Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 08:35 PM EST

PDB ID	:	6U0L
EMDB ID	:	EMD-20605
Title	:	Asymmetrically open conformational state (Class I) of HIV-1 Env trimer BG505 SOSIP.664 in complex with sCD4 and E51 Fab
Authors	:	Yang, Z.; Bjorkman, P.J.
Deposited on	:	2019-08-14
Resolution	:	3.30 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:

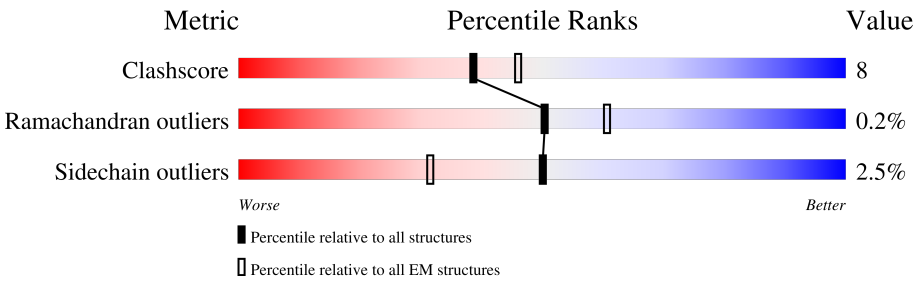
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.30 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	481	62% 14% 24%
1	B	481	63% 13% 24%
1	C	481	58% 17% • 24%
2	D	192	5% 41% 8% • 49%
2	E	192	5% 40% 9% • 49%
2	F	192	40% 8% • 49%
3	H	235	43% 14% 44%
3	I	235	46% 9% 44%

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Mol	Chain	Length	Quality of chain
3	P	235	42% 13% 44%
4	J	213	14% 46% 6% 48%
4	L	213	15% 42% 9% 48%
4	Q	213	11% 38% 13% 48%
5	X	153	76% 10% 13%
5	Y	153	79% 8% 13%
5	Z	153	70% 8% 21%
6	G	2	100%
6	M	2	50% 50%
6	N	2	50% 50%
6	R	2	100%
7	K	5	20% 80%
7	S	5	20% 80%
8	O	7	14% 14% 57% 29%

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
9	NAG	C	611	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19611 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	365	2791	1771	486	510	24	0	0
1	B	367	2781	1763	494	500	24	0	0
1	C	365	2814	1779	493	518	24	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
B	332	ASN	THR	conflict	UNP Q2N0S6
B	501	CYS	ALA	conflict	UNP Q2N0S6
B	509	ARG	-	expression tag	UNP Q2N0S6
B	510	ARG	-	expression tag	UNP Q2N0S6
B	511	ARG	-	expression tag	UNP Q2N0S6
B	512	ARG	-	expression tag	UNP Q2N0S6
B	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	97	767	481	134	150	2	0	0
2	E	97	767	481	134	150	2	0	0
2	F	97	767	481	134	150	2	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	ILE	-	expression tag	UNP P01730
D	184	ASP	-	expression tag	UNP P01730
D	185	GLY	-	expression tag	UNP P01730
D	186	ARG	-	expression tag	UNP P01730
D	187	HIS	-	expression tag	UNP P01730
D	188	HIS	-	expression tag	UNP P01730
D	189	HIS	-	expression tag	UNP P01730
D	190	HIS	-	expression tag	UNP P01730
D	191	HIS	-	expression tag	UNP P01730
D	192	HIS	-	expression tag	UNP P01730
E	183	ILE	-	expression tag	UNP P01730
E	184	ASP	-	expression tag	UNP P01730
E	185	GLY	-	expression tag	UNP P01730
E	186	ARG	-	expression tag	UNP P01730
E	187	HIS	-	expression tag	UNP P01730
E	188	HIS	-	expression tag	UNP P01730
E	189	HIS	-	expression tag	UNP P01730
E	190	HIS	-	expression tag	UNP P01730
E	191	HIS	-	expression tag	UNP P01730
E	192	HIS	-	expression tag	UNP P01730
F	183	ILE	-	expression tag	UNP P01730
F	184	ASP	-	expression tag	UNP P01730
F	185	GLY	-	expression tag	UNP P01730
F	186	ARG	-	expression tag	UNP P01730
F	187	HIS	-	expression tag	UNP P01730
F	188	HIS	-	expression tag	UNP P01730
F	189	HIS	-	expression tag	UNP P01730
F	190	HIS	-	expression tag	UNP P01730
F	191	HIS	-	expression tag	UNP P01730
F	192	HIS	-	expression tag	UNP P01730

- Molecule 3 is a protein called E51 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	132	998	621	173	197	7	1	0
3	I	132	998	621	173	197	7	1	0
3	P	132	992	618	172	196	6	0	0

- Molecule 4 is a protein called E51 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	110	812	503	135	171	3	2	0
4	L	110	806	500	134	170	2	1	0
4	Q	110	800	497	133	168	2	0	0

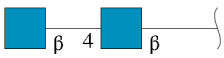
- Molecule 5 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	X	133	984	633	169	177	5	0	0
5	Y	133	1012	647	177	183	5	0	0
5	Z	121	911	577	160	169	5	0	0

There are 6 discrepancies between the modelled and reference sequences:

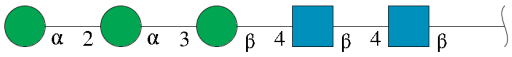
Chain	Residue	Modelled	Actual	Comment	Reference
X	559	PRO	ILE	conflict	UNP Q2N0S6
X	605	CYS	THR	conflict	UNP Q2N0S6
Y	559	PRO	ILE	conflict	UNP Q2N0S6
Y	605	CYS	THR	conflict	UNP Q2N0S6
Z	559	PRO	ILE	conflict	UNP Q2N0S6
Z	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



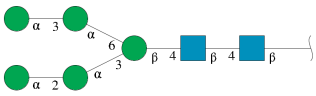
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	G	2	28	16	2	10	0	0
6	M	2	28	16	2	10	0	0
6	N	2	28	16	2	10	0	0
6	R	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



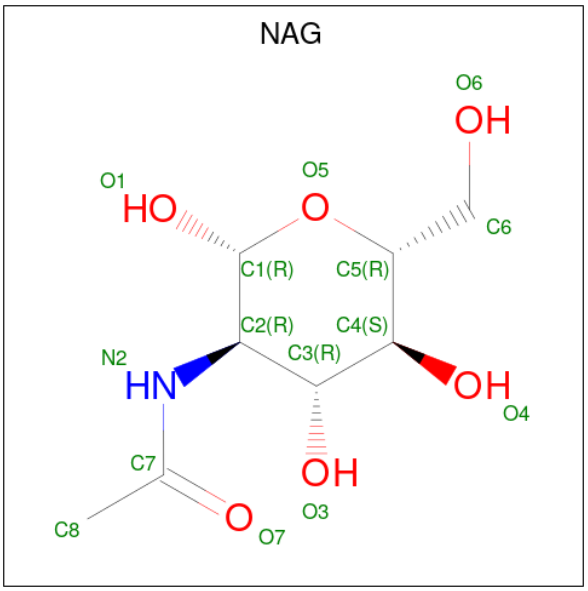
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	K	5	61	34	2	25	0	0
7	S	5	61	34	2	25	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O		
8	O	7	83	46	2	35	0	0

- Molecule 9 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	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	A	1	84	48	6	30	0
			Total	C	N	O	
9	B	1	70	40	5	25	0
			Total	C	N	O	
9	B	1	70	40	5	25	0
			Total	C	N	O	
9	B	1	70	40	5	25	0
			Total	C	N	O	
9	B	1	70	40	5	25	0
			Total	C	N	O	
9	B	1	70	40	5	25	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0

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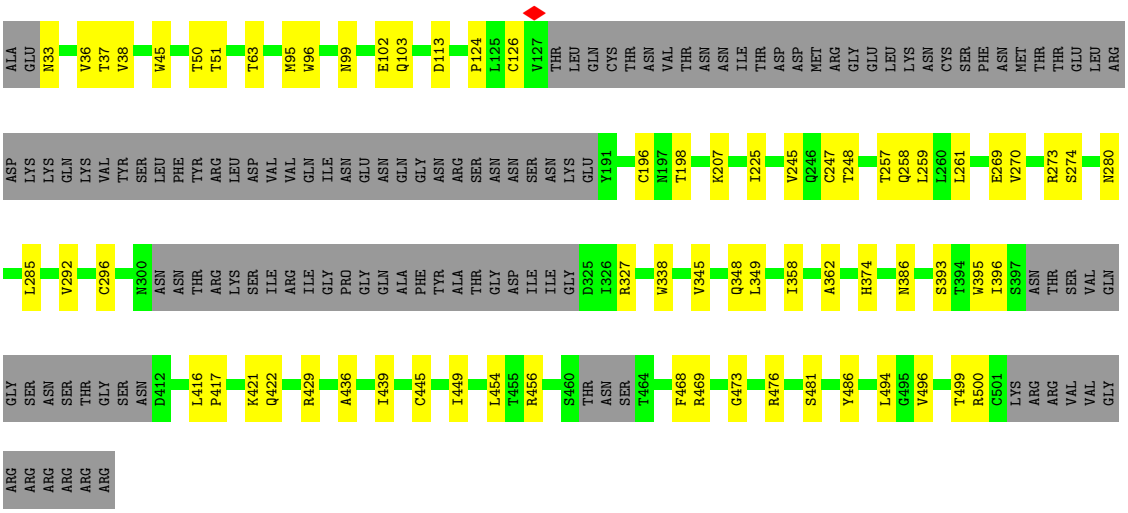
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	C	1	126	72	9	45	0
			Total	C	N	O	
9	X	1	14	8	1	5	0

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.

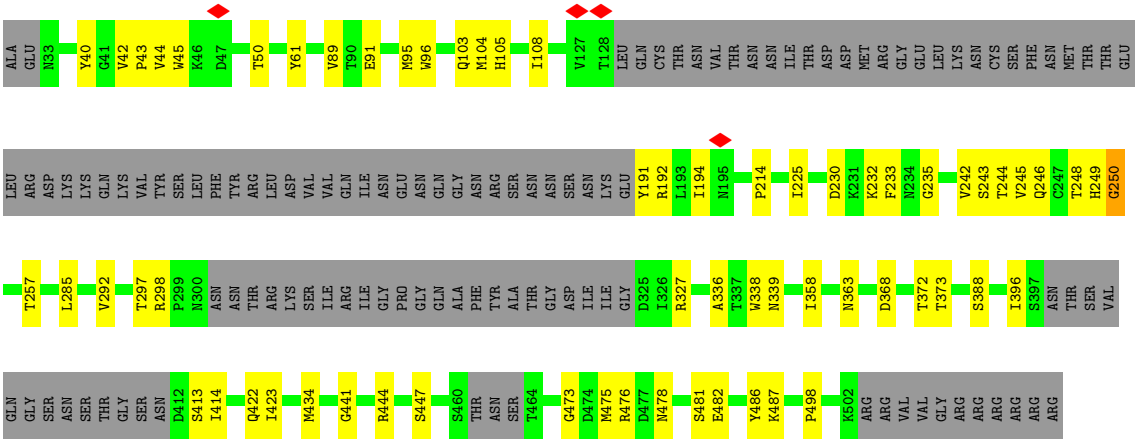
• Molecule 1: Envelope glycoprotein gp120

Chain A: 62% 14% 24%



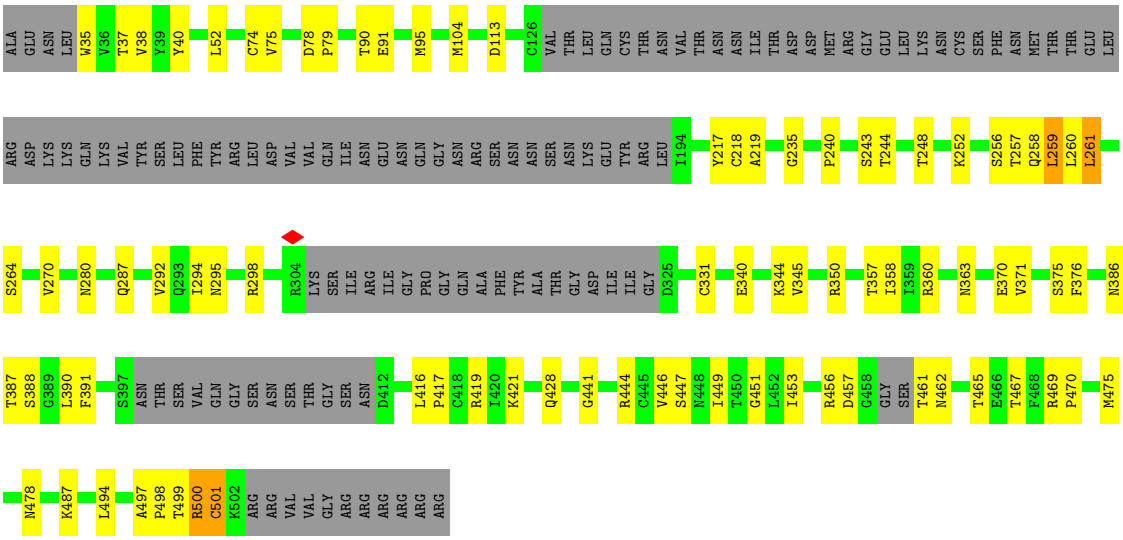
• Molecule 1: Envelope glycoprotein gp120

Chain B: 63% 13% 24%



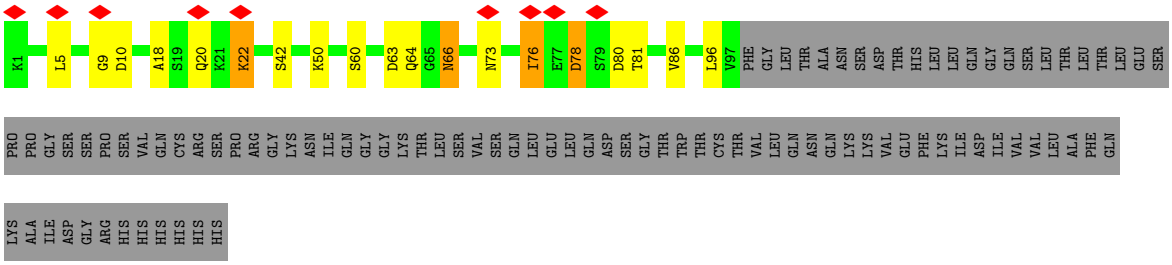
• Molecule 1: Envelope glycoprotein gp120

Chain C:



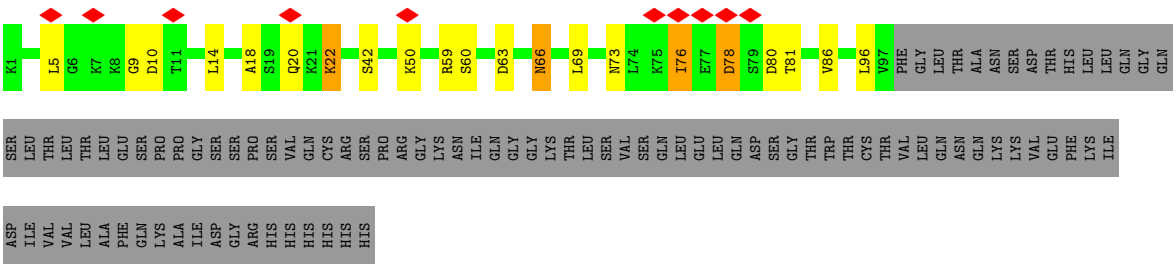
- Molecule 2: T-cell surface glycoprotein CD4

Chain D:



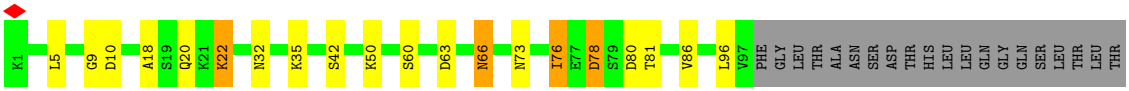
- Molecule 2: T-cell surface glycoprotein CD4

Chain E:

