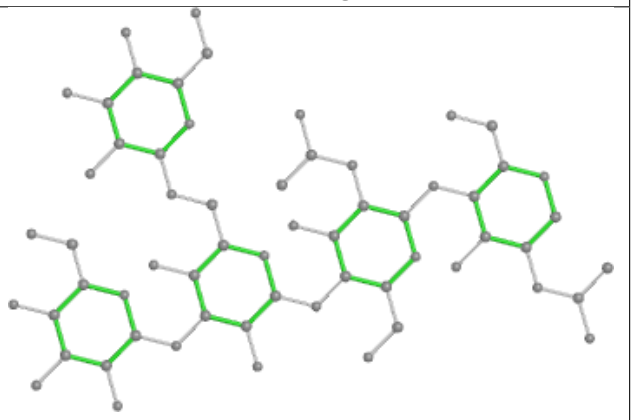
Bond lengths



Bond angles

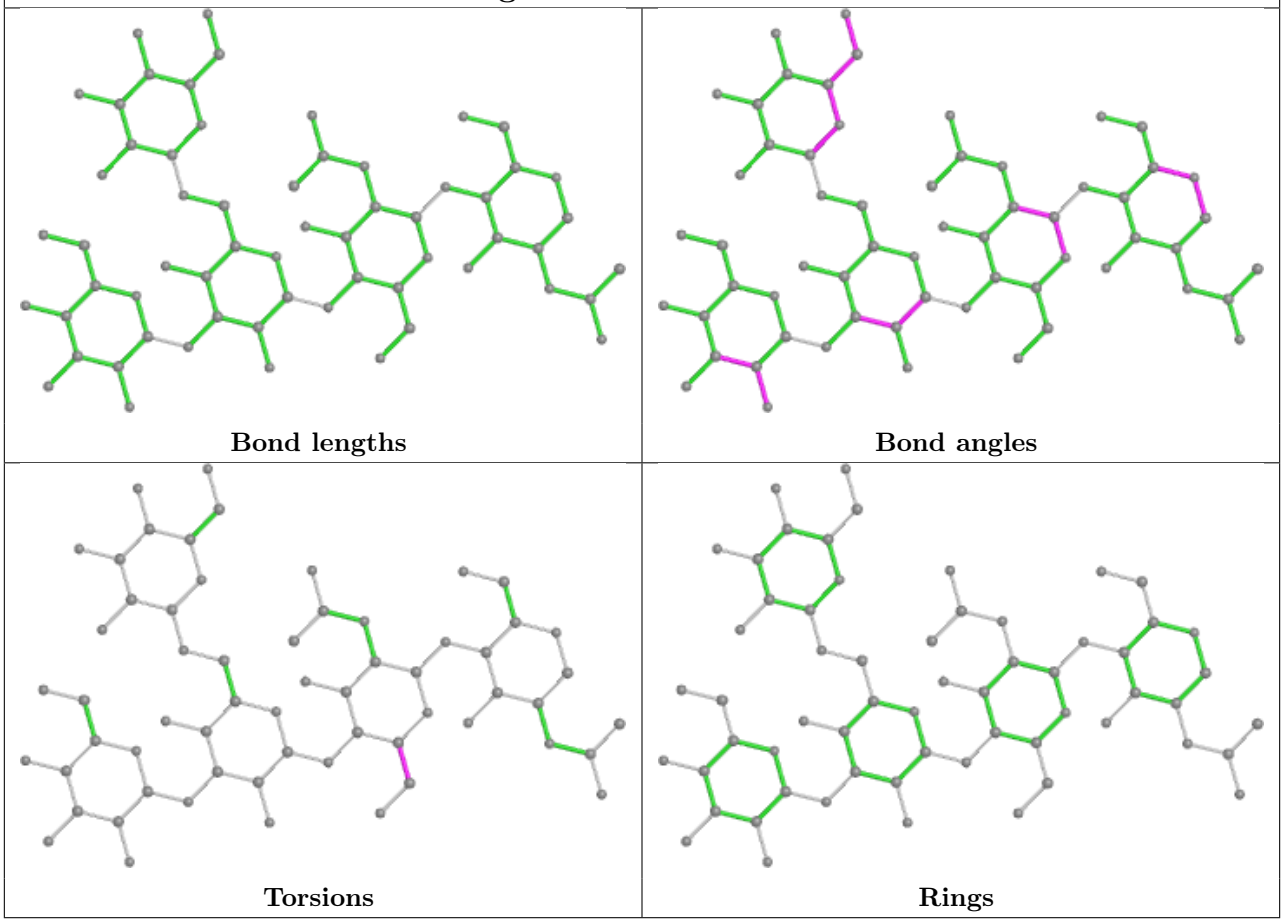


Torsions



Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
11	NAG	E	603	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
11	NAG	A	603	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
11	NAG	F	603	1	14,14,15	0.32	0	17,19,21	0.88	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	E	603	1	-	0/6/23/26	0/1/1/1
11	NAG	A	603	1	-	0/6/23/26	0/1/1/1
11	NAG	F	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	603	NAG	C1-O5-C5	2.61	115.73	112.19
11	E	603	NAG	C1-O5-C5	2.58	115.69	112.19
11	A	603	NAG	C1-O5-C5	2.57	115.68	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

