Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 10:21 PM EDT

PDB ID	:	7S0Q
EMDB ID	:	EMD-24791
Title	:	Head region of a complex of IGF-I with the ectodomain of a hybrid insulin receptor / type 1 insulin-like growth factor receptor
Authors	:	Xu, Y.; Lawrence, M.C.
Deposited on	:	2021-08-30
Resolution	:	3.70 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 ⓘ symbol.

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

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

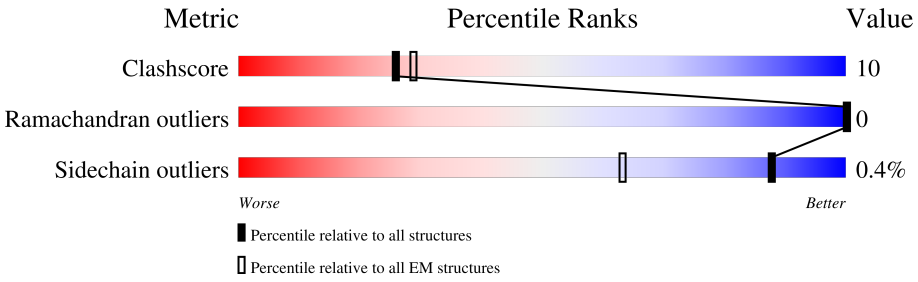
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	952	45% 15% 40%
2	B	961	25% 8% 66%
3	D	70	11% 79% 9% 13%
4	C	3	100%
4	F	3	33% 33% 67%
5	E	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15551 atoms, of which 7660 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	575	9039	2888	4453	789	866	43	0	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	906	ARG	-	expression tag	UNP P08069
A	907	MET	-	expression tag	UNP P08069
A	908	LYS	-	expression tag	UNP P08069
A	909	GLN	-	expression tag	UNP P08069
A	910	LEU	-	expression tag	UNP P08069
A	911	GLU	-	expression tag	UNP P08069
A	912	ASP	-	expression tag	UNP P08069
A	913	LYS	-	expression tag	UNP P08069
A	914	VAL	-	expression tag	UNP P08069
A	915	GLU	-	expression tag	UNP P08069
A	916	GLU	-	expression tag	UNP P08069
A	917	LEU	-	expression tag	UNP P08069
A	918	LEU	-	expression tag	UNP P08069
A	919	SER	-	expression tag	UNP P08069
A	920	LYS	-	expression tag	UNP P08069
A	921	ASN	-	expression tag	UNP P08069
A	922	TYR	-	expression tag	UNP P08069
A	923	HIS	-	expression tag	UNP P08069
A	924	LEU	-	expression tag	UNP P08069
A	925	GLU	-	expression tag	UNP P08069
A	926	ASN	-	expression tag	UNP P08069
A	927	GLU	-	expression tag	UNP P08069
A	928	VAL	-	expression tag	UNP P08069
A	929	ALA	-	expression tag	UNP P08069
A	930	ARG	-	expression tag	UNP P08069
A	931	LEU	-	expression tag	UNP P08069
A	932	LYS	-	expression tag	UNP P08069
A	933	LYS	-	expression tag	UNP P08069

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Chain	Residue	Modelled	Actual	Comment	Reference
A	934	LEU	-	expression tag	UNP P08069
A	935	VAL	-	expression tag	UNP P08069
A	936	GLY	-	expression tag	UNP P08069
A	937	GLU	-	expression tag	UNP P08069
A	938	ARG	-	expression tag	UNP P08069
A	939	SER	-	expression tag	UNP P08069
A	940	SER	-	expression tag	UNP P08069
A	941	SER	-	expression tag	UNP P08069
A	942	GLU	-	expression tag	UNP P08069
A	943	GLN	-	expression tag	UNP P08069
A	944	LYS	-	expression tag	UNP P08069
A	945	LEU	-	expression tag	UNP P08069
A	946	ILE	-	expression tag	UNP P08069
A	947	SER	-	expression tag	UNP P08069
A	948	GLU	-	expression tag	UNP P08069
A	949	GLU	-	expression tag	UNP P08069
A	950	ASP	-	expression tag	UNP P08069
A	951	LEU	-	expression tag	UNP P08069
A	952	ASN	-	expression tag	UNP P08069