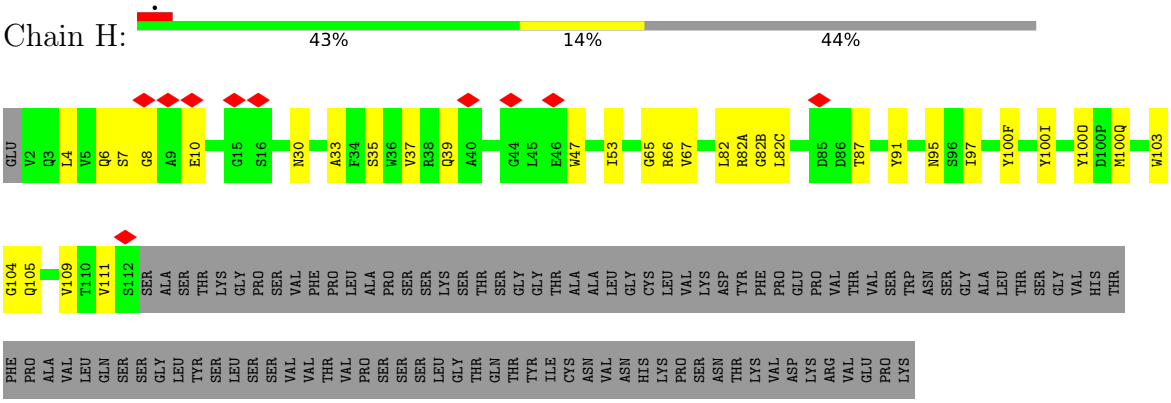


- Molecule 2: T-cell surface glycoprotein CD4

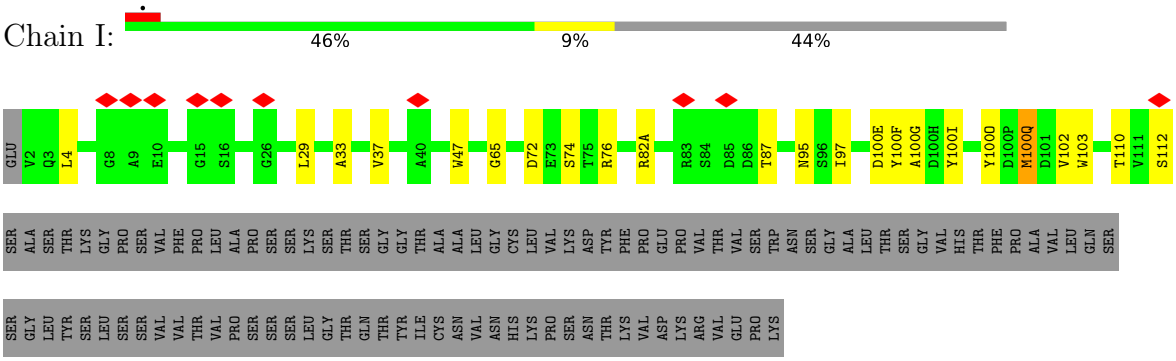
Chain F:



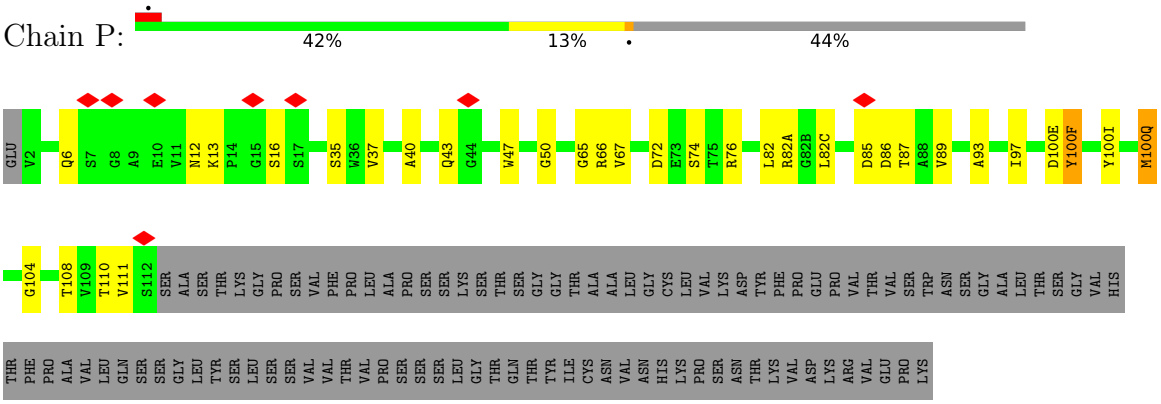
• Molecule 3: E51 Fab heavy chain



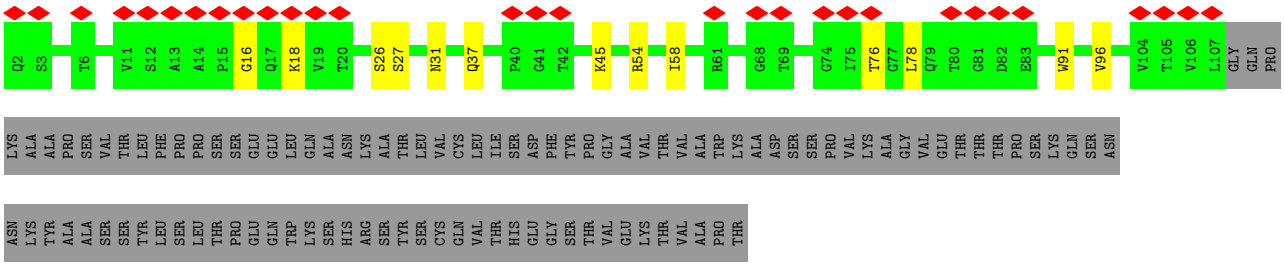
• Molecule 3: E51 Fab heavy chain



• Molecule 3: E51 Fab heavy chain

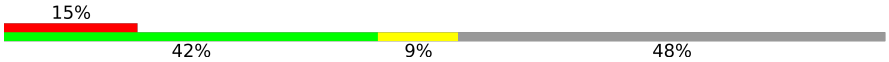


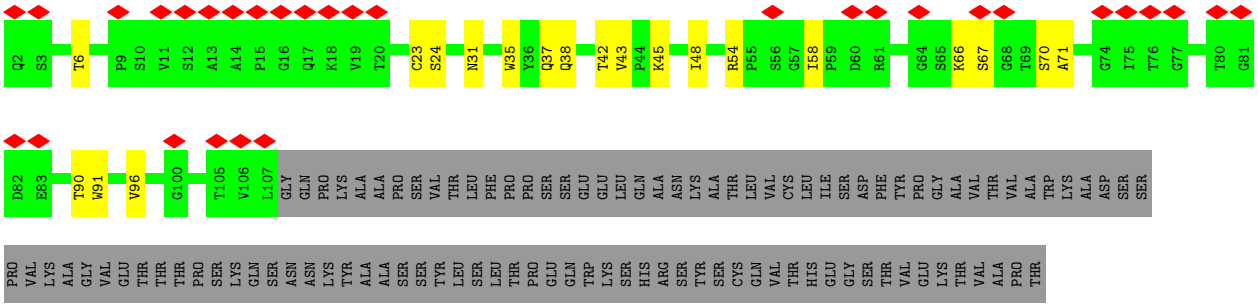
• Molecule 4: E51 Fab light chain



• Molecule 4: E51 Fab light chain

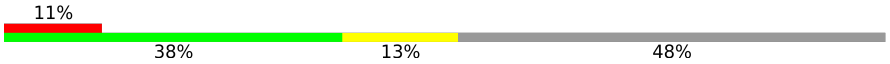
Chain L:

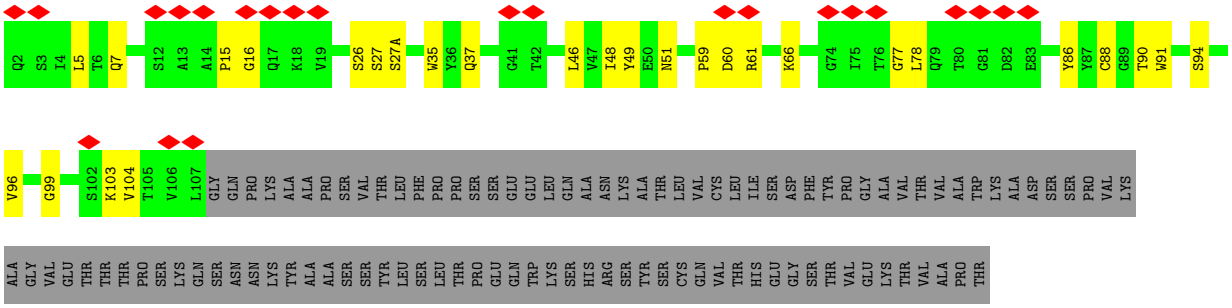




• Molecule 4: E51 Fab light chain

Chain Q:



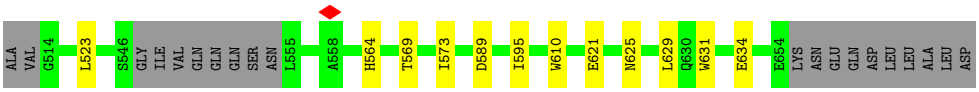


• Molecule 5: Envelope glycoprotein gp41

Chain X:

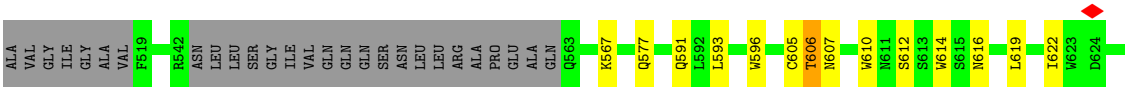
• Molecule 5: Envelope glycoprotein gp41

Chain Y:



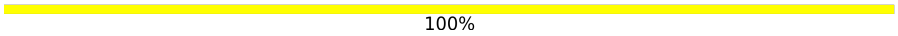
• Molecule 5: Envelope glycoprotein gp41

Chain Z:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

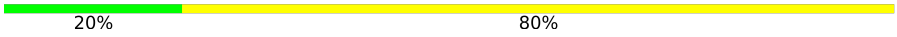
Chain N:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

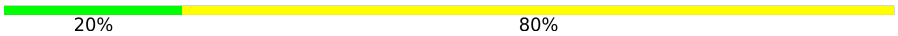
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



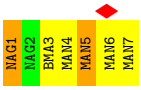
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320895	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	380.52002, 380.52002, 380.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TYS, MAN, NAG, 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	0.59	0/2856	0.59	0/3892
1	B	0.51	0/2846	0.59	0/3883
1	C	0.57	0/2878	0.60	0/3920
2	D	0.43	0/777	0.56	0/1045
2	E	0.43	0/777	0.56	0/1045
2	F	0.43	0/777	0.56	0/1045
3	H	0.39	0/985	0.59	0/1336
3	I	0.39	0/985	0.57	0/1336
3	P	0.40	0/979	0.55	0/1328
4	J	0.33	0/829	0.55	0/1130
4	L	0.35	0/823	0.58	0/1122
4	Q	0.31	0/817	0.52	0/1114
5	X	0.48	0/1004	0.60	0/1371
5	Y	0.46	0/1032	0.56	0/1405
5	Z	0.50	0/929	0.57	0/1267
All	All	0.48	0/19294	0.58	0/26239