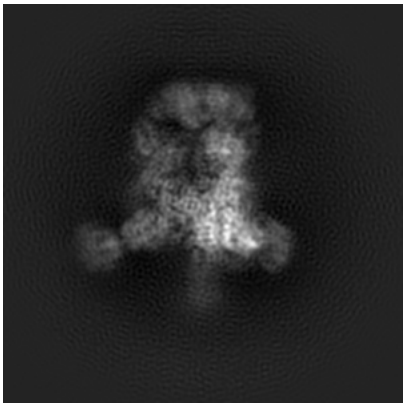
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8240. These allow visual inspection of the internal detail of the map and identification of artifacts.

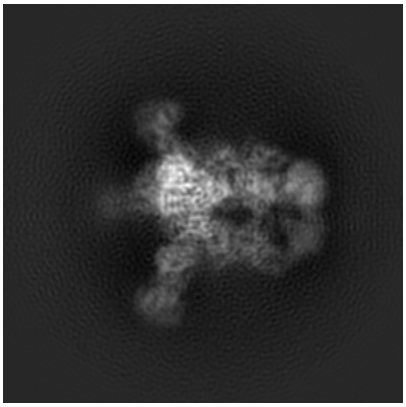
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

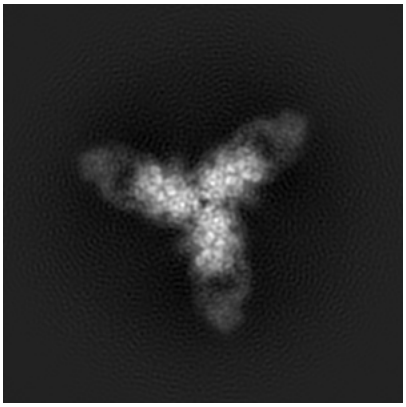
6.1.1 Primary map



X



Y

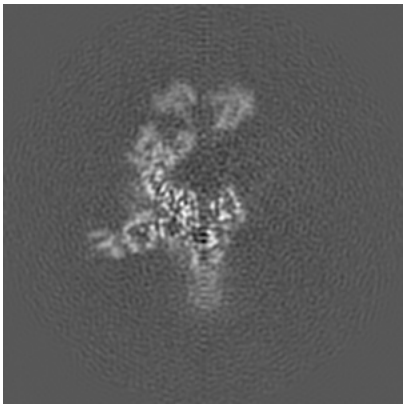


Z

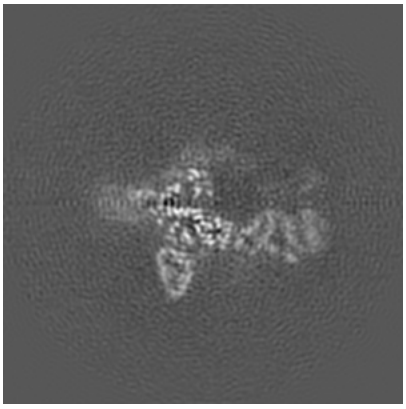
The images above show the map projected in three orthogonal directions.