- Molecule 2 is a protein called Insulin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	322	Total	C	H	N	O	S	0	0
			5190	1668	2572	449	490	11		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	929	ARG	-	expression tag	UNP P06213
B	930	MET	-	expression tag	UNP P06213
B	931	LYS	-	expression tag	UNP P06213
B	932	GLN	-	expression tag	UNP P06213
B	933	LEU	-	expression tag	UNP P06213
B	934	GLU	-	expression tag	UNP P06213
B	935	ASP	-	expression tag	UNP P06213
B	936	LYS	-	expression tag	UNP P06213
B	937	VAL	-	expression tag	UNP P06213
B	938	GLU	-	expression tag	UNP P06213
B	939	GLU	-	expression tag	UNP P06213
B	940	LEU	-	expression tag	UNP P06213
B	941	LEU	-	expression tag	UNP P06213

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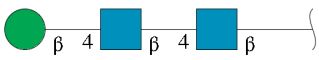
Chain	Residue	Modelled	Actual	Comment	Reference
B	942	SER	-	expression tag	UNP P06213
B	943	LYS	-	expression tag	UNP P06213
B	944	ASN	-	expression tag	UNP P06213
B	945	TYR	-	expression tag	UNP P06213
B	946	HIS	-	expression tag	UNP P06213
B	947	LEU	-	expression tag	UNP P06213
B	948	GLU	-	expression tag	UNP P06213
B	949	ASN	-	expression tag	UNP P06213
B	950	GLU	-	expression tag	UNP P06213
B	951	VAL	-	expression tag	UNP P06213
B	952	ALA	-	expression tag	UNP P06213
B	953	ARG	-	expression tag	UNP P06213
B	954	LEU	-	expression tag	UNP P06213
B	955	LYS	-	expression tag	UNP P06213
B	956	LYS	-	expression tag	UNP P06213
B	957	LEU	-	expression tag	UNP P06213
B	958	VAL	-	expression tag	UNP P06213
B	959	GLY	-	expression tag	UNP P06213
B	960	GLU	-	expression tag	UNP P06213
B	961	ARG	-	expression tag	UNP P06213

- Molecule 3 is a protein called Insulin-like growth factor I.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	61	Total	C	H	N	O	S	0	0
			913	292	441	83	90	7		

- Molecule 4 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.

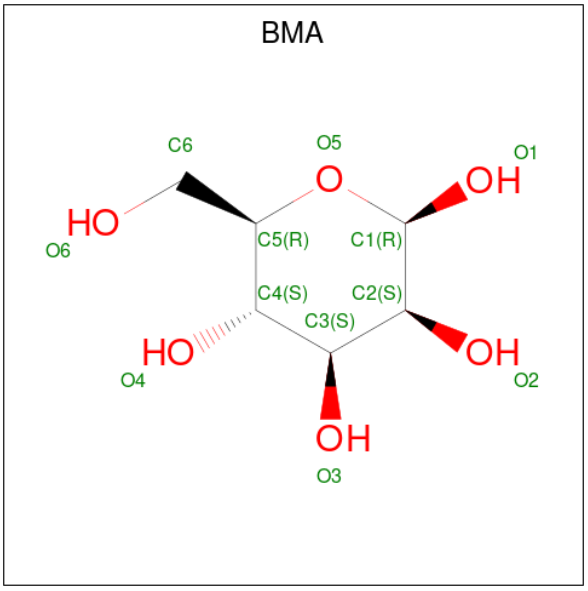


Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
4	F	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