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2791	0	2687	54	0
1	B	2781	0	2673	50	0
1	C	2814	0	2729	78	0
2	D	767	0	773	7	0
2	E	767	0	773	8	0
2	F	767	0	773	8	0
3	H	998	0	931	21	0
3	I	998	0	929	13	0
3	P	992	0	927	20	0
4	J	812	0	773	7	0
4	L	806	0	770	13	0
4	Q	800	0	766	17	0
5	X	984	0	933	18	0
5	Y	1012	0	982	12	0
5	Z	911	0	843	19	0
6	G	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	R	28	0	25	0	0
7	K	61	0	52	0	0
7	S	61	0	52	0	0
8	O	83	0	70	2	0
9	A	84	0	78	0	0
9	B	70	0	65	0	0
9	C	126	0	117	8	0
9	X	14	0	13	0	0
All	All	19611	0	18809	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ASN:HD21	9:C:611:NAG:C1	0.92	1.57
1:C:386:ASN:ND2	9:C:611:NAG:C1	1.75	1.40
1:C:388:SER:HB2	9:C:611:NAG:O7	1.25	1.30
1:A:248:THR:HB	1:A:486:TYR:CZ	1.80	1.17
1:C:257:THR:HG21	1:C:371:VAL:HA	1.23	1.14
1:C:257:THR:CG2	1:C:371:VAL:HA	2.01	0.90
1:C:388:SER:HB2	9:C:611:NAG:C7	2.02	0.90
1:A:248:THR:HB	1:A:486:TYR:CE2	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:SER:CB	9:C:611:NAG:O7	2.20	0.85
1:C:257:THR:HG21	1:C:370:GLU:O	1.78	0.84
1:A:248:THR:CB	1:A:486:TYR:CZ	2.63	0.81
1:C:260:LEU:HD21	1:C:453:ILE:HD11	1.64	0.80
1:B:225:ILE:HB	1:B:245:VAL:O	1.82	0.79
1:C:37:THR:HG21	1:C:499:THR:HB	1.64	0.78
1:C:386:ASN:CG	9:C:611:NAG:C1	2.53	0.76
1:A:259:LEU:HB2	1:A:374:HIS:CD2	2.21	0.76
1:B:248:THR:HB	1:B:486:TYR:CZ	2.21	0.74
1:C:35:TRP:HB2	1:C:500:ARG:HA	1.68	0.74
1:C:257:THR:HG21	1:C:371:VAL:CA	2.13	0.72
1:A:248:THR:HB	1:A:486:TYR:OH	1.90	0.71
1:C:37:THR:CG2	1:C:499:THR:HB	2.22	0.70
1:C:258:GLN:HG3	1:C:470:PRO:HB2	1.73	0.69
3:H:87:THR:HG22	3:H:111:VAL:H	1.57	0.69
1:C:259:LEU:HD11	1:C:449:ILE:HD11	1.75	0.69
1:B:45:TRP:CE3	5:Y:629:LEU:HD21	2.29	0.68
1:A:261:LEU:HD11	1:A:374:HIS:CE1	2.30	0.67
1:C:52:LEU:HD12	1:C:219:ALA:HA	1.77	0.66
1:B:475:MET:SD	1:B:478:ASN:ND2	2.68	0.66
1:A:45:TRP:HD1	5:X:523:LEU:HD11	1.62	0.64
1:C:257:THR:CG2	1:C:370:GLU:O	2.46	0.64
1:C:258:GLN:O	1:C:258:GLN:HG2	2.00	0.62
5:Y:621:GLU:HA	5:Y:625:ASN:HD21	1.63	0.62
1:B:45:TRP:HH2	1:B:89:VAL:HG21	1.64	0.62
1:C:444:ARG:HH21	9:C:609:NAG:H81	1.65	0.62
1:B:441:GLY:HA3	8:O:5:MAN:H62	1.81	0.61
3:H:39:GLN:HE22	4:L:38:GLN:HE22	1.48	0.61
4:Q:35:TRP:HB2	4:Q:48:ILE:HB	1.83	0.61
1:C:386:ASN:HB3	1:C:417:PRO:HD2	1.83	0.61
1:C:243:SER:OG	1:C:244:THR:N	2.34	0.60
1:C:419:ARG:HG2	3:P:100(F):TYS:HE1	1.83	0.60
1:A:225:ILE:HB	1:A:245:VAL:O	2.01	0.60
5:X:545:LEU:CD1	5:Z:591:GLN:OE1	2.48	0.60
5:X:569:THR:HG22	5:Y:569:THR:HG21	1.83	0.60
1:C:257:THR:CB	1:C:370:GLU:O	2.50	0.60
5:X:518:VAL:HG21	5:X:545:LEU:HG	1.84	0.59
1:C:461:THR:N	2:F:32:ASN:OD1	2.35	0.59
4:L:23:CYS:HB3	4:L:71:ALA:HB3	1.84	0.59
1:C:37:THR:OG1	1:C:499:THR:OG1	2.11	0.59
1:B:45:TRP:CZ3	5:Y:629:LEU:HD21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:CE1	1:B:482:GLU:HG2	2.38	0.59
1:C:360:ARG:HB3	1:C:467:THR:HG22	1.85	0.59
1:A:362:ALA:HB3	1:A:469:ARG:HG2	1.85	0.58
1:C:260:LEU:HD21	1:C:453:ILE:CD1	2.34	0.58
1:C:294:ILE:HG23	1:C:447:SER:HB2	1.86	0.58
3:H:65:GLY:O	3:H:82(A):ARG:NH2	2.37	0.58
3:P:37:VAL:HG12	3:P:47:TRP:HA	1.85	0.58
3:H:33:ALA:HB2	3:H:97:ILE:HD13	1.86	0.58
1:C:74:CYS:O	5:X:564:HIS:NE2	2.36	0.57
1:C:363:ASN:O	1:C:469:ARG:NH1	2.37	0.57
4:J:54:ARG:NH1	4:J:58:ILE:O	2.37	0.57
1:C:90:THR:HG22	1:C:240:PRO:HA	1.86	0.57
1:C:258:GLN:HE21	1:C:391:PHE:HE2	1.51	0.57
1:C:295:ASN:HB3	1:C:446:VAL:HG12	1.87	0.57
1:C:358:ILE:HB	1:C:465:THR:HG22	1.86	0.57
1:B:298:ARG:NH2	1:B:441:GLY:O	2.37	0.56
2:E:78:ASP:N	2:E:78:ASP:OD1	2.39	0.56
1:C:456:ARG:O	2:F:35:LYS:NZ	2.39	0.56
1:B:327:ARG:HE	1:B:422:GLN:HE21	1.54	0.56
3:P:66:ARG:NH2	3:P:86:ASP:OD2	2.39	0.56
3:P:67:VAL:HG22	3:P:82:LEU:HD13	1.88	0.56
1:A:285:LEU:HD13	1:A:481:SER:HB2	1.88	0.55
2:D:78:ASP:OD1	2:D:78:ASP:N	2.39	0.55
3:H:91:TYR:HE2	4:L:43:VAL:HG22	1.71	0.55
2:D:20:GLN:HB3	2:D:22:LYS:HG2	1.88	0.55
2:E:20:GLN:HB3	2:E:22:LYS:HG2	1.88	0.55
1:B:50:THR:O	1:B:103:GLN:NE2	2.40	0.55
3:P:100(Q):MET:SD	3:P:100(Q):MET:N	2.76	0.55
1:A:33:ASN:N	5:X:607:ASN:OD1	2.39	0.55
2:F:20:GLN:HB3	2:F:22:LYS:HG2	1.88	0.55
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.89	0.55
4:J:31:ASN:ND2	4:J:91:TRP:O	2.37	0.54
1:B:230:ASP:HB3	1:B:233:PHE:HB2	1.90	0.54
1:C:258:GLN:NE2	1:C:387:THR:OG1	2.37	0.54
1:A:50:THR:OG1	1:A:51:THR:N	2.41	0.54
3:H:95:ASN:ND2	3:H:100(O):TYR:O	2.41	0.54
3:H:66:ARG:NH2	3:H:82(B):GLY:O	2.40	0.54
1:C:298:ARG:NH2	1:C:441:GLY:O	2.38	0.54
1:C:498:PRO:HB3	5:Z:610:TRP:CZ2	2.42	0.54
2:F:78:ASP:OD1	2:F:78:ASP:N	2.39	0.54
4:J:26:SER:OG	4:J:27:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HE	1:A:422:GLN:HE21	1.56	0.53
3:P:93:ALA:HB1	3:P:100(Q):MET:HG3	1.89	0.53
1:C:52:LEU:HG	1:C:218:CYS:O	2.07	0.53
3:H:10:GLU:HB2	3:H:109:VAL:HG12	1.90	0.53
1:A:270:VAL:HG11	1:A:345:VAL:HG22	1.91	0.53
1:A:207:LYS:HD3	1:A:436:ALA:HB3	1.90	0.53
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.43	0.53
1:B:447:SER:HB3	8:O:1:NAG:HN2	1.74	0.53
1:A:50:THR:O	1:A:103:GLN:NE2	2.42	0.53
1:C:256:SER:HB2	1:C:376:PHE:CB	2.39	0.53
1:C:498:PRO:HB2	5:Z:619:LEU:HD22	1.90	0.52
1:B:105:HIS:CD2	1:B:476:ARG:HE	2.27	0.52
1:C:292:VAL:HB	1:C:449:ILE:HG23	1.91	0.52
4:L:31:ASN:O	4:L:66:LYS:NZ	2.37	0.52
1:A:393:SER:OG	1:A:395:TRP:NE1	2.40	0.52
1:A:259:LEU:HD22	1:A:449:ILE:CG2	2.40	0.52
3:P:89:VAL:HA	3:P:108:THR:HA	1.91	0.52
1:C:217:TYR:O	1:C:248:THR:HG23	2.10	0.52
3:I:65:GLY:O	3:I:82(A):ARG:NH2	2.43	0.52
1:B:413:SER:OG	1:B:414:ILE:N	2.42	0.52
1:C:498:PRO:HB3	5:Z:610:TRP:NE1	2.25	0.52
1:C:104:MET:HA	1:C:217:TYR:OH	2.10	0.52
5:X:652:GLN:O	5:X:656:ASN:ND2	2.42	0.51
1:A:126:CYS:O	2:D:64:GLN:NE2	2.44	0.51
1:B:91:GLU:HB3	1:B:242:VAL:HG21	1.92	0.51
3:H:37:VAL:HG12	3:H:47:TRP:HA	1.91	0.51
1:A:113:ASP:OD2	1:A:429:ARG:NH2	2.35	0.51
1:C:256:SER:HB2	1:C:376:PHE:HB3	1.90	0.51
3:H:95:ASN:HB3	3:H:100(Q):MET:HA	1.92	0.51
1:A:259:LEU:HD22	1:A:449:ILE:HG21	1.92	0.51
1:B:368:ASP:OD2	2:E:59:ARG:NH1	2.35	0.51
4:L:42:THR:OG1	4:L:43:VAL:N	2.43	0.51
1:A:248:THR:CB	1:A:486:TYR:CE2	2.88	0.51
1:C:95:MET:HE2	1:C:235:GLY:HA3	1.93	0.51
2:F:66:ASN:OD1	2:F:66:ASN:N	2.44	0.51
1:C:280:ASN:ND2	1:C:457:ASP:O	2.44	0.50
1:C:331:CYS:HB2	1:C:416:LEU:HB2	1.93	0.50
2:D:66:ASN:OD1	2:D:66:ASN:N	2.44	0.50
1:A:280:ASN:OD1	1:A:456:ARG:NH2	2.44	0.50
1:C:37:THR:HG22	5:Z:605:CYS:HA	1.93	0.50
3:P:12:ASN:ND2	3:P:16:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:47:TRP:CG	4:Q:96:VAL:HB	2.47	0.50
1:A:261:LEU:HD11	1:A:374:HIS:HE1	1.74	0.50
1:B:45:TRP:CH2	1:B:89:VAL:HG21	2.46	0.50
1:C:261:LEU:HD23	1:C:449:ILE:HB	1.94	0.50
2:E:66:ASN:N	2:E:66:ASN:OD1	2.44	0.50
1:C:498:PRO:HB3	5:Z:610:TRP:HE1	1.77	0.50
1:A:259:LEU:HB2	1:A:374:HIS:NE2	2.27	0.50
3:P:72:ASP:OD1	3:P:74:SER:OG	2.28	0.50
4:L:54:ARG:NH1	4:L:58:ILE:O	2.45	0.49
1:C:270:VAL:HG11	1:C:345:VAL:HG22	1.94	0.49
3:I:33:ALA:HB2	3:I:97:ILE:HD13	1.94	0.49
3:I:100(Q):MET:SD	3:I:100(Q):MET:N	2.75	0.49
3:I:37:VAL:HG12	3:I:47:TRP:HA	1.93	0.49
1:C:78:ASP:N	1:C:78:ASP:OD1	2.45	0.49
1:C:340:GLU:O	1:C:344:LYS:N	2.46	0.49
1:B:61:TYR:HB3	5:Y:564:HIS:CE1	2.47	0.49
1:A:257:THR:HG22	1:A:473:GLY:HA2	1.95	0.49
1:C:390:LEU:HD13	1:C:416:LEU:HD21	1.94	0.49
4:Q:59:PRO:HB2	4:Q:61:ARG:HG2	1.94	0.49
1:B:292:VAL:HG11	1:B:338:TRP:HE3	1.77	0.49
1:C:113:ASP:OD1	1:C:428:GLN:NE2	2.47	0.48
3:P:6:GLN:HE21	3:P:104:GLY:HA3	1.77	0.48
1:A:270:VAL:O	1:A:348:GLN:NE2	2.45	0.48
1:B:42:VAL:HG13	1:B:44:VAL:HG23	1.95	0.48
4:Q:7:GLN:HE21	4:Q:99:GLY:HA3	1.77	0.48
1:B:96:TRP:HH2	1:B:285:LEU:HD13	1.78	0.48
5:X:545:LEU:HD11	5:Z:591:GLN:OE1	2.12	0.48
1:A:37:THR:HG22	5:X:605:CYS:HB3	1.93	0.48
1:A:102:GLU:OE2	1:A:476:ARG:NH2	2.46	0.48
4:Q:60:ASP:OD2	4:Q:60:ASP:N	2.43	0.48
1:B:358:ILE:HD12	1:B:396:ILE:HA	1.94	0.48
1:A:96:TRP:NE1	1:A:274:SER:O	2.47	0.48
3:I:95:ASN:ND2	3:I:100(O):TYR:O	2.47	0.48
3:P:87:THR:HG22	3:P:110:THR:HA	1.94	0.48
3:I:37:VAL:HG21	3:I:103:TRP:HZ3	1.79	0.47
1:C:494:LEU:HD11	5:Z:593:LEU:HD21	1.96	0.47
2:E:9:GLY:HA2	2:E:73:ASN:HA	1.97	0.47
1:A:38:VAL:HG12	1:A:496:VAL:HG12	1.95	0.47
4:Q:26:SER:OG	4:Q:27:SER:N	2.48	0.47
1:C:264:SER:O	1:C:287:GLN:NE2	2.47	0.47
1:C:498:PRO:HB3	5:Z:610:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:GLY:HA2	2:D:73:ASN:HA	1.97	0.47
1:A:292:VAL:HG11	1:A:338:TRP:HE3	1.80	0.47
1:C:259:LEU:HD11	1:C:449:ILE:CD1	2.44	0.47
1:B:423:ILE:HG23	1:B:434:MET:HG2	1.97	0.47
4:J:16:GLY:N	4:J:78:LEU:O	2.45	0.47
4:J:18:LYS:HG2	4:J:76:THR:HA	1.97	0.47
1:C:259:LEU:HD12	1:C:451:GLY:O	2.14	0.47
1:B:285:LEU:HD23	1:B:481:SER:HB2	1.96	0.47
1:B:249:HIS:HE2	1:B:482:GLU:CG	2.28	0.46
3:P:65:GLY:O	3:P:82(A):ARG:NH2	2.47	0.46
4:Q:103:LYS:NZ	4:Q:104:VAL:O	2.41	0.46
3:I:95:ASN:OD1	3:I:95:ASN:N	2.48	0.46
4:Q:37:GLN:HE21	4:Q:86:TYR:HE2	1.64	0.46
3:H:6:GLN:H	3:H:105:GLN:HE22	1.63	0.46
4:L:37:GLN:O	4:L:45:LYS:N	2.47	0.46
1:A:124:PRO:HA	1:A:198:THR:HA	1.96	0.46
1:C:501:CYS:HB2	5:Z:605:CYS:HB3	1.75	0.46
3:H:7:SER:OG	3:H:8:GLY:N	2.48	0.46
1:C:498:PRO:CB	5:Z:610:TRP:HE1	2.28	0.46
3:P:12:ASN:HD22	3:P:82(C):LEU:HD23	1.80	0.46
5:X:544:LEU:O	5:X:544:LEU:HD12	2.16	0.46
2:F:76:ILE:H	2:F:76:ILE:HG12	1.49	0.45
2:F:9:GLY:HA2	2:F:73:ASN:HA	1.97	0.45
1:A:358:ILE:HG23	1:A:396:ILE:HA	1.98	0.45
3:H:47:TRP:CG	4:L:96:VAL:HB	2.52	0.45
3:I:87:THR:HG23	3:I:110:THR:HA	1.99	0.45
1:A:454:LEU:HD13	1:A:468:PHE:HB3	1.97	0.45
3:H:67:VAL:HG22	3:H:82:LEU:HD13	1.97	0.45
1:A:126:CYS:HA	1:A:196:CYS:HA	1.98	0.45
1:B:42:VAL:CG2	1:B:43:PRO:HD2	2.46	0.45
3:H:37:VAL:HG21	3:H:103:TRP:HZ3	1.82	0.45
1:A:386:ASN:HB3	1:A:417:PRO:HD2	1.98	0.45
1:B:244:THR:HG23	1:B:244:THR:O	2.17	0.45
3:H:30:ASN:HB3	3:H:53:ILE:HD13	1.99	0.45
3:P:85:ASP:OD2	3:P:85:ASP:N	2.49	0.45
1:A:269:GLU:HG2	1:A:270:VAL:H	1.81	0.44
1:C:91:GLU:OE1	1:C:487:LYS:NZ	2.50	0.44
1:B:95:MET:HB3	1:B:95:MET:HE2	1.73	0.44
1:B:225:ILE:HD12	1:B:246:GLN:O	2.18	0.44
1:C:350:ARG:HA	1:C:357:THR:HG21	2.00	0.44
4:Q:15:PRO:HA	4:Q:78:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:13:LYS:O	3:P:16:SER:OG	2.32	0.44
3:P:35:SER:HA	3:P:50:GLY:HA2	1.98	0.44
1:A:36:VAL:HG22	5:X:610:TRP:HE3	1.82	0.44
1:B:257:THR:HG22	1:B:473:GLY:HA2	2.00	0.44
1:C:75:VAL:HG12	5:X:568:LEU:HD21	1.99	0.44
2:F:18:ALA:HB2	2:F:86:VAL:HG11	2.00	0.44
5:X:545:LEU:HD13	5:Z:591:GLN:OE1	2.18	0.44
5:X:586:TYR:OH	5:Z:591:GLN:NE2	2.51	0.44
3:I:47:TRP:CG	4:J:96:VAL:HB	2.52	0.44
4:Q:5:LEU:HD11	4:Q:90:THR:HG22	1.99	0.44
1:C:252:LYS:HB3	1:C:252:LYS:HE2	1.80	0.44
1:C:386:ASN:OD1	9:C:611:NAG:C1	2.65	0.44
2:D:76:ILE:H	2:D:76:ILE:HG12	1.49	0.44
1:B:95:MET:HE1	1:B:235:GLY:HA3	2.00	0.43
4:Q:90:THR:OG1	4:Q:91:TRP:N	2.51	0.43
1:A:99:ASN:HD21	1:A:103:GLN:HE21	1.65	0.43
2:E:18:ALA:HB2	2:E:86:VAL:HG11	2.00	0.43
3:H:6:GLN:HE21	3:H:104:GLY:HA3	1.83	0.43
4:L:90:THR:OG1	4:L:91:TRP:N	2.51	0.43
1:A:248:THR:CG2	1:A:486:TYR:CZ	3.02	0.43
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.84	0.43
1:B:249:HIS:NE2	1:B:482:GLU:HG2	2.32	0.43
3:P:97:ILE:HD12	3:P:97:ILE:HA	1.82	0.43
4:Q:27(A):SER:HG	4:Q:94:SER:H	1.67	0.43
1:A:296:CYS:HB2	1:A:445:CYS:HB3	1.99	0.43
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.87	0.43
1:A:248:THR:HG22	1:A:486:TYR:CD1	2.52	0.43
1:B:498:PRO:HB3	5:Y:610:TRP:CG	2.53	0.43
2:D:18:ALA:HB2	2:D:86:VAL:HG11	2.00	0.43
5:Z:610:TRP:HE3	5:Z:614:TRP:HE3	1.67	0.43
1:B:43:PRO:HB3	5:Y:523:LEU:HA	2.01	0.43
1:A:257:THR:C	1:A:259:LEU:H	2.22	0.43
1:C:40:TYR:HD2	1:C:494:LEU:HD13	1.84	0.43
4:Q:46:LEU:HD11	4:Q:49:TYR:HB3	2.01	0.43
1:A:439:ILE:HD12	1:A:439:ILE:HA	1.92	0.42
3:P:40:ALA:HB3	3:P:43:GLN:HB2	2.00	0.42
5:X:540:GLN:O	5:X:544:LEU:HG	2.18	0.42
1:C:79:PRO:HB3	5:Z:567:LYS:HD3	2.01	0.42
4:Q:16:GLY:HA2	4:Q:77:GLY:HA2	2.01	0.42
3:I:112:SER:OG	3:I:112:SER:O	2.35	0.42
1:B:214:PRO:HB2	1:B:250:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:37:GLN:N	4:L:45:LYS:O	2.42	0.42
5:Y:631:TRP:HA	5:Y:634:GLU:HB2	2.01	0.42
5:X:573:ILE:HD11	5:Y:573:ILE:HG12	2.02	0.42
5:Z:612:SER:HA	5:Z:616:ASN:HD21	1.85	0.42
1:C:38:VAL:HG11	5:Z:596:TRP:HZ3	1.85	0.42
1:A:37:THR:HA	5:X:605:CYS:HA	2.01	0.42
1:C:475:MET:SD	1:C:478:ASN:ND2	2.93	0.42
1:B:358:ILE:H	1:B:358:ILE:HG12	1.69	0.42
2:E:76:ILE:H	2:E:76:ILE:HG12	1.49	0.42
1:C:257:THR:N	1:C:375:SER:O	2.51	0.42
3:H:35:SER:OG	3:H:47:TRP:NE1	2.53	0.42
1:B:297:THR:HG22	1:B:444:ARG:HA	2.02	0.41
4:Q:7:GLN:HE22	4:Q:88:CYS:H	1.67	0.41
1:A:499:THR:OG1	1:A:500:ARG:N	2.51	0.41
1:B:363:ASN:ND2	1:B:388:SER:OG	2.51	0.41
3:I:29:LEU:HD11	3:I:76:ARG:HA	2.02	0.41
4:Q:5:LEU:HB2	4:Q:99:GLY:HA2	2.02	0.41
1:B:40:TYR:OH	5:Y:589:ASP:OD2	2.31	0.41
1:C:421:LYS:HB3	1:C:421:LYS:HE2	1.83	0.41
5:Y:595:ILE:HD13	5:Y:595:ILE:HA	1.92	0.41
3:P:82(C):LEU:HG	3:P:111:VAL:HG21	2.02	0.41
1:B:45:TRP:CE3	5:Y:629:LEU:CD2	3.03	0.41
1:B:243:SER:OG	1:B:244:THR:N	2.54	0.41
1:B:372:THR:HG23	1:B:373:THR:HG23	2.03	0.41
3:H:4:LEU:HD23	3:H:4:LEU:HA	1.83	0.41
4:L:6:THR:OG1	4:L:24:SER:OG	2.33	0.41
1:A:198:THR:O	1:A:198:THR:OG1	2.34	0.41
1:B:91:GLU:OE2	1:B:487:LYS:NZ	2.47	0.41
1:C:461:THR:OG1	1:C:462:ASN:N	2.54	0.41
3:I:72:ASP:OD2	3:I:74:SER:OG	2.36	0.41
4:L:67:SER:HG	4:L:70[A]:SER:HG	1.62	0.41
5:X:576:LEU:HD11	5:Z:577:GLN:HG2	2.03	0.41
1:B:191:TYR:O	1:B:192:ARG:NE	2.53	0.41
1:B:232:LYS:HD2	1:B:232:LYS:HA	1.95	0.41
3:I:4:LEU:HG	3:I:102:VAL:HG12	2.03	0.41
2:E:14:LEU:HD12	2:E:69:LEU:HD23	2.03	0.40
4:J:37:GLN:O	4:J:45:LYS:N	2.50	0.40
1:B:194:ILE:H	1:B:194:ILE:HG13	1.62	0.40
1:B:214:PRO:HB2	1:B:250:GLY:CA	2.51	0.40
1:B:336:ALA:HA	1:B:339:ASN:HB3	2.03	0.40
1:C:497:ALA:HB1	1:C:498:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:82(C):LEU:HD22	3:H:111:VAL:HG21	2.02	0.40
5:Z:606:THR:OG1	5:Z:607:ASN:N	2.54	0.40
4:Q:51:ASN:HB3	4:Q:66:LYS:HB2	2.04	0.40
1:A:95:MET:HE2	1:A:273:ARG:HD3	2.03	0.40
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.93	0.40
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.84	0.40
1:B:104:MET:HE2	1:B:108:ILE:HD11	2.03	0.40
3:H:97:ILE:HD12	3:H:97:ILE:HA	1.92	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	355/481 (74%)	303 (85%)	51 (14%)	1 (0%)	41	71
1	B	357/481 (74%)	320 (90%)	36 (10%)	1 (0%)	41	71
1	C	355/481 (74%)	320 (90%)	34 (10%)	1 (0%)	41	71
2	D	95/192 (50%)	82 (86%)	13 (14%)	0	100	100
2	E	95/192 (50%)	82 (86%)	13 (14%)	0	100	100
2	F	95/192 (50%)	82 (86%)	13 (14%)	0	100	100
3	H	129/235 (55%)	121 (94%)	8 (6%)	0	100	100
3	I	129/235 (55%)	116 (90%)	11 (8%)	2 (2%)	9	36
3	P	128/235 (54%)	119 (93%)	8 (6%)	1 (1%)	19	51
4	J	110/213 (52%)	103 (94%)	7 (6%)	0	100	100
4	L	109/213 (51%)	102 (94%)	7 (6%)	0	100	100
4	Q	108/213 (51%)	101 (94%)	7 (6%)	0	100	100
5	X	129/153 (84%)	124 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	129/153 (84%)	122 (95%)	7 (5%)	0	100	100
5	Z	117/153 (76%)	104 (89%)	13 (11%)	0	100	100
All	All	2440/3822 (64%)	2201 (90%)	233 (10%)	6 (0%)	50	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	100(E)	ASP
1	B	250	GLY
1	C	501	CYS
3	I	100(G)	ALA
1	A	258	GLN
3	I	100(E)	ASP