6.2 Central slices

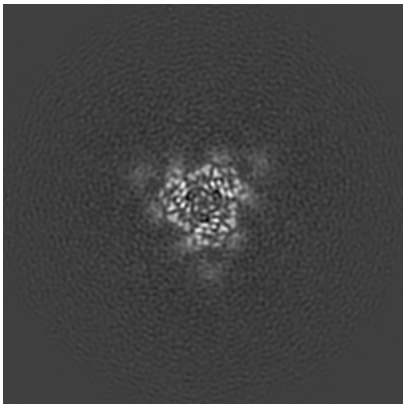
6.2.1 Primary map



X Index: 122



Y Index: 122

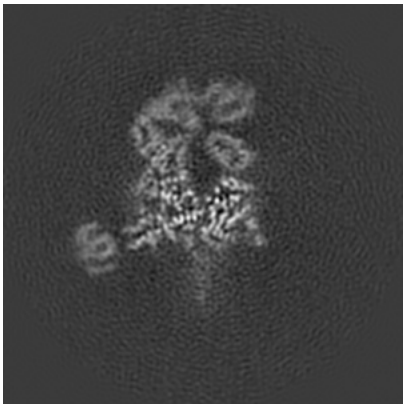


Z Index: 122

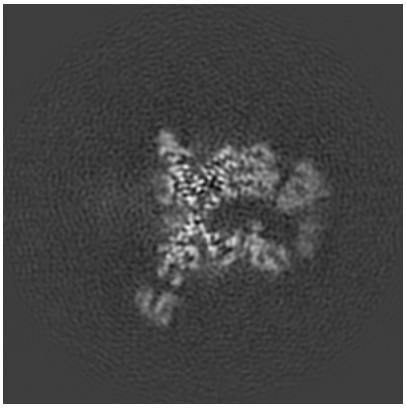
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

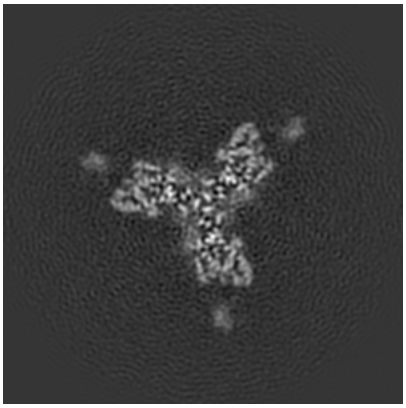
6.3.1 Primary map



X Index: 132



Y Index: 136

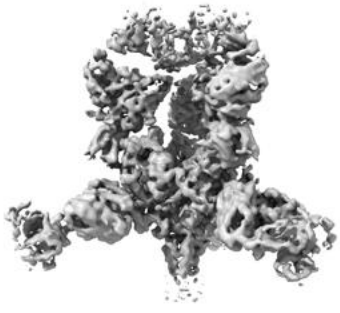


Z Index: 108

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

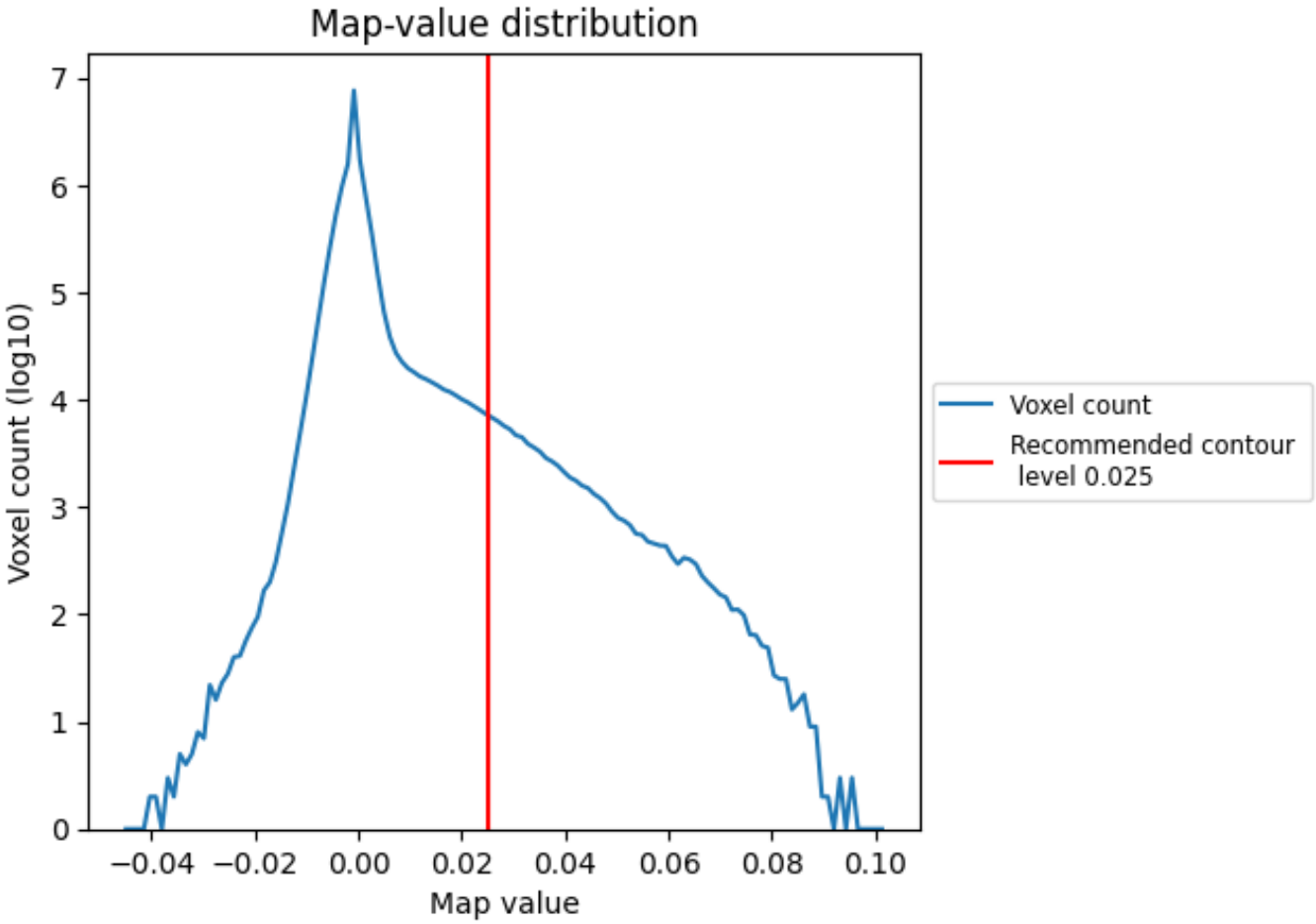
6.5 Mask visualisation (i)