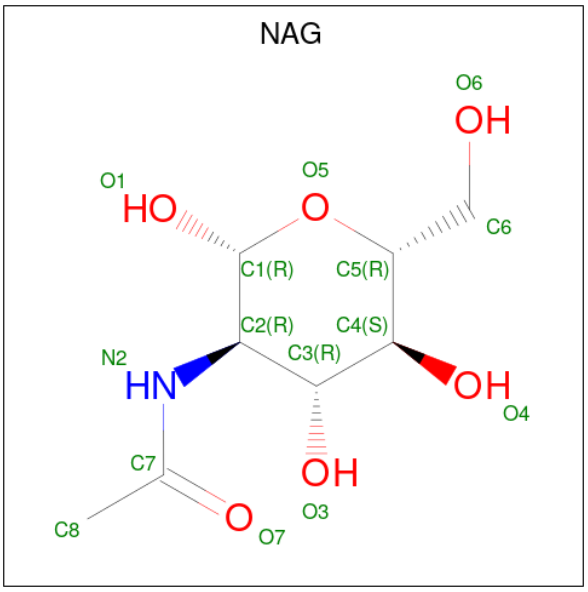
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	H	O	0
			21	6	10	5	

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



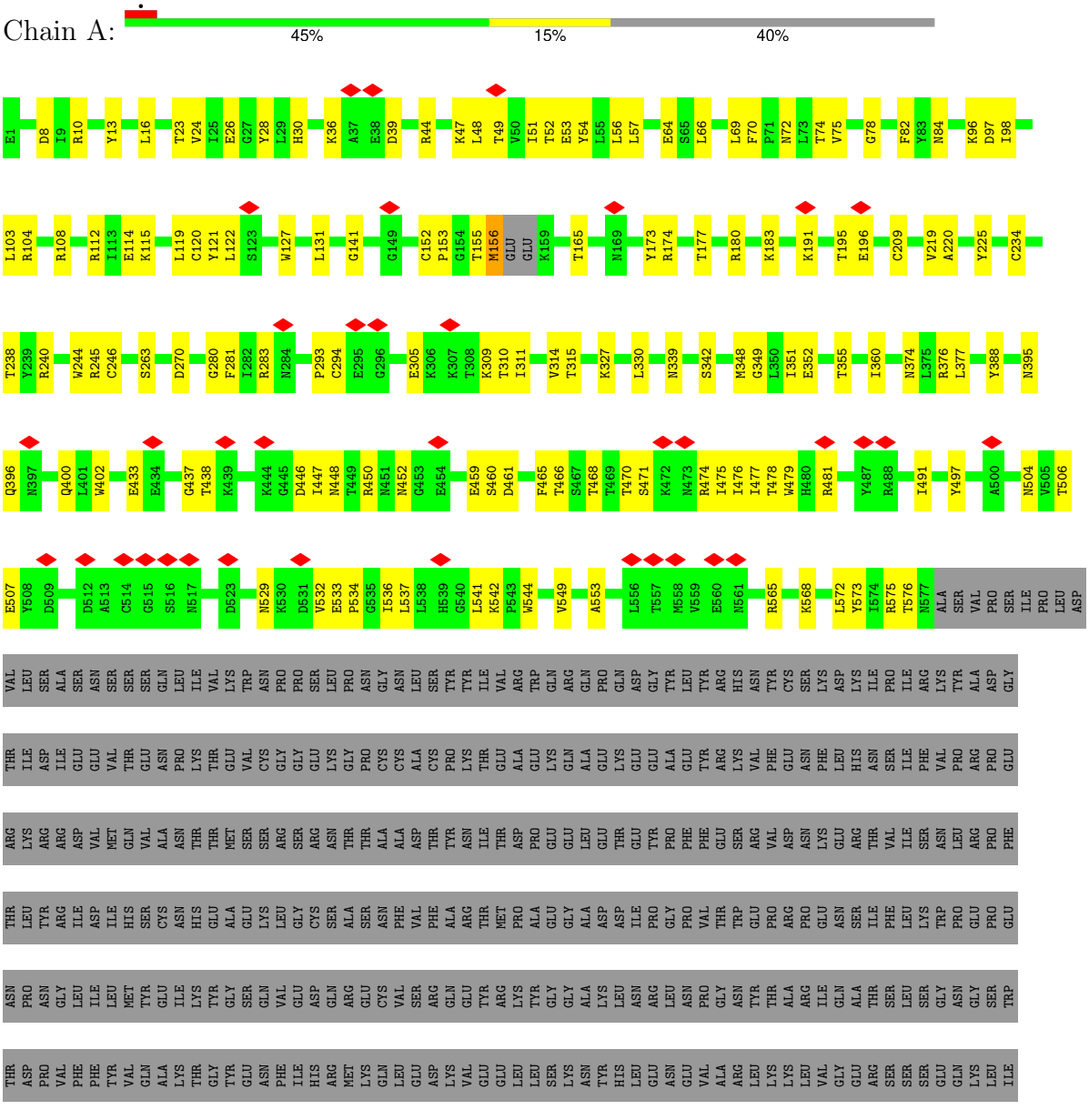
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
7	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