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	304/428 (71%)	302 (99%)	2 (1%)	84	90
1	B	300/428 (70%)	300 (100%)	0	100	100
1	C	312/428 (73%)	309 (99%)	3 (1%)	76	86
2	D	87/173 (50%)	74 (85%)	13 (15%)	3	13
2	E	87/173 (50%)	74 (85%)	13 (15%)	3	13
2	F	87/173 (50%)	74 (85%)	13 (15%)	3	13
3	H	98/189 (52%)	98 (100%)	0	100	100
3	I	98/189 (52%)	97 (99%)	1 (1%)	76	86
3	P	97/189 (51%)	95 (98%)	2 (2%)	53	75
4	J	93/179 (52%)	93 (100%)	0	100	100
4	L	92/179 (51%)	92 (100%)	0	100	100
4	Q	91/179 (51%)	91 (100%)	0	100	100
5	X	94/129 (73%)	93 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Y	102/129 (79%)	102 (100%)	0	100	100
5	Z	89/129 (69%)	87 (98%)	2 (2%)	52	74
All	All	2031/3294 (62%)	1981 (98%)	50 (2%)	50	72

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	247	CYS
1	C	259	LEU
1	C	261	LEU
1	C	500	ARG
2	D	5	LEU
2	D	10	ASP
2	D	22	LYS
2	D	42	SER
2	D	50	LYS
2	D	60	SER
2	D	63	ASP
2	D	66	ASN
2	D	76	ILE
2	D	78	ASP
2	D	80	ASP
2	D	81	THR
2	D	96	LEU
2	E	5	LEU
2	E	10	ASP
2	E	22	LYS
2	E	42	SER
2	E	50	LYS
2	E	60	SER
2	E	63	ASP
2	E	66	ASN
2	E	76	ILE
2	E	78	ASP
2	E	80	ASP
2	E	81	THR
2	E	96	LEU
2	F	5	LEU
2	F	10	ASP
2	F	22	LYS

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Mol	Chain	Res	Type
2	F	42	SER
2	F	50	LYS
2	F	60	SER
2	F	63	ASP
2	F	66	ASN
2	F	76	ILE
2	F	78	ASP
2	F	80	ASP
2	F	81	THR
2	F	96	LEU
3	I	100(Q)	MET
3	P	76	ARG
3	P	100(Q)	MET
5	X	545	LEU
5	Z	606	THR
5	Z	622	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	99	ASN
1	A	352	HIS
1	A	374	HIS
1	A	422	GLN
1	A	425	ASN
1	B	195	ASN
1	B	279	ASN
1	B	422	GLN
1	C	197	ASN
1	C	258	GLN
1	C	280	ASN
1	C	287	GLN
1	C	293	GLN
1	C	386	ASN
1	C	478	ASN
2	D	27	HIS
2	F	32	ASN
3	H	39	GLN
3	H	81	HIS
3	I	12	ASN
3	I	81	HIS

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Mol	Chain	Res	Type
4	L	30	ASN
3	P	6	GLN
3	P	12	ASN
3	P	32	HIS
4	Q	7	GLN
4	Q	37	GLN
5	X	590	GLN
5	X	591	GLN
5	X	607	ASN
5	X	656	ASN
5	Y	543	ASN
5	Y	625	ASN
5	Z	616	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	TYS	I	100(I)	3	15,16,17	1.86	3 (20%)	18,22,24	1.05	1 (5%)
3	TYS	P	100(I)	3	15,16,17	1.85	3 (20%)	18,22,24	1.07	1 (5%)
3	TYS	I	100(F)	3	15,16,17	1.64	3 (20%)	18,22,24	0.85	0
3	TYS	P	100(F)	3	15,16,17	1.69	3 (20%)	18,22,24	0.86	0
3	TYS	H	100(I)	3	15,16,17	1.57	3 (20%)	18,22,24	1.23	1 (5%)
3	TYS	H	100(F)	3	15,16,17	1.39	3 (20%)	18,22,24	1.07	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
3	TYS	I	100(I)	3	-	3/10/11/13	0/1/1/1
3	TYS	P	100(I)	3	-	2/10/11/13	0/1/1/1
3	TYS	I	100(F)	3	-	3/10/11/13	0/1/1/1
3	TYS	P	100(F)	3	-	3/10/11/13	0/1/1/1
3	TYS	H	100(I)	3	-	1/10/11/13	0/1/1/1
3	TYS	H	100(F)	3	-	1/10/11/13	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	100(F)	TYS	O1-S	4.37	1.64	1.45
3	P	100(F)	TYS	O1-S	4.31	1.63	1.45
3	P	100(I)	TYS	O2-S	4.18	1.63	1.45
3	I	100(I)	TYS	O1-S	4.12	1.62	1.45
3	H	100(I)	TYS	OH-S	-4.00	1.52	1.58
3	I	100(I)	TYS	OH-S	-3.93	1.52	1.58
3	P	100(I)	TYS	OH-S	-3.82	1.52	1.58
3	P	100(I)	TYS	OH-CZ	-3.72	1.36	1.42
3	I	100(I)	TYS	OH-CZ	-3.71	1.36	1.42
3	H	100(I)	TYS	OH-CZ	-3.55	1.36	1.42
3	H	100(F)	TYS	OH-CZ	-3.39	1.37	1.42
3	P	100(F)	TYS	OH-CZ	-3.22	1.37	1.42
3	I	100(F)	TYS	OH-CZ	-3.08	1.37	1.42
3	P	100(F)	TYS	OH-S	-3.05	1.53	1.58
3	H	100(F)	TYS	OH-S	-2.94	1.53	1.58
3	I	100(F)	TYS	OH-S	-2.54	1.54	1.58
3	H	100(F)	TYS	O3-S	2.14	1.63	1.50
3	H	100(I)	TYS	O3-S	2.02	1.62	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	100(I)	TYS	CG-CB-CA	-3.98	106.05	114.10
3	I	100(I)	TYS	CG-CB-CA	-3.39	107.23	114.10
3	H	100(F)	TYS	CG-CB-CA	-2.43	109.18	114.10
3	P	100(I)	TYS	O3-S-OH	2.24	111.23	105.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	100(F)	TYS	O-C-CA-CB
3	I	100(F)	TYS	CE1-CZ-OH-S
3	I	100(F)	TYS	CE2-CZ-OH-S
3	P	100(F)	TYS	CZ-OH-S-O3
3	H	100(I)	TYS	O-C-CA-CB
3	I	100(I)	TYS	O-C-CA-CB
3	I	100(I)	TYS	CE1-CZ-OH-S
3	I	100(I)	TYS	CE2-CZ-OH-S
3	P	100(I)	TYS	CE1-CZ-OH-S
3	P	100(I)	TYS	CE2-CZ-OH-S
3	P	100(F)	TYS	CZ-OH-S-O1
3	I	100(F)	TYS	CZ-OH-S-O3
3	P	100(F)	TYS	CZ-OH-S-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	100(F)	TYS	1	0

5.5 Carbohydrates (i)

25 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	$\#\|Z\| > 2$
6	NAG	G	1	6,1	14,14,15	0.59	1 (7%)	17,19,21	0.66	0
6	NAG	G	2	6	14,14,15	0.95	1 (7%)	17,19,21	0.97	1 (5%)
7	NAG	K	1	7,1	14,14,15	0.70	1 (7%)	17,19,21	0.65	0
7	NAG	K	2	7	14,14,15	0.26	0	17,19,21	0.49	0
7	BMA	K	3	7	11,11,12	0.71	0	15,15,17	1.00	2 (13%)
7	MAN	K	4	7	11,11,12	0.96	0	15,15,17	1.89	2 (13%)
7	MAN	K	5	7	11,11,12	0.74	0	15,15,17	1.13	2 (13%)
6	NAG	M	1	6,1	14,14,15	1.36	2 (14%)	17,19,21	1.56	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	M	2	6	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	N	1	6,1	14,14,15	0.40	0	17,19,21	0.55	0
6	NAG	N	2	6	14,14,15	0.70	1 (7%)	17,19,21	0.97	1 (5%)
8	NAG	O	1	8,1	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
8	NAG	O	2	8	14,14,15	0.27	0	17,19,21	0.55	0
8	BMA	O	3	8	11,11,12	0.87	0	15,15,17	1.23	1 (6%)
8	MAN	O	4	8	11,11,12	1.04	0	15,15,17	1.88	2 (13%)
8	MAN	O	5	8	11,11,12	0.56	0	15,15,17	1.23	2 (13%)
8	MAN	O	6	8	11,11,12	0.91	0	15,15,17	1.09	2 (13%)
8	MAN	O	7	8	11,11,12	1.12	1 (9%)	15,15,17	1.63	4 (26%)
6	NAG	R	1	6,1	14,14,15	0.24	0	17,19,21	0.58	0
6	NAG	R	2	6	14,14,15	0.40	0	17,19,21	0.48	0
7	NAG	S	1	7,1	14,14,15	0.68	1 (7%)	17,19,21	0.81	1 (5%)
7	NAG	S	2	7	14,14,15	0.35	0	17,19,21	0.59	0
7	BMA	S	3	7	11,11,12	0.93	0	15,15,17	1.07	2 (13%)
7	MAN	S	4	7	11,11,12	0.93	0	15,15,17	1.93	2 (13%)
7	MAN	S	5	7	11,11,12	0.83	0	15,15,17	1.15	2 (13%)