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

7 Map analysis

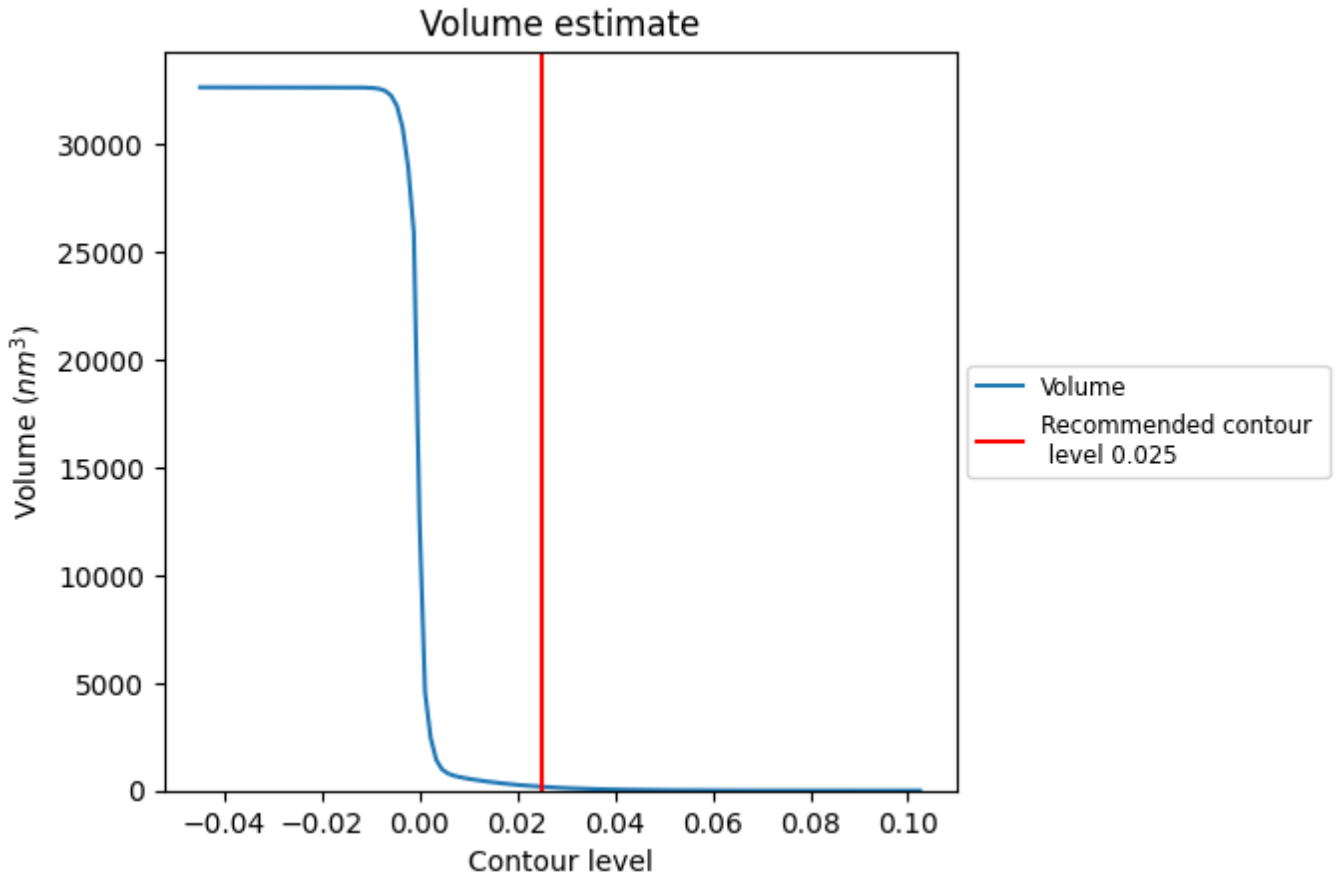
This section contains the results of statistical analysis of the map.