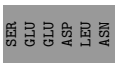
3 Residue-property plots (i)

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: Insulin-like growth factor 1 receptor

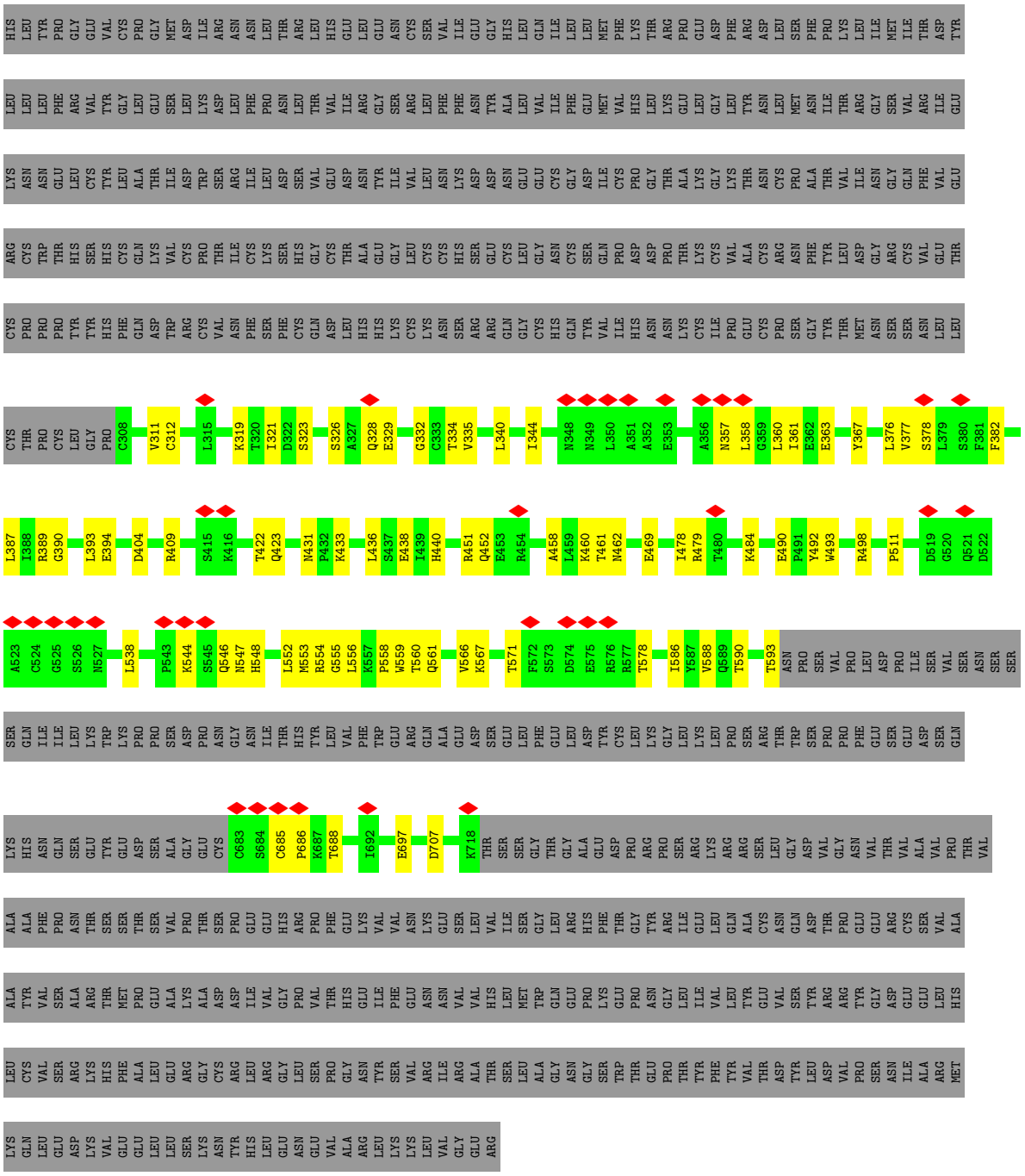
Chain A:





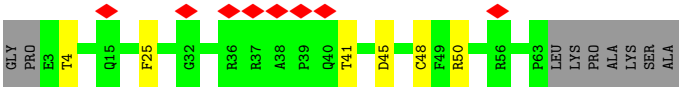
• Molecule 2: Insulin receptor

Chain B:



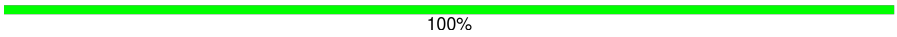
• Molecule 3: Insulin-like growth factor I

Chain D:



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

Chain C:



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

Chain F:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.061	Depositor
Minimum map value	-0.141	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.1529	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/4686	0.44	0/6351
2	B	0.26	0/2678	0.42	0/3622
3	D	0.27	0/481	0.40	0/647
All	All	0.27	0/7845	0.43	0/10620

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

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	4586	4453	4453	101	0
2	B	2618	2572	2572	53	0
3	D	472	441	441	4	0
4	C	39	34	34	0	0
4	F	39	34	34	1	0
5	E	28	25	25	1	0
6	A	11	10	10	1	0
7	A	56	52	52	1	0
7	B	42	39	39	1	0
All	All	7891	7660	7660	155	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 10.

All (155) 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:A:155:THR:OG1	1:A:156:MET:SD	2.31	0.87
1:A:23:THR:OG1	1:A:47:LYS:O	1.93	0.86
1:A:240:ARG:NH2	1:A:270:ASP:O	2.09	0.84
1:A:238:THR:OG1	1:A:246:CYS:SG	2.34	0.83
2:B:458:ALA:O	2:B:462:ASN:ND2	2.13	0.81
1:A:470:THR:HG22	1:A:475:ILE:HD12	1.63	0.81
1:A:36:LYS:NZ	1:A:39:ASP:OD2	2.17	0.77
2:B:389:ARG:O	2:B:423:GLN:NE2	2.17	0.77
2:B:498:ARG:NH2	2:B:707:ASP:OD1	2.17	0.76
3:D:41:THR:OG1	3:D:45:ASP:OD2	2.03	0.76
2:B:560:THR:N	2:B:590:THR:OG1	2.19	0.75
1:A:400:GLN:NE2	1:A:402:TRP:O	2.19	0.74
1:A:78:GLY:O	1:A:108:ARG:NH1	2.21	0.74
2:B:571:THR:O	2:B:578:THR:OG1	2.06	0.74
1:A:448:ASN:OD1	1:A:452:ASN:ND2	2.21	0.74
1:A:544:TRP:O	1:A:575:ARG:NH2	2.20	0.73
1:A:474:ARG:HA	1:A:541:LEU:HD13	1.70	0.73
1:A:450:ARG:NE	2:B:404:ASP:OD1	2.22	0.73
1:A:479:TRP:HZ3	1:A:536:ILE:HG22	1.53	0.72
2:B:559:TRP:N	2:B:590:THR:OG1	2.22	0.72
4:F:1:NAG:O6	4:F:2:NAG:O7	2.05	0.72
1:A:28:TYR:N	1:A:53:GLU:OE1	2.23	0.72
1:A:119:LEU:HG	1:A:122:LEU:HD11	1.72	0.70
1:A:470:THR:HB	1:A:576:THR:HG22	1.73	0.70
1:A:84:ASN:OD1	1:A:314:VAL:N	2.26	0.69
1:A:460:SER:OG	1:A:568:LYS:N	2.25	0.69
1:A:24:VAL:HG11	1:A:244:TRP:CH2	2.27	0.69