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
6	NAG	G	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
8	NAG	O	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	O	4	8	-	1/2/19/22	0/1/1/1
8	MAN	O	5	8	-	2/2/19/22	0/1/1/1
8	MAN	O	6	8	-	0/2/19/22	0/1/1/1
8	MAN	O	7	8	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
7	NAG	S	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	2/2/19/22	0/1/1/1
7	MAN	S	5	7	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1	NAG	O5-C1	-4.42	1.36	1.43
6	G	2	NAG	C1-C2	3.18	1.57	1.52
8	O	7	MAN	C1-C2	3.09	1.59	1.52
7	K	1	NAG	O5-C1	-2.38	1.39	1.43
6	N	2	NAG	C1-C2	2.25	1.55	1.52
7	S	1	NAG	O5-C1	-2.13	1.40	1.43
6	M	1	NAG	C1-C2	-2.04	1.49	1.52
6	G	1	NAG	O5-C1	-2.01	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	4	MAN	C1-O5-C5	6.17	120.55	112.19
7	S	4	MAN	C1-O5-C5	5.67	119.87	112.19
7	K	4	MAN	C1-O5-C5	5.63	119.82	112.19
6	M	1	NAG	C3-C4-C5	3.86	117.12	110.24
6	M	1	NAG	C1-O5-C5	3.65	117.14	112.19
7	K	4	MAN	O2-C2-C3	-3.53	103.06	110.14
7	S	4	MAN	O2-C2-C3	-3.35	103.44	110.14
8	O	5	MAN	C1-O5-C5	3.26	116.61	112.19
6	G	2	NAG	C2-N2-C7	3.05	127.25	122.90
8	O	7	MAN	C1-O5-C5	3.05	116.32	112.19
8	O	3	BMA	C1-C2-C3	-3.03	105.94	109.67
6	N	2	NAG	C2-N2-C7	2.97	127.12	122.90
8	O	7	MAN	C1-C2-C3	2.90	113.23	109.67
7	K	5	MAN	O2-C2-C3	-2.72	104.69	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	5	MAN	O2-C2-C3	-2.69	104.74	110.14
7	S	3	BMA	O2-C2-C3	-2.66	104.82	110.14
8	O	7	MAN	O5-C1-C2	2.60	114.79	110.77
8	O	6	MAN	C1-O5-C5	2.56	115.66	112.19
7	S	5	MAN	C1-O5-C5	2.56	115.66	112.19
8	O	4	MAN	O2-C2-C3	-2.55	105.04	110.14
7	K	3	BMA	C1-O5-C5	2.50	115.58	112.19
7	S	1	NAG	C1-O5-C5	2.45	115.51	112.19
7	K	5	MAN	C1-O5-C5	2.45	115.51	112.19
8	O	5	MAN	O2-C2-C3	-2.41	105.31	110.14
7	S	3	BMA	C1-O5-C5	2.31	115.33	112.19
7	K	3	BMA	O2-C2-C3	-2.23	105.67	110.14
8	O	1	NAG	C1-O5-C5	2.16	115.12	112.19
8	O	6	MAN	O2-C2-C3	-2.16	105.81	110.14
8	O	7	MAN	O2-C2-C3	-2.13	105.87	110.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	2	NAG	O5-C5-C6-O6
7	K	4	MAN	C4-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
7	S	4	MAN	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
7	S	4	MAN	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
8	O	5	MAN	C4-C5-C6-O6
7	S	3	BMA	C4-C5-C6-O6
8	O	2	NAG	C8-C7-N2-C2
8	O	2	NAG	O7-C7-N2-C2
8	O	5	MAN	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	N	1	NAG	O5-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
6	G	2	NAG	C3-C2-N2-C7
6	N	2	NAG	C3-C2-N2-C7
8	O	4	MAN	O5-C5-C6-O6

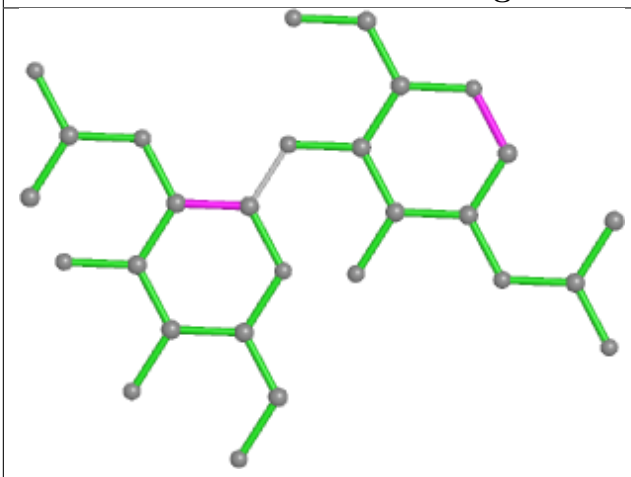
There are no ring outliers.

2 monomers are involved in 2 short contacts:

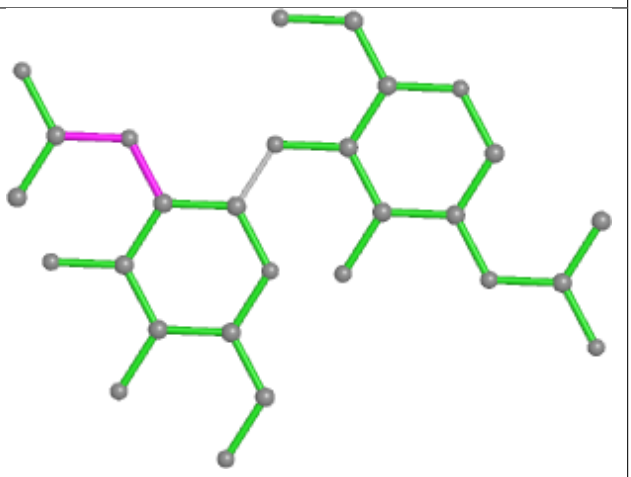
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	1	NAG	1	0
8	O	5	MAN	1	0

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

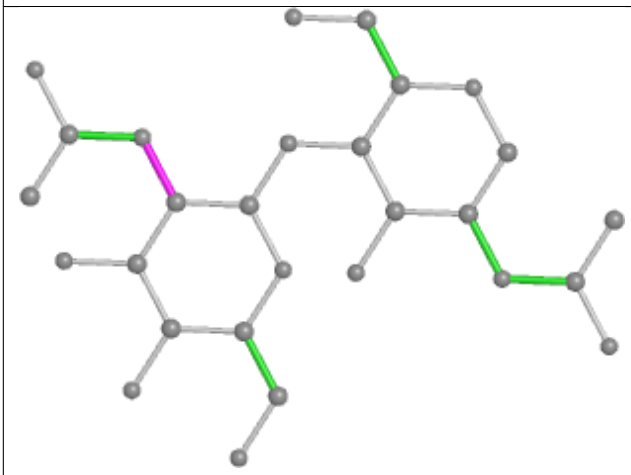
Oligosaccharide Chain G



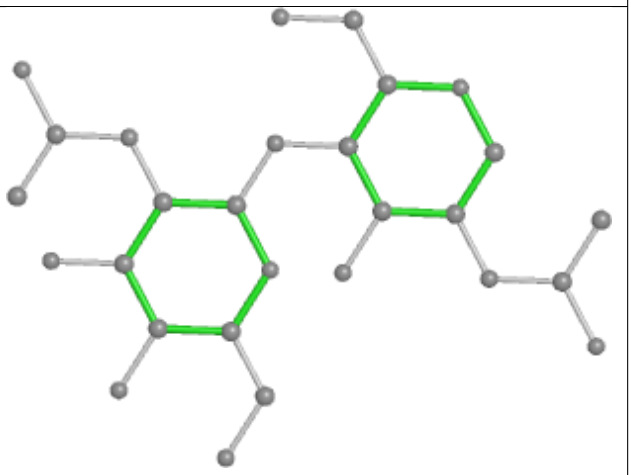
Bond lengths



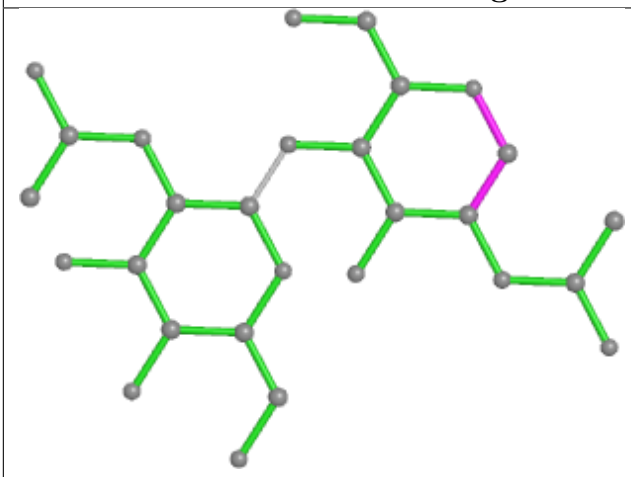
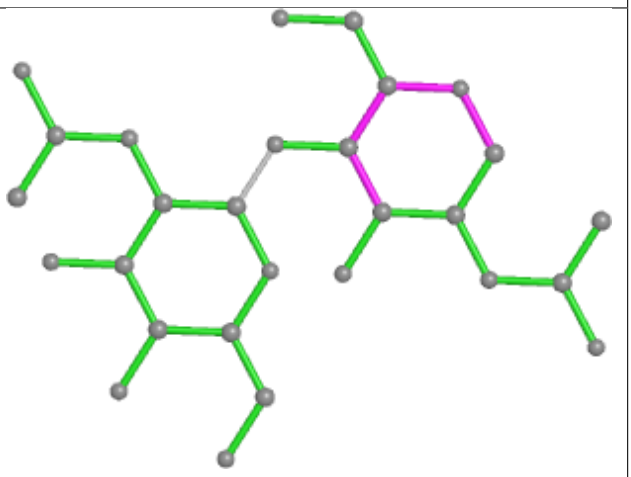
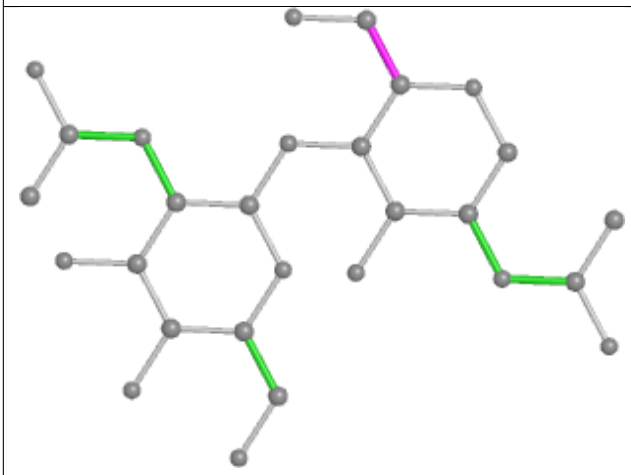
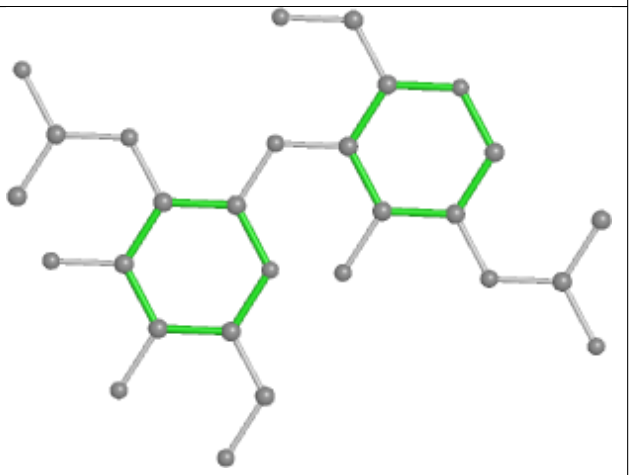
Bond angles

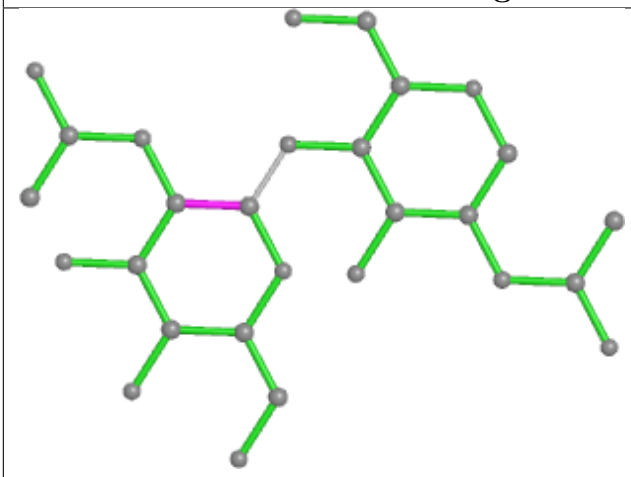
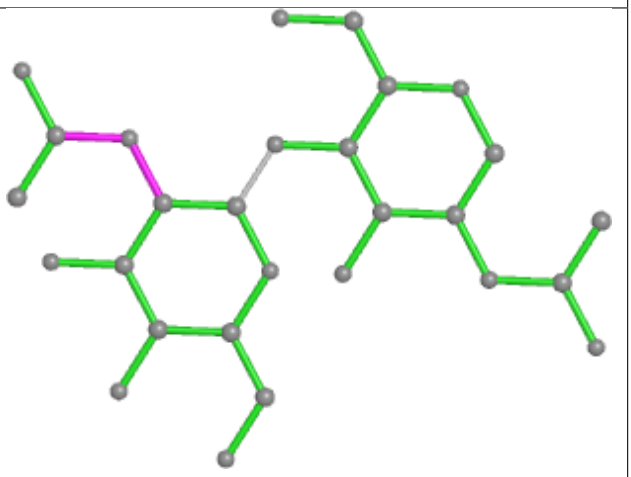
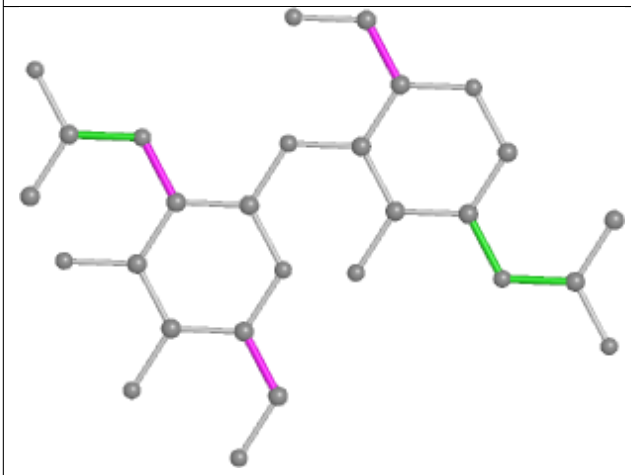
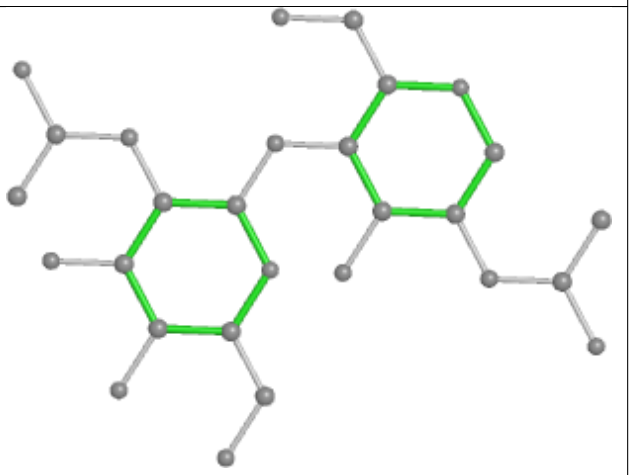


Torsions

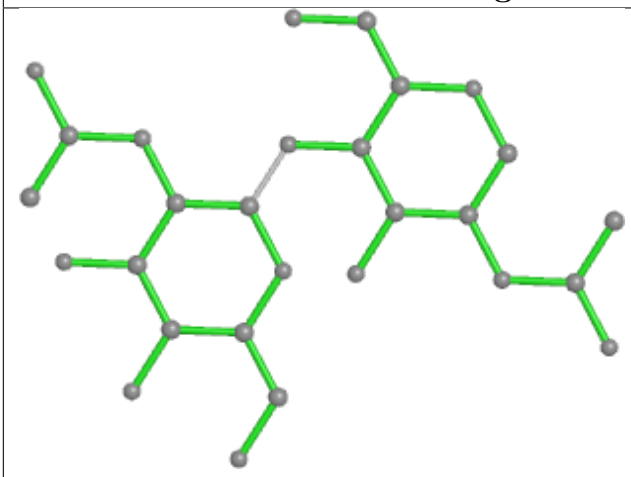


Rings

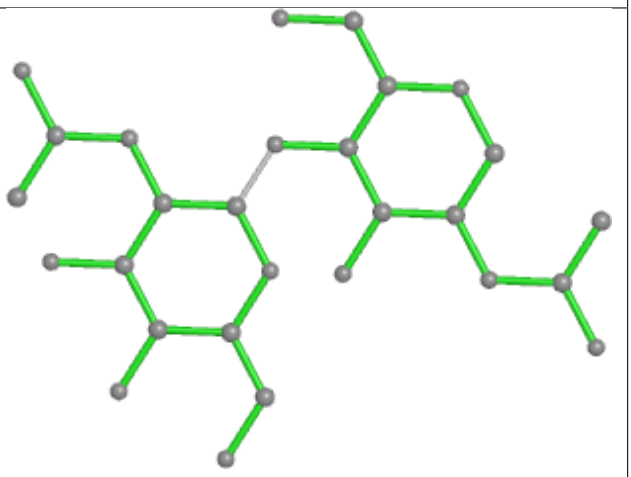
Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