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.

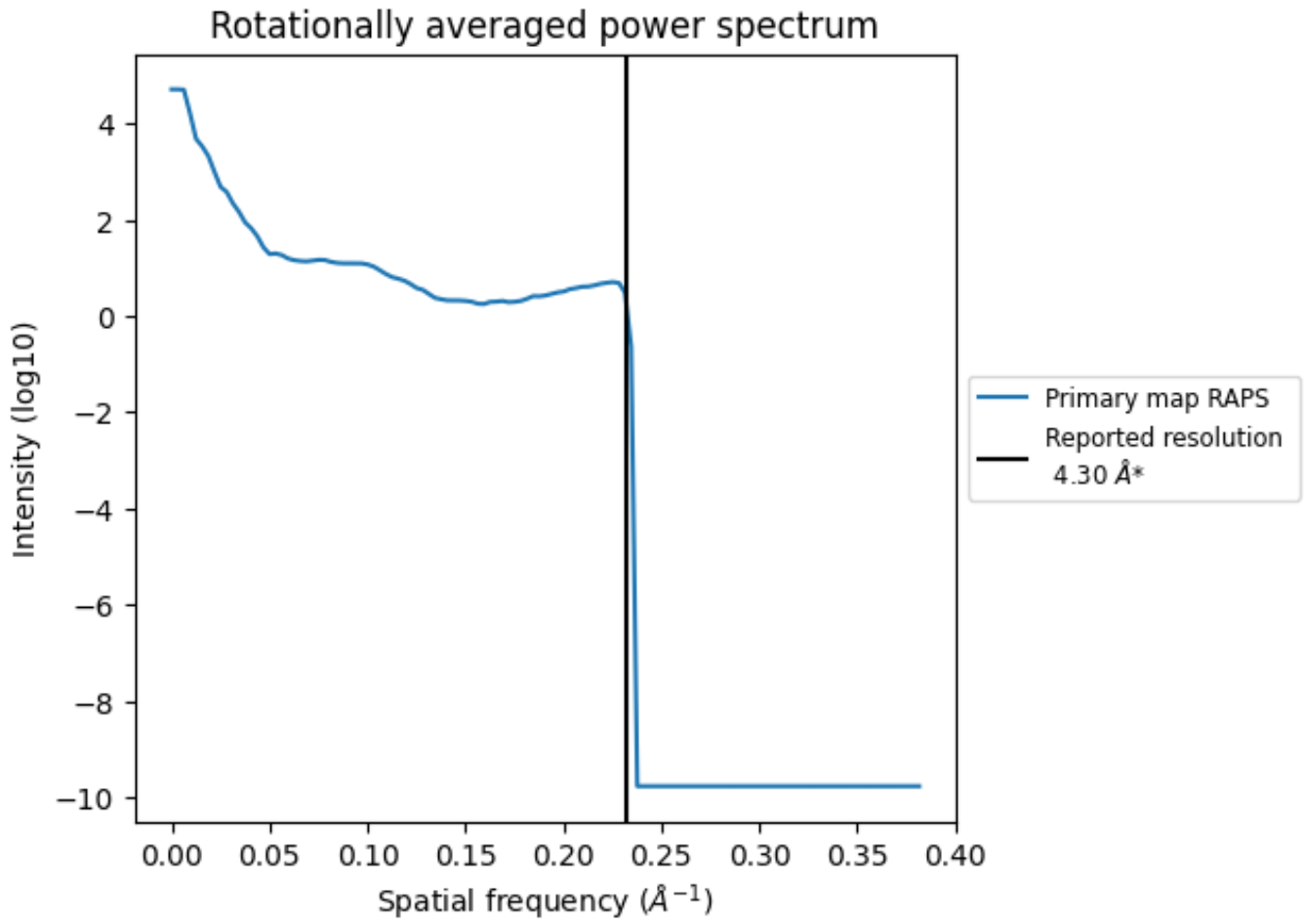
7.2 Volume estimate



The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 160 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)