2:B:321:ILE:HD12	2:B:340:LEU:HD22	1.73	0.69
1:A:542:LYS:O	1:A:576:THR:OG1	2.10	0.68
2:B:452:GLN:OE1	2:B:452:GLN:N	2.27	0.67
2:B:493:TRP:NE1	2:B:546:GLN:OE1	2.28	0.66
2:B:323:SER:O	2:B:326:SER:OG	2.11	0.66
3:D:45:ASP:O	3:D:50:ARG:NH1	2.29	0.65
1:A:481:ARG:NH1	1:A:532:VAL:O	2.30	0.64
2:B:367:TYR:HB3	2:B:393:LEU:HD23	1.79	0.64
1:A:479:TRP:CZ3	1:A:536:ILE:HG22	2.33	0.64
2:B:460:LYS:O	2:B:462:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:LEU:O	2:B:440:HIS:ND1	2.31	0.63
1:A:360:ILE:HG22	1:A:395:ASN:OD1	2.00	0.62
2:B:558:PRO:CB	2:B:593:THR:HG22	2.30	0.62
1:A:461:ASP:O	1:A:568:LYS:N	2.32	0.62
6:A:1001:BMA:O5	5:E:2:NAG:O4	2.18	0.61
1:A:44:ARG:HA	1:A:69:LEU:HD12	1.83	0.60
1:A:468:THR:HG22	1:A:477:ILE:HG13	1.84	0.60
1:A:474:ARG:HB3	1:A:537:LEU:HD11	1.82	0.60
1:A:127:TRP:O	1:A:131:LEU:N	2.35	0.59
1:A:66:LEU:HD11	1:A:70:PHE:CD2	2.37	0.59
1:A:305:GLU:N	1:A:305:GLU:OE1	2.35	0.58
2:B:553:MET:HG3	2:B:556:LEU:HD11	1.85	0.58
1:A:450:ARG:NH2	2:B:404:ASP:OD2	2.35	0.58
2:B:319:LYS:NZ	2:B:329:GLU:OE1	2.34	0.58
1:A:470:THR:HG22	1:A:475:ILE:CD1	2.31	0.58
1:A:507:GLU:N	1:A:507:GLU:OE1	2.37	0.58
1:A:97:ASP:OD1	1:A:98:ILE:N	2.38	0.57
1:A:82:PHE:O	1:A:315:THR:HG21	2.04	0.57
1:A:30:HIS:NE2	1:A:54:TYR:OH	2.33	0.56
1:A:196:GLU:OE1	1:A:196:GLU:N	2.37	0.56
2:B:390:GLY:HA2	2:B:393:LEU:HD21	1.87	0.56
1:A:48:LEU:HD23	1:A:70:PHE:CD1	2.40	0.56
1:A:471:SER:OG	1:A:474:ARG:N	2.38	0.56
1:A:388:TYR:OH	2:B:460:LYS:NZ	2.39	0.55
2:B:484:LYS:HB3	2:B:552:LEU:HD11	1.87	0.55
1:A:173:TYR:O	1:A:174:ARG:NE	2.39	0.55
2:B:332:GLY:HA2	2:B:360:LEU:HD12	1.89	0.54
1:A:52:THR:HG21	1:A:244:TRP:NE1	2.23	0.54
1:A:311:ILE:HD12	1:A:330:LEU:HD11	1.90	0.54
1:A:352:GLU:OE1	1:A:376:ARG:NE	2.41	0.54
2:B:552:LEU:O	2:B:554:ARG:NH1	2.41	0.53
2:B:328:GLN:NE2	2:B:357:ASN:OD1	2.43	0.52
1:A:219:VAL:O	1:A:225:TYR:OH	2.27	0.52
1:A:165:THR:O	1:A:174:ARG:NH1	2.43	0.51
1:A:52:THR:HG21	1:A:244:TRP:CE2	2.46	0.51
1:A:26:GLU:OE2	1:A:245:ARG:NE	2.43	0.51
1:A:23:THR:HG23	1:A:24:VAL:HG23	1.93	0.50
1:A:327:LYS:HA	1:A:355:THR:HG22	1.94	0.50
3:D:4:THR:OG1	3:D:48:CYS:O	2.30	0.50
2:B:688:THR:HG23	2:B:688:THR:O	2.12	0.49
1:A:497:TYR:HB2	1:A:549:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:OD1	1:A:342:SER:OG	2.31	0.49