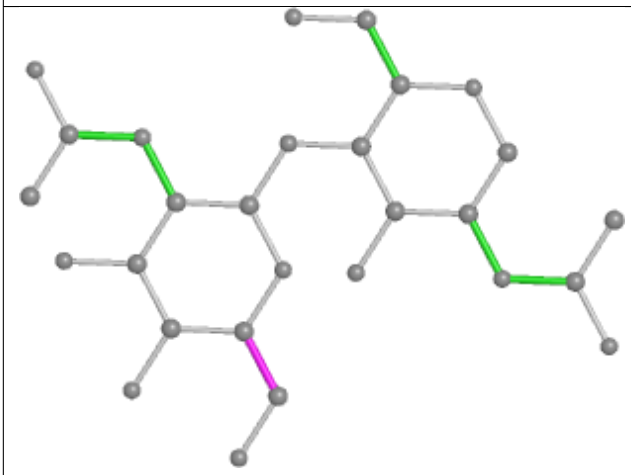
Oligosaccharide Chain R



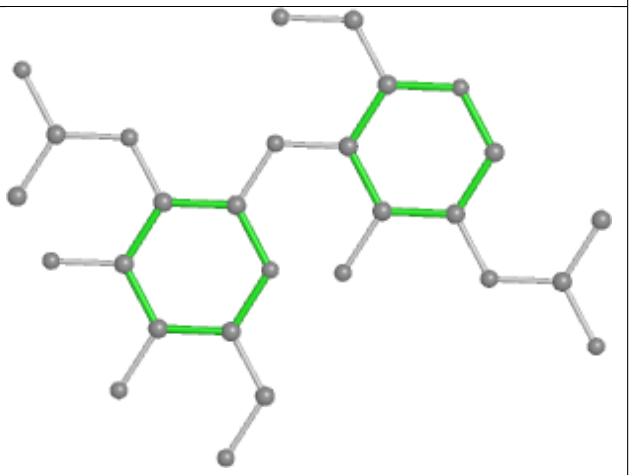
Bond lengths



Bond angles

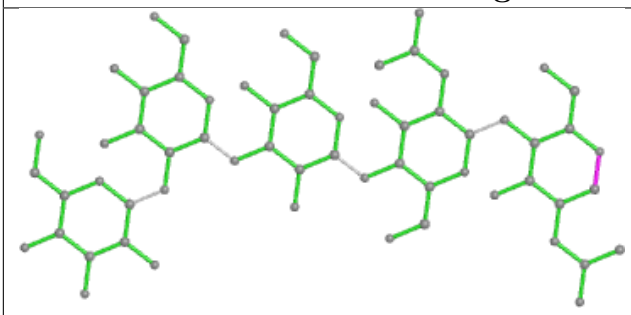


Torsions

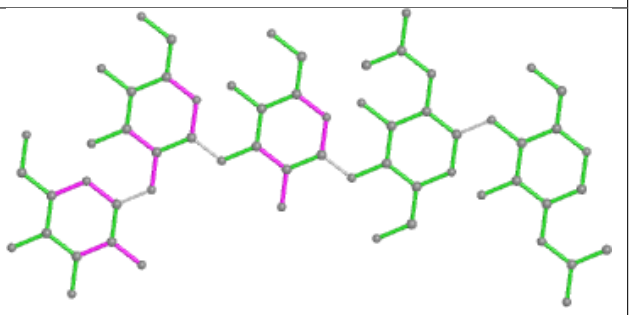


Rings

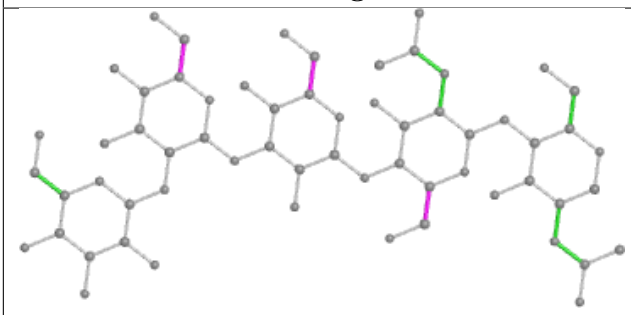
Oligosaccharide Chain K



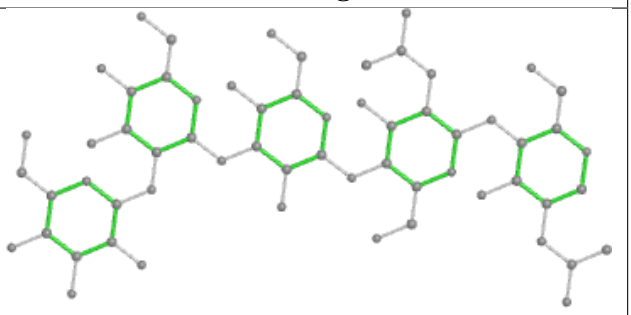
Bond lengths



Bond angles

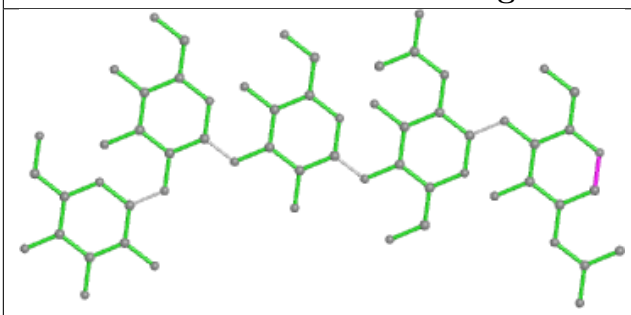


Torsions

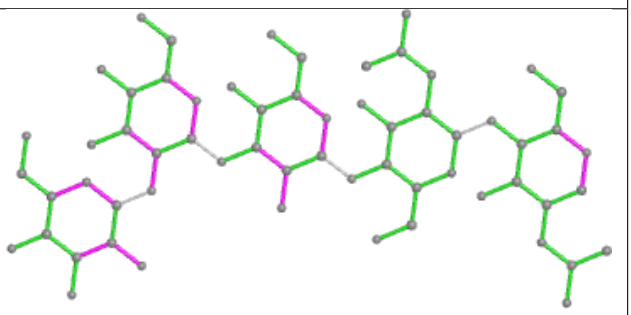


Rings

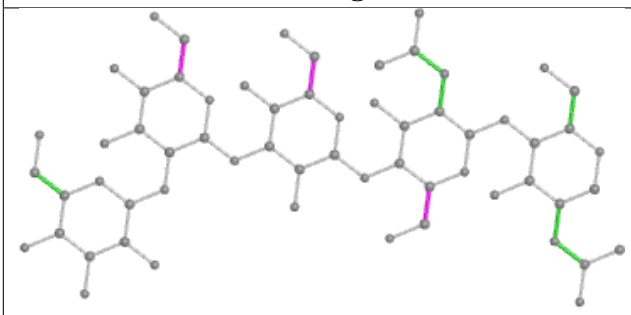
Oligosaccharide Chain S



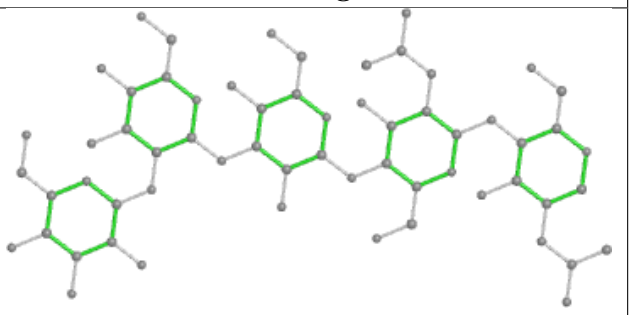
Bond lengths



Bond angles

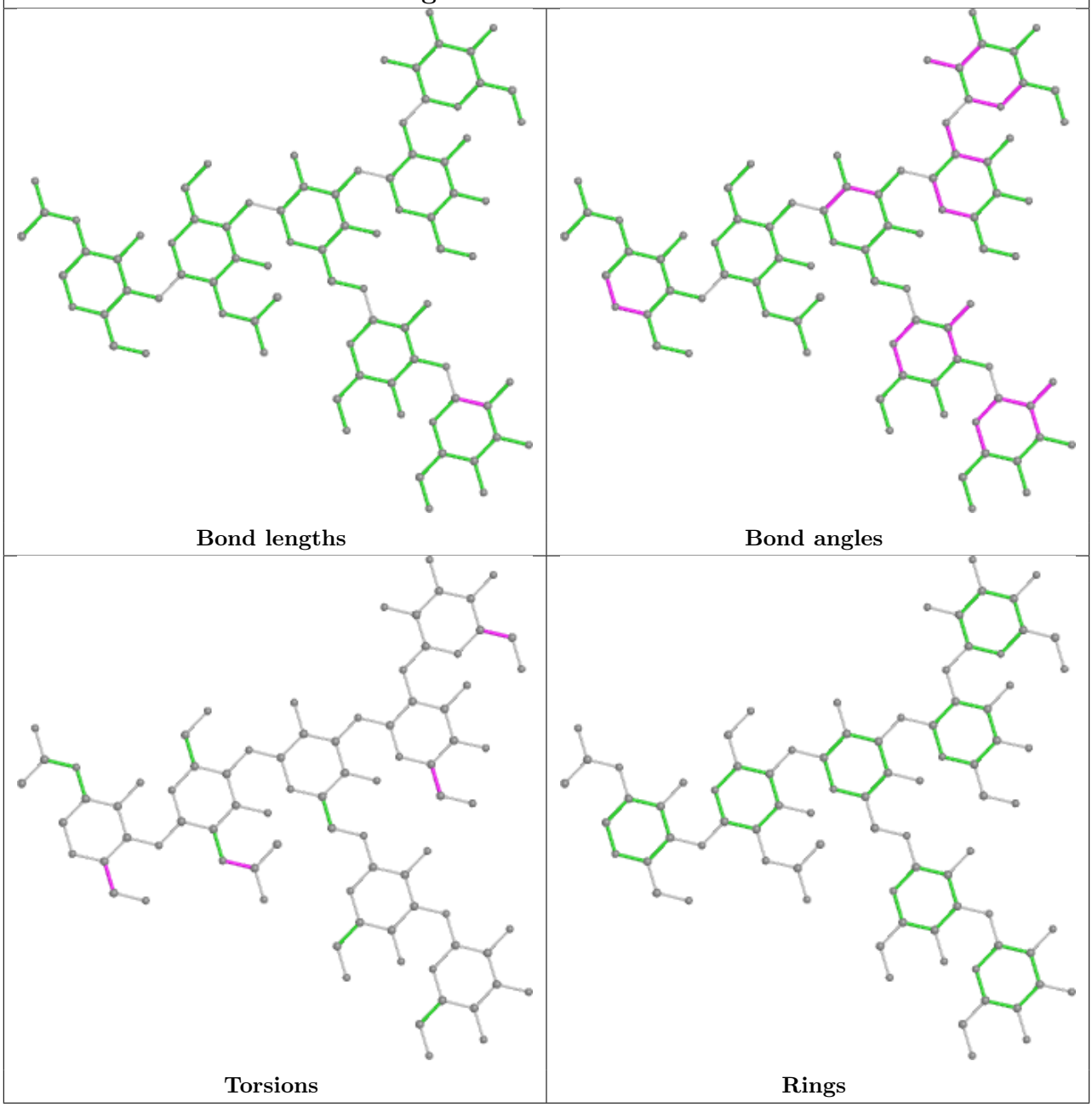


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
9	NAG	B	605	1	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	C	613	1	14,14,15	0.49	0	17,19,21	0.52	0
9	NAG	B	615	1	14,14,15	0.33	0	17,19,21	0.52	0
9	NAG	C	610	1	14,14,15	0.27	0	17,19,21	0.50	0
9	NAG	C	608	1	14,14,15	0.53	0	17,19,21	0.64	1 (5%)
9	NAG	A	614	1	14,14,15	0.46	0	17,19,21	0.43	0
9	NAG	A	604	1	14,14,15	0.21	0	17,19,21	0.69	0
9	NAG	C	614	1	14,14,15	0.27	0	17,19,21	0.69	0
9	NAG	C	611	-	14,14,15	0.35	0	17,19,21	0.42	0
9	NAG	A	615	1	14,14,15	0.39	0	17,19,21	0.56	0
9	NAG	C	601	1	14,14,15	0.37	0	17,19,21	0.54	0
9	NAG	B	604	1	14,14,15	0.21	0	17,19,21	0.58	0
9	NAG	C	612	1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
9	NAG	A	613	1	14,14,15	0.93	1 (7%)	17,19,21	0.98	1 (5%)
9	NAG	B	601	1	14,14,15	0.34	0	17,19,21	0.45	0
9	NAG	A	612	1	14,14,15	0.23	0	17,19,21	0.45	0
9	NAG	A	601	1	14,14,15	0.60	0	17,19,21	0.74	1 (5%)
9	NAG	X	701	5	14,14,15	0.28	0	17,19,21	0.56	0
9	NAG	C	609	1	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
9	NAG	B	616	1	14,14,15	0.27	0	17,19,21	0.59	0
9	NAG	C	607	1	14,14,15	0.18	0	17,19,21	0.67	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
9	NAG	B	605	1	-	2/6/23/26	0/1/1/1
9	NAG	C	613	1	-	2/6/23/26	0/1/1/1
9	NAG	B	615	1	-	2/6/23/26	0/1/1/1
9	NAG	C	610	1	-	2/6/23/26	0/1/1/1
9	NAG	C	608	1	-	2/6/23/26	0/1/1/1
9	NAG	A	614	1	-	0/6/23/26	0/1/1/1
9	NAG	A	604	1	-	2/6/23/26	0/1/1/1
9	NAG	C	614	1	-	0/6/23/26	0/1/1/1
9	NAG	C	611	-	-	2/6/23/26	0/1/1/1
9	NAG	A	615	1	-	3/6/23/26	0/1/1/1
9	NAG	C	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	604	1	-	2/6/23/26	0/1/1/1
9	NAG	C	612	1	-	0/6/23/26	0/1/1/1
9	NAG	A	613	1	-	1/6/23/26	0/1/1/1
9	NAG	B	601	1	-	0/6/23/26	0/1/1/1
9	NAG	A	612	1	-	2/6/23/26	0/1/1/1
9	NAG	A	601	1	-	0/6/23/26	0/1/1/1
9	NAG	X	701	5	-	0/6/23/26	0/1/1/1
9	NAG	C	609	1	-	2/6/23/26	0/1/1/1
9	NAG	B	616	1	-	2/6/23/26	0/1/1/1
9	NAG	C	607	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	613	NAG	C1-C2	2.92	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	613	NAG	C1-O5-C5	3.40	116.80	112.19
9	C	609	NAG	C1-O5-C5	2.62	115.74	112.19
9	C	612	NAG	C1-O5-C5	2.56	115.65	112.19
9	A	601	NAG	C1-O5-C5	2.40	115.44	112.19
9	C	607	NAG	C1-O5-C5	2.31	115.32	112.19
9	C	608	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	616	NAG	O5-C5-C6-O6
9	C	608	NAG	O5-C5-C6-O6
9	A	612	NAG	O5-C5-C6-O6
9	C	609	NAG	O5-C5-C6-O6
9	C	613	NAG	O5-C5-C6-O6
9	B	616	NAG	C4-C5-C6-O6
9	C	611	NAG	O5-C5-C6-O6
9	A	612	NAG	C4-C5-C6-O6
9	A	604	NAG	C8-C7-N2-C2
9	A	604	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	A	615	NAG	C8-C7-N2-C2
9	A	615	NAG	O7-C7-N2-C2
9	B	605	NAG	C8-C7-N2-C2
9	B	605	NAG	O7-C7-N2-C2
9	C	601	NAG	C8-C7-N2-C2
9	C	601	NAG	O7-C7-N2-C2
9	B	604	NAG	O5-C5-C6-O6
9	C	608	NAG	C4-C5-C6-O6
9	C	611	NAG	C4-C5-C6-O6
9	C	613	NAG	C4-C5-C6-O6
9	C	609	NAG	C4-C5-C6-O6
9	B	615	NAG	O5-C5-C6-O6
9	C	610	NAG	O5-C5-C6-O6
9	C	607	NAG	O5-C5-C6-O6
9	B	615	NAG	C4-C5-C6-O6
9	B	604	NAG	C4-C5-C6-O6
9	C	607	NAG	C4-C5-C6-O6
9	C	610	NAG	C4-C5-C6-O6
9	A	615	NAG	O5-C5-C6-O6
9	A	613	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	611	NAG	7	0
9	C	609	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

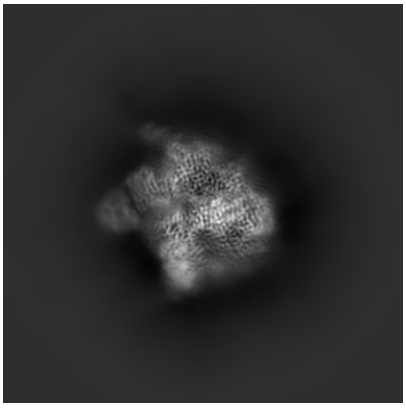
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20605. These allow visual inspection of the internal detail of the map and identification of artifacts.