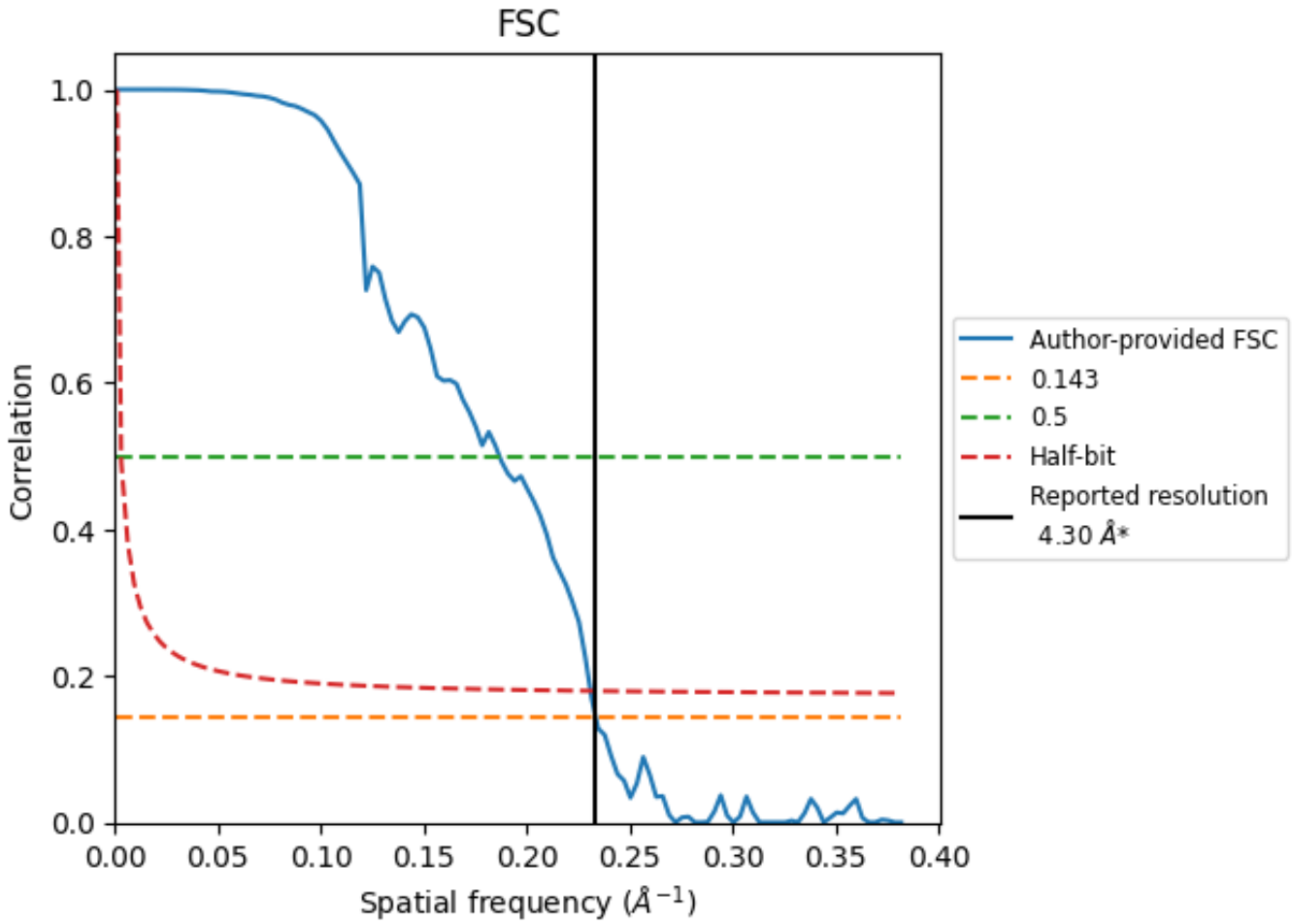


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

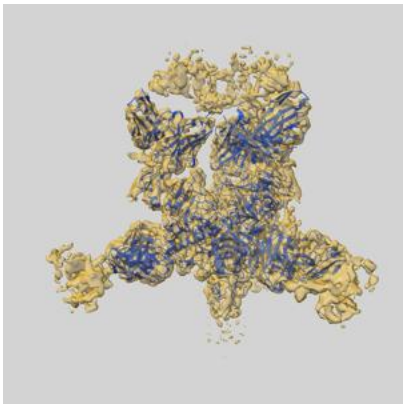
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	5.36	4.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

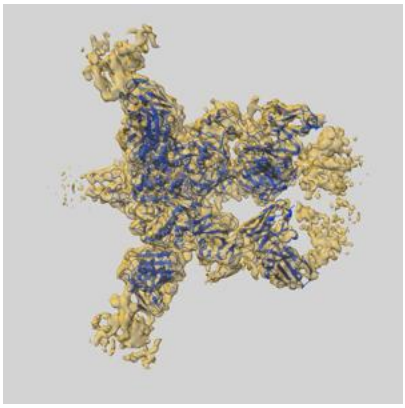
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8240 and PDB model 5KEL. Per-residue inclusion information can be found in section 3 on page 10.