2:B:363:GLU:OE2	2:B:387:LEU:HD23	2.13	0.48
1:A:120:CYS:O	1:A:121:TYR:HB2	2.14	0.48
1:A:476:ILE:HG13	1:A:537:LEU:HD13	1.96	0.48
2:B:438:GLU:OE1	2:B:438:GLU:N	2.44	0.48
1:A:112:ARG:NE	1:A:114:GLU:OE2	2.38	0.48
1:A:396:GLN:NE2	2:B:697:GLU:OE2	2.47	0.47
1:A:465:PHE:CE1	1:A:477:ILE:HD11	2.49	0.47
1:A:572:LEU:HD12	1:A:573:TYR:N	2.29	0.47
2:B:511:PRO:O	2:B:561:GLN:NE2	2.48	0.47
2:B:593:THR:O	2:B:593:THR:HG23	2.14	0.47
1:A:305:GLU:OE1	1:A:309:LYS:NZ	2.43	0.47
2:B:431:ASN:N	2:B:461:THR:O	2.47	0.47
1:A:195:THR:HG22	1:A:209:CYS:O	2.15	0.47
1:A:104:ARG:NH2	1:A:183:LYS:O	2.47	0.47
2:B:319:LYS:HE3	2:B:321:ILE:HD11	1.97	0.46
2:B:538:LEU:H	2:B:538:LEU:HD23	1.79	0.46
1:A:339:ASN:O	1:A:342:SER:OG	2.33	0.46
2:B:566:VAL:HG22	2:B:567:LYS:N	2.31	0.46
1:A:47:LYS:O	1:A:49:THR:HG23	2.16	0.46
1:A:8:ASP:OD1	1:A:8:ASP:N	2.48	0.46
1:A:115:LYS:N	1:A:141:GLY:O	2.36	0.46
2:B:344:ILE:HG21	2:B:376:LEU:HD21	1.97	0.46
1:A:156:MET:SD	1:A:156:MET:N	2.89	0.46
2:B:358:LEU:HB3	2:B:361:ILE:HD12	1.97	0.46
1:A:466:THR:OG1	1:A:478:THR:O	2.35	0.45
1:A:82:PHE:C	1:A:315:THR:HG21	2.37	0.45
2:B:358:LEU:HD23	2:B:382:PHE:HE1	1.81	0.45
1:A:152:CYS:HB2	1:A:153:PRO:HD2	1.98	0.45
1:A:433:GLU:O	1:A:437:GLY:N	2.47	0.45
2:B:311:VAL:HG12	2:B:312:CYS:H	1.83	0.44
2:B:558:PRO:HB3	2:B:593:THR:HG22	2.00	0.44
1:A:504:ASN:OD1	7:A:1004:NAG:N2	2.50	0.44
1:A:466:THR:OG1	1:A:533:GLU:OE2	2.13	0.44
2:B:311:VAL:HG12	2:B:312:CYS:N	2.33	0.44
1:A:75:VAL:HG21	1:A:220:ALA:CB	2.47	0.44
2:B:555:GLY:C	2:B:556:LEU:HD12	2.38	0.44
1:A:348:MET:HB3	1:A:351:ILE:HD12	1.99	0.43
1:A:376:ARG:NH1	1:A:377:LEU:HD12	2.32	0.43
1:A:51:ILE:HG22	1:A:52:THR:N	2.34	0.43
1:A:497:TYR:CB	1:A:549:VAL:HG12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NH1	3:D:25:PHE:HB2	2.34	0.43
2:B:685:CYS:N	2:B:686:PRO:HD2	2.34	0.43
1:A:281:PHE:N	1:A:294:CYS:SG	2.92	0.43
1:A:529:ASN:HB3	1:A:532:VAL:HG12	2.00	0.43
1:A:120:CYS:C	1:A:122:LEU:HD12	2.40	0.43
1:A:177:THR:OG1	1:A:180:ARG:N	2.44	0.42
1:A:506:THR:OG1	1:A:507:GLU:N	2.51	0.42
2:B:422:THR:O	2:B:451:ARG:NH2	2.52	0.42
1:A:74:THR:O	1:A:103:LEU:HD12	2.20	0.42
1:A:349:GLY:O	1:A:374:ASN:ND2	2.43	0.42
2:B:394:GLU:O	7:B:1002:NAG:H81	2.20	0.42