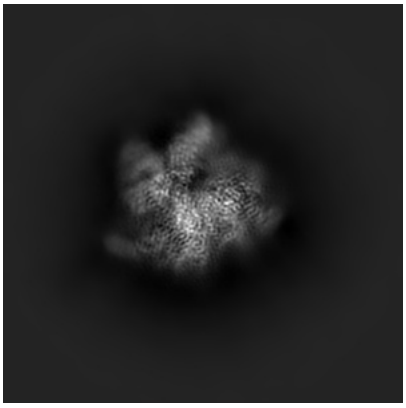
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

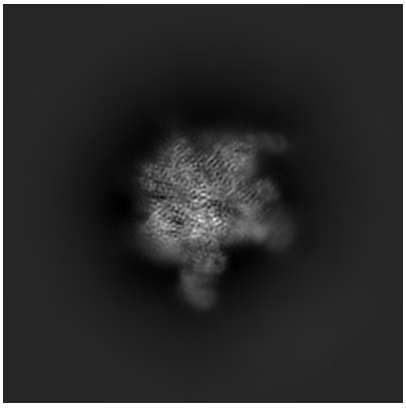
6.1.1 Primary map



X



Y

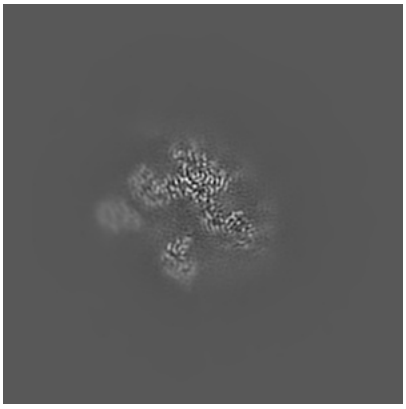


Z

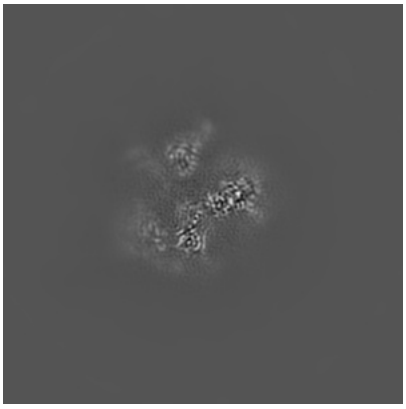
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

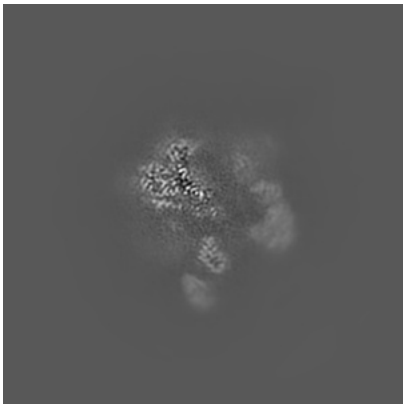
6.2.1 Primary map



X Index: 180



Y Index: 180

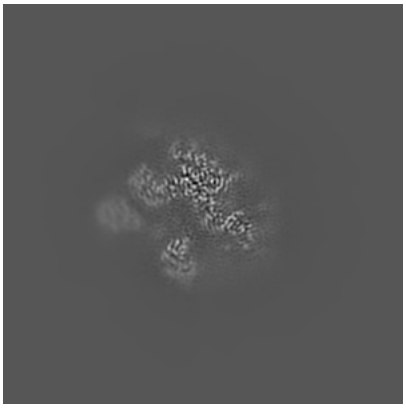


Z Index: 180

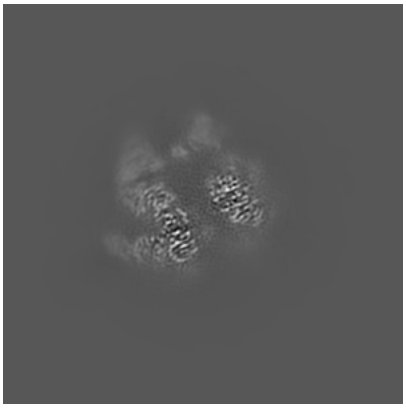
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

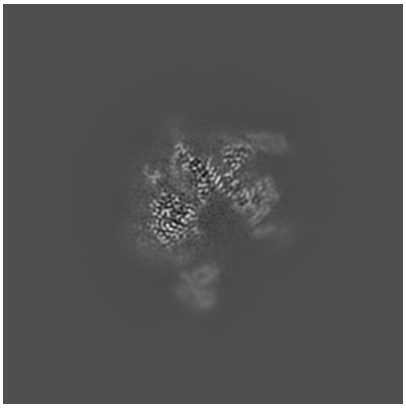
6.3.1 Primary map



X Index: 179



Y Index: 162

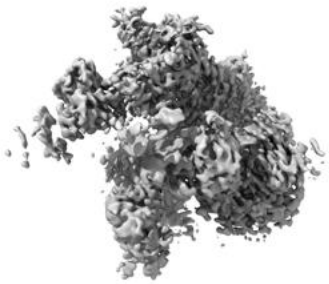


Z Index: 165

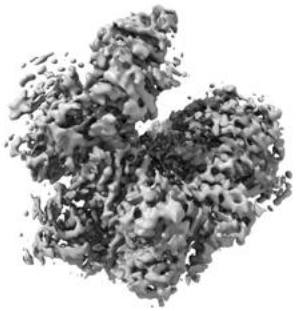
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

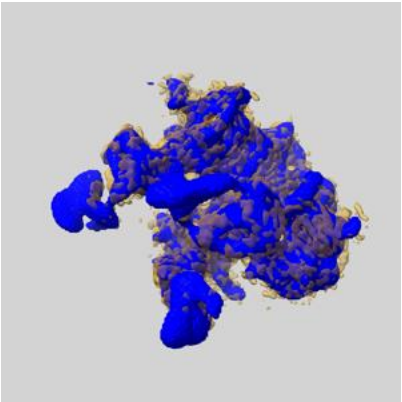
6.5 Mask visualisation (i)

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

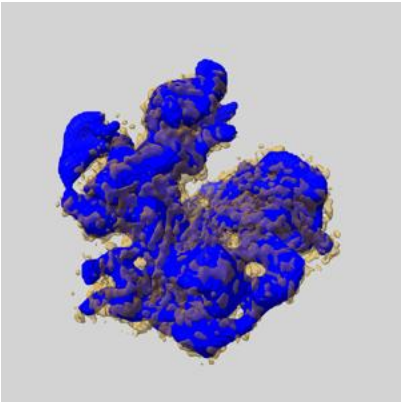
A mask typically either:

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

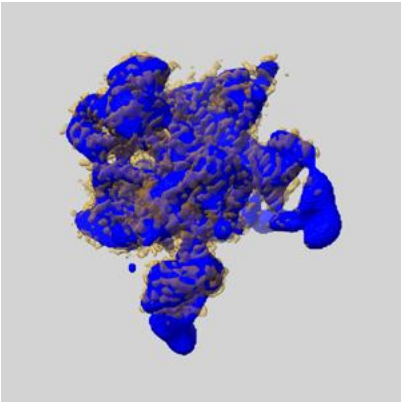
6.5.1 emd_20605_msk_1.map (i)



X



Y

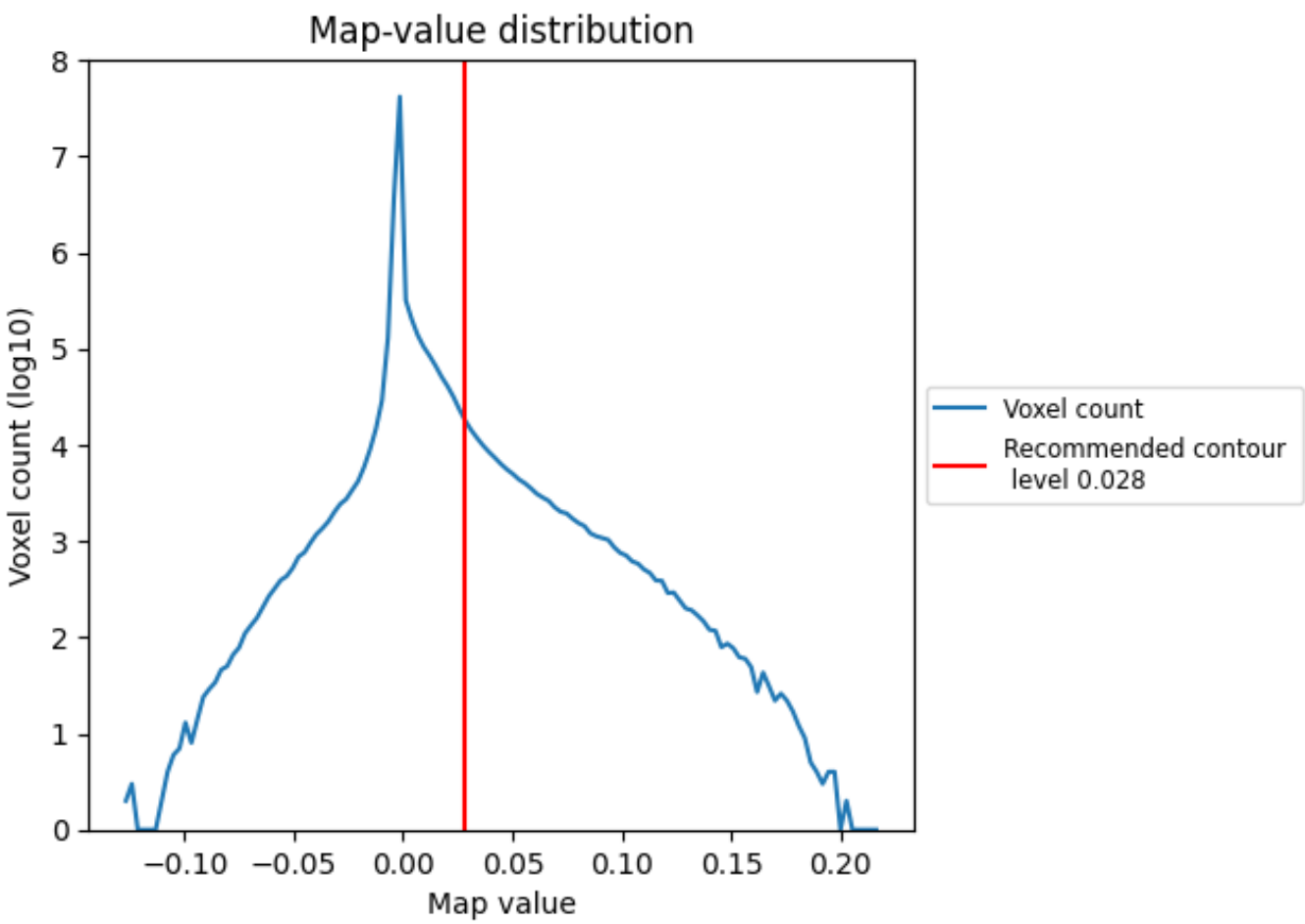


Z

7 Map analysis (i)

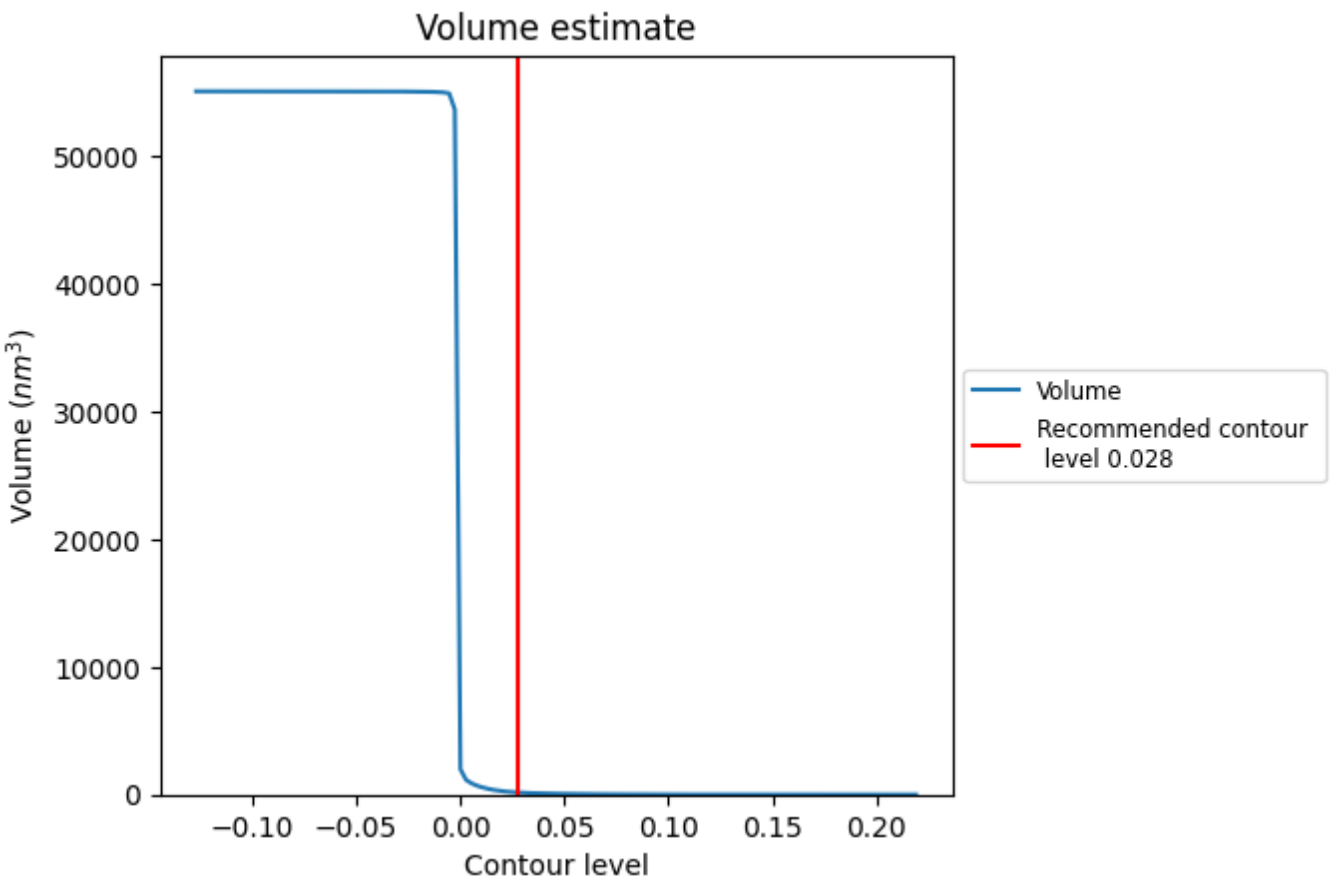
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