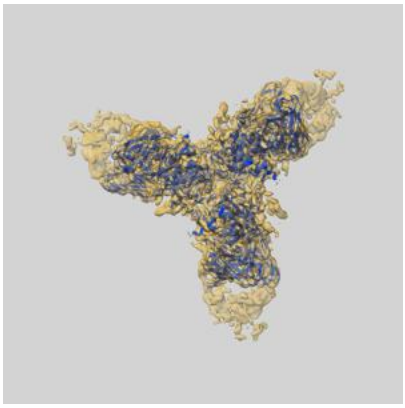
9.1 Map-model overlay



X



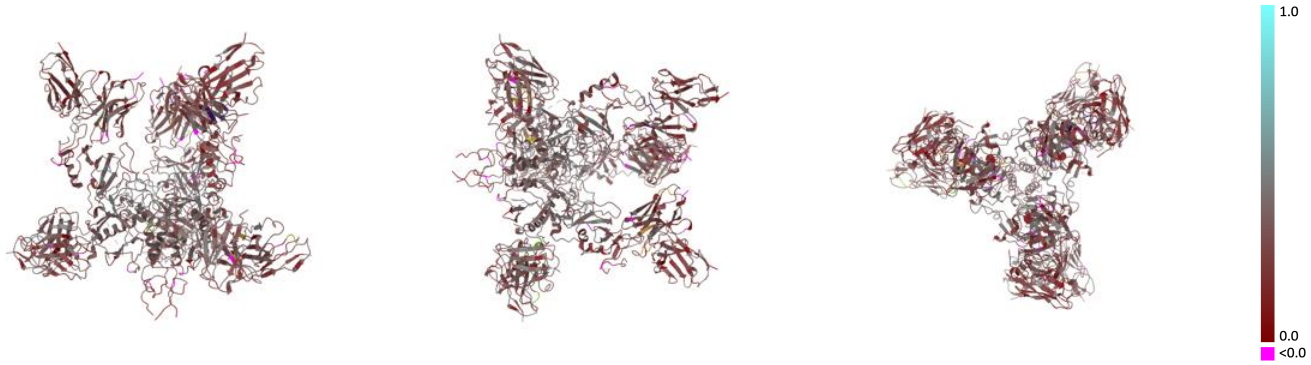
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

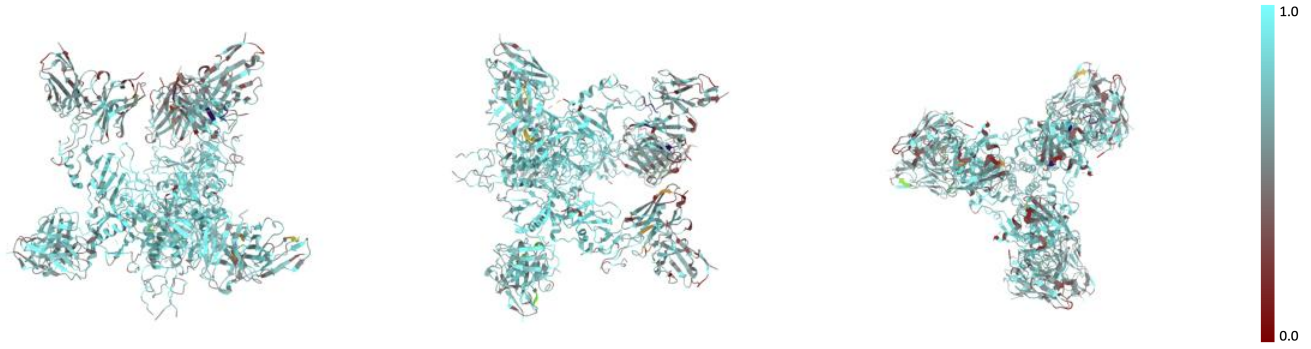
9.2 Q-score mapped to coordinate model (i)



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.

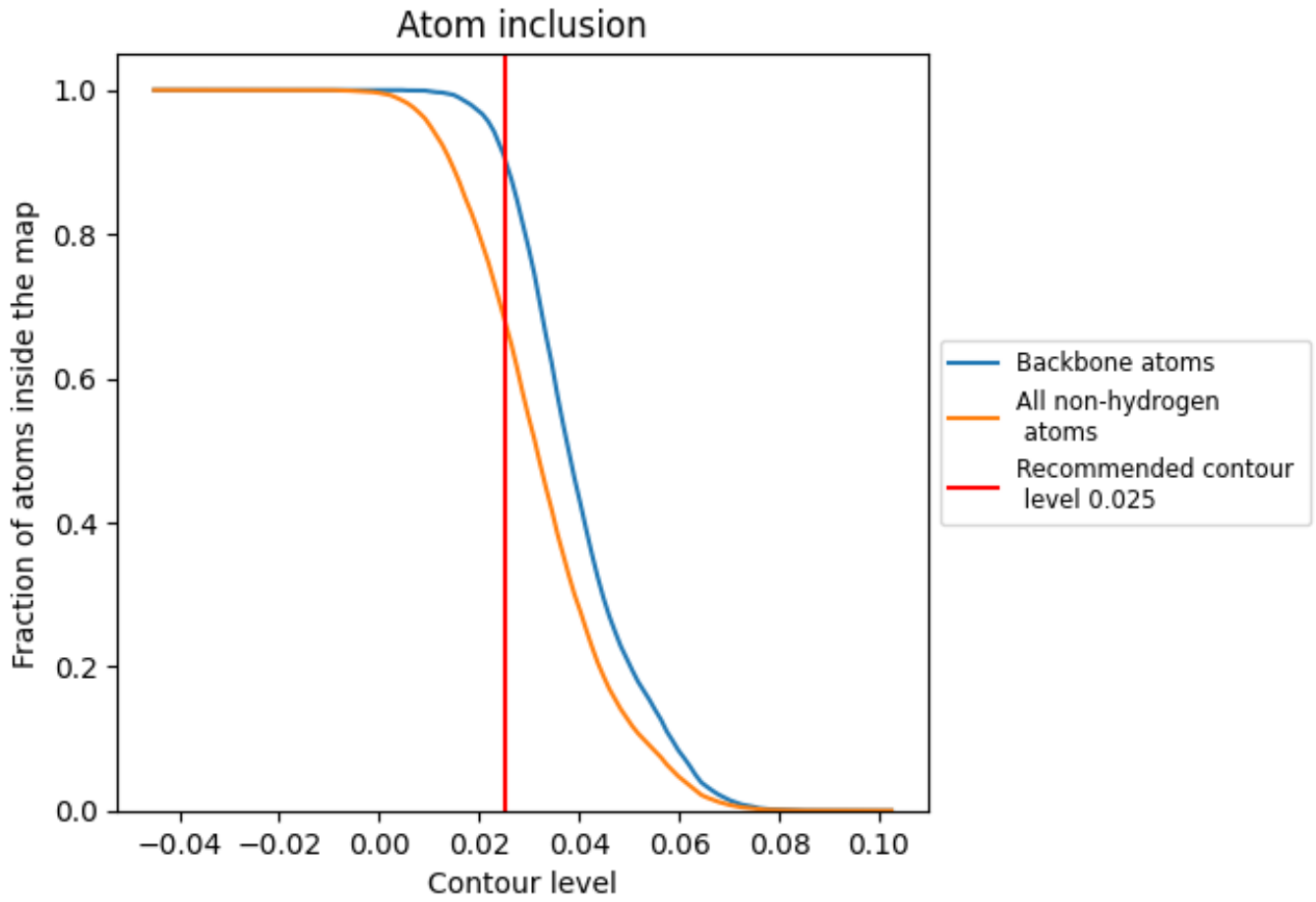
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 68% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6839	0.3090
A	0.7642	0.3330
B	0.8050	0.3420
C	0.5763	0.2770
D	0.5500	0.2690
E	0.7691	0.3330
F	0.7658	0.3310
G	0.7993	0.3410
H	0.6688	0.2900
I	0.8016	0.3410
J	0.5785	0.2740
K	0.2143	0.2460
L	0.6914	0.3180
M	0.5807	0.2730
N	0.5525	0.2710
O	0.5500	0.2690
P	0.6710	0.2880
Q	0.6710	0.2890
R	0.4615	0.3690
S	0.3600	0.2860
T	0.6939	0.3160
U	0.6815	0.3170
V	0.6721	0.3660
W	0.2143	0.2240
X	0.4615	0.3640
Y	0.3400	0.2900
Z	0.6557	0.3640
a	0.2143	0.2180
b	0.4615	0.3800
c	0.3200	0.3060
d	0.6393	0.3630