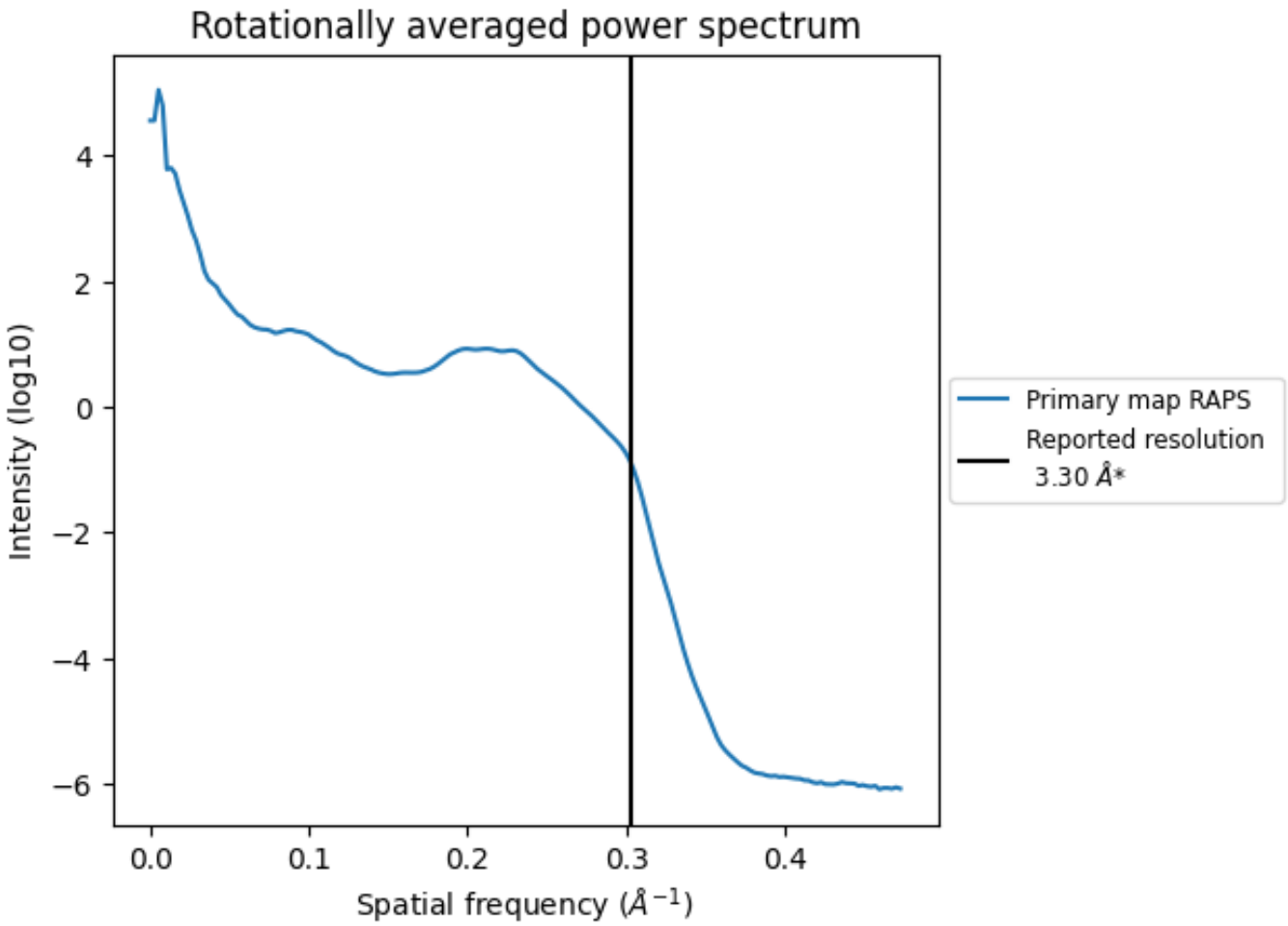
7.2 Volume estimate (i)



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 143 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)

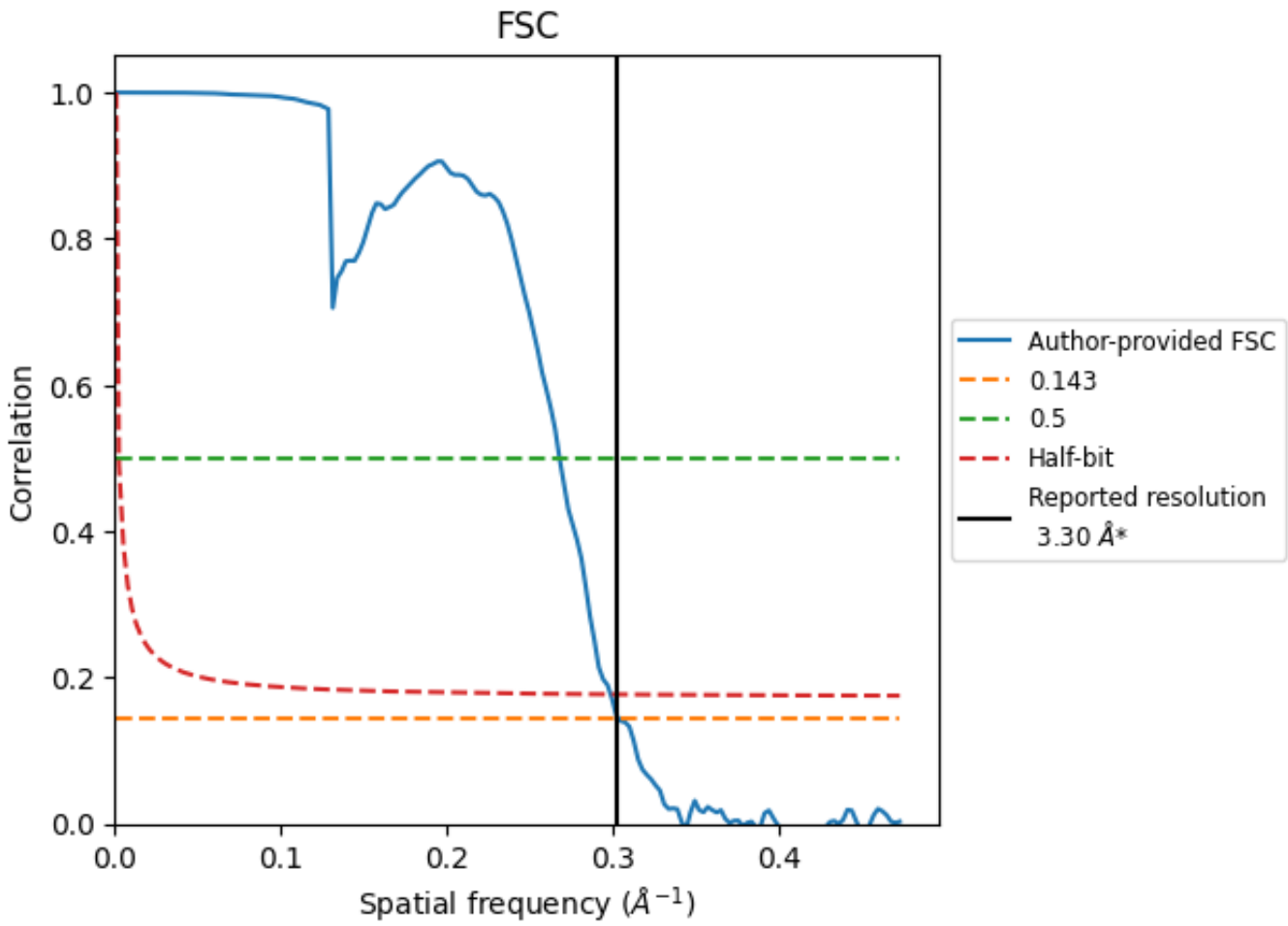


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

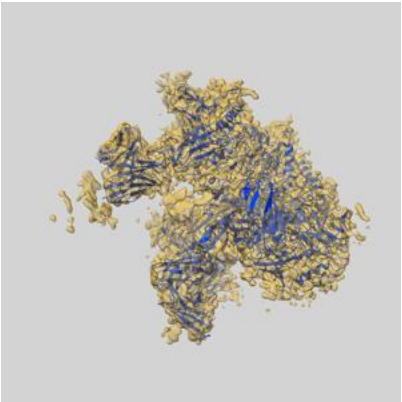
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.73	3.35
Unmasked-calculated*	-	-	-

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

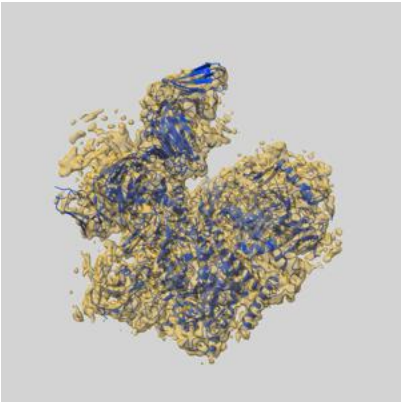
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20605 and PDB model 6U0L. Per-residue inclusion information can be found in section 3 on page 10.

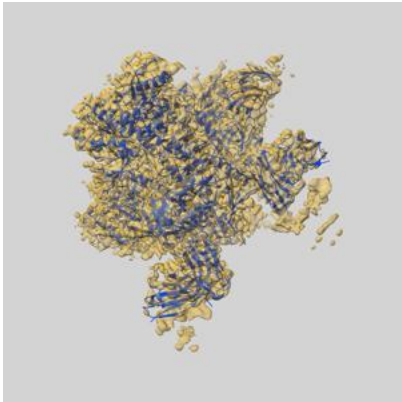
9.1 Map-model overlay (i)



X



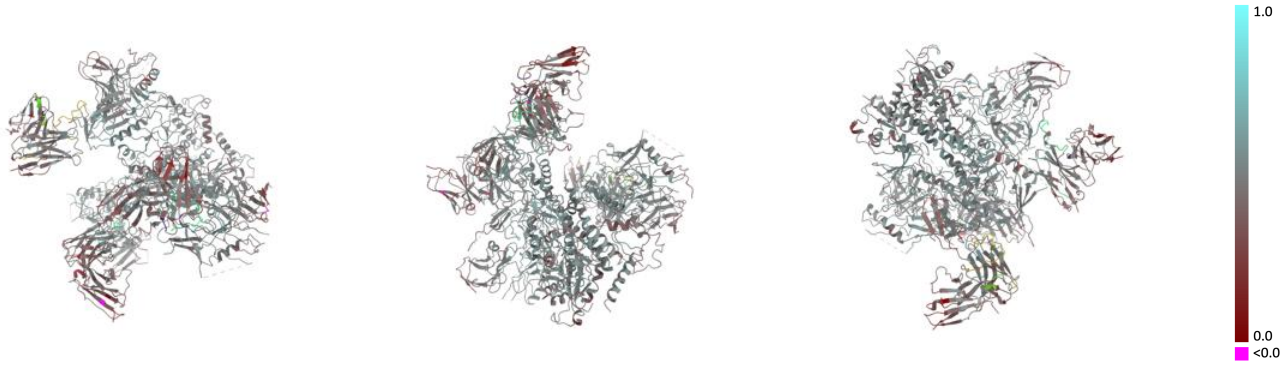
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

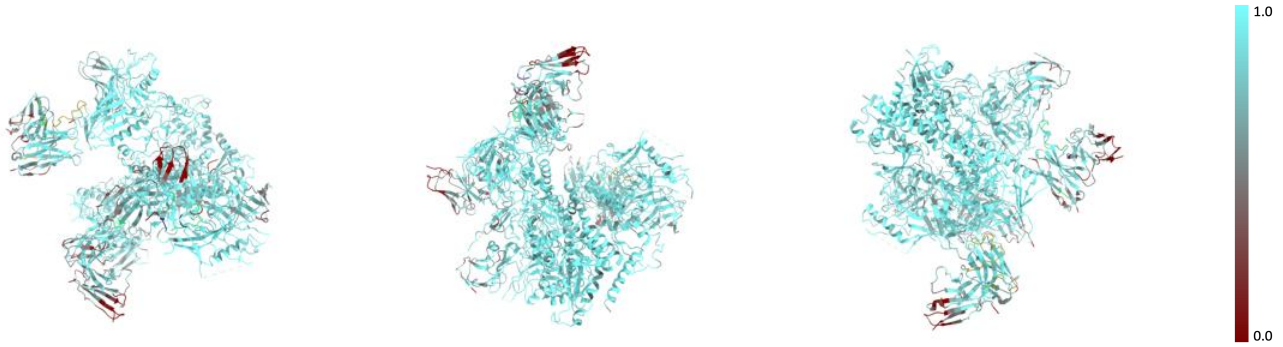
9.2 Q-score mapped to coordinate model (i)



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.

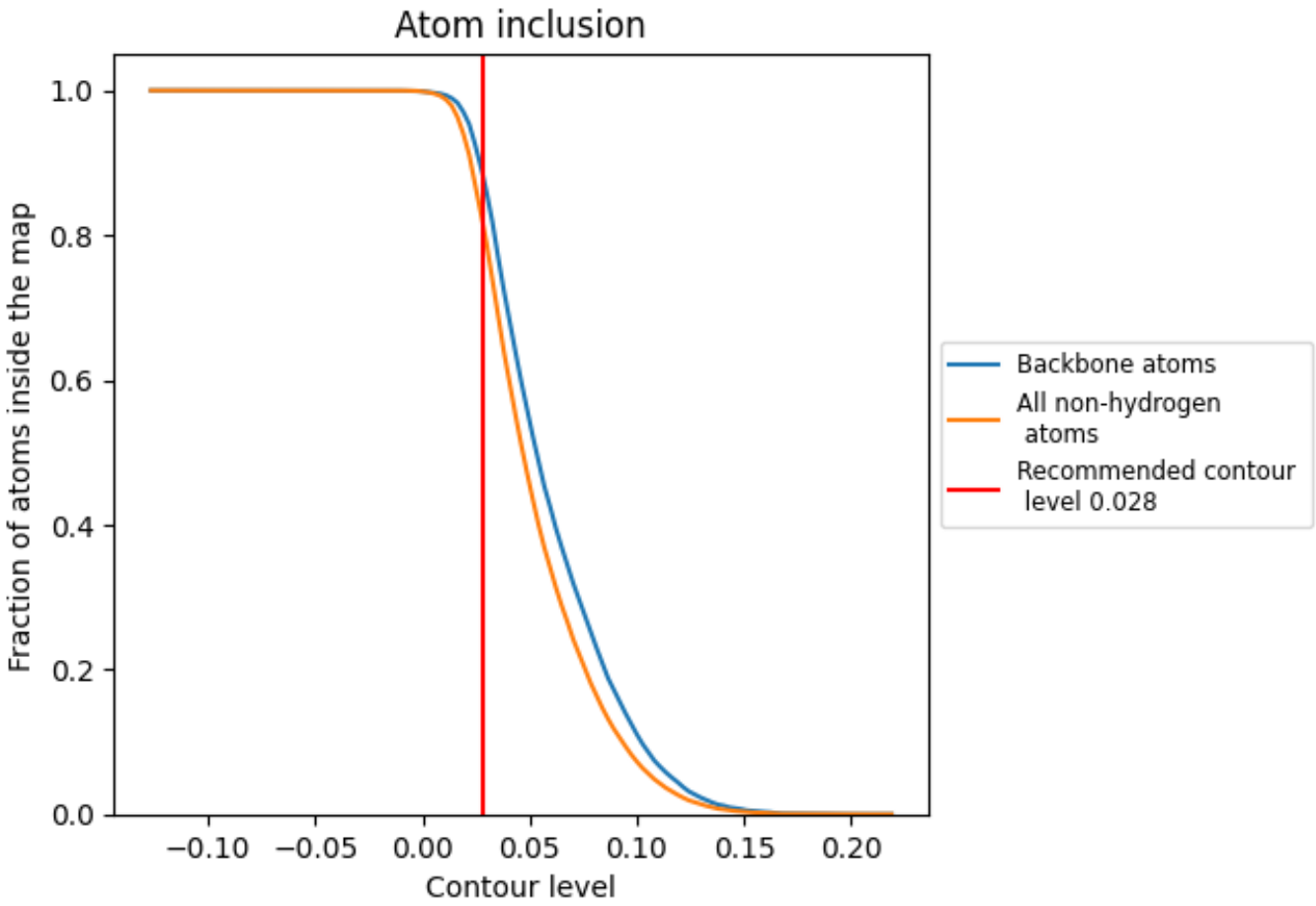
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8198	0.4740
A	0.9111	0.5240
B	0.8841	0.5070
C	0.8989	0.5110
D	0.7375	0.4460
E	0.7177	0.4210
F	0.7916	0.4410
G	0.8929	0.4680
H	0.7717	0.4420
I	0.7417	0.4370
J	0.5709	0.3760
K	1.0000	0.5500
L	0.5620	0.3710
M	0.7500	0.4130
N	0.7857	0.4270
O	0.6867	0.4450
P	0.7913	0.4520
Q	0.6241	0.3950
R	0.6429	0.4180
S	1.0000	0.5590
X	0.8880	0.4920
Y	0.8690	0.4830
Z	0.9048	0.4920