1:A:122:LEU:HD12	1:A:122:LEU:N	2.35	0.42
1:A:64:GLU:O	1:A:96:LYS:N	2.43	0.42
2:B:484:LYS:CB	2:B:552:LEU:HD11	2.50	0.42
1:A:234:CYS:SG	1:A:238:THR:OG1	2.77	0.41
1:A:310:THR:O	1:A:310:THR:HG23	2.20	0.41
1:A:459:GLU:OE2	1:A:565:ARG:NH2	2.53	0.41
2:B:469:GLU:OE1	2:B:469:GLU:N	2.50	0.41
1:A:49:THR:HG22	1:A:72:ASN:ND2	2.34	0.41
1:A:446:ASP:OD1	1:A:447:ILE:N	2.46	0.41
1:A:481:ARG:HG2	1:A:534:PRO:HD3	2.03	0.41
2:B:334:THR:OG1	2:B:335:VAL:N	2.53	0.41
2:B:490:GLU:OE1	2:B:492:TYR:N	2.54	0.41
1:A:56:LEU:HD12	1:A:57:LEU:N	2.36	0.41
2:B:547:ASN:OD1	2:B:548:HIS:N	2.54	0.41
1:A:438:THR:O	1:A:438:THR:HG22	2.20	0.41
1:A:541:LEU:N	1:A:541:LEU:HD12	2.36	0.41
2:B:478:ILE:HG22	2:B:479:ARG:N	2.36	0.41
1:A:280:GLY:O	1:A:293:PRO:HA	2.21	0.41
1:A:263:SER:OG	1:A:283:ARG:NH1	2.55	0.40
2:B:377:VAL:HG13	2:B:378:SER:N	2.37	0.40
2:B:586:ILE:HG22	2:B:588:VAL:HG23	2.03	0.40
2:B:409:ARG:HD2	2:B:433:LYS:HB3	2.03	0.40
1:A:13:TYR:HD1	1:A:16:LEU:HD11	1.87	0.40
1:A:475:ILE:O	1:A:475:ILE:HG23	2.21	0.40
1:A:491:ILE:HD11	1:A:553:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/952 (60%)	513 (90%)	58 (10%)	0	100	100
2	B	318/961 (33%)	287 (90%)	31 (10%)	0	100	100
3	D	59/70 (84%)	54 (92%)	5 (8%)	0	100	100
All	All	948/1983 (48%)	854 (90%)	94 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	513/852 (60%)	511 (100%)	2 (0%)	89	93
2	B	290/870 (33%)	289 (100%)	1 (0%)	91	94
3	D	51/57 (90%)	51 (100%)	0	100	100
All	All	854/1779 (48%)	851 (100%)	3 (0%)	88	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	MET
1	A	191	LYS
2	B	544	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	223	HIS
1	A	254	ASN
1	A	275	GLN
1	A	287	GLN
1	A	338	ASN
2	B	328	GLN
2	B	348	ASN
2	B	561	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1	4,1	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	C	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	BMA	C	3	4	11,11,12	0.69	0	15,15,17	0.86	0
5	NAG	E	1	5,1	14,14,15	0.16	0	17,19,21	0.47	0
5	NAG	E	2	5	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	F	1	4,1	14,14,15	0.17	0	17,19,21	0.52	0
4	NAG	F	2	4	14,14,15	0.17	0	17,19,21	0.48	0
4	BMA	F	3	4	11,11,12	0.53	0	15,15,17	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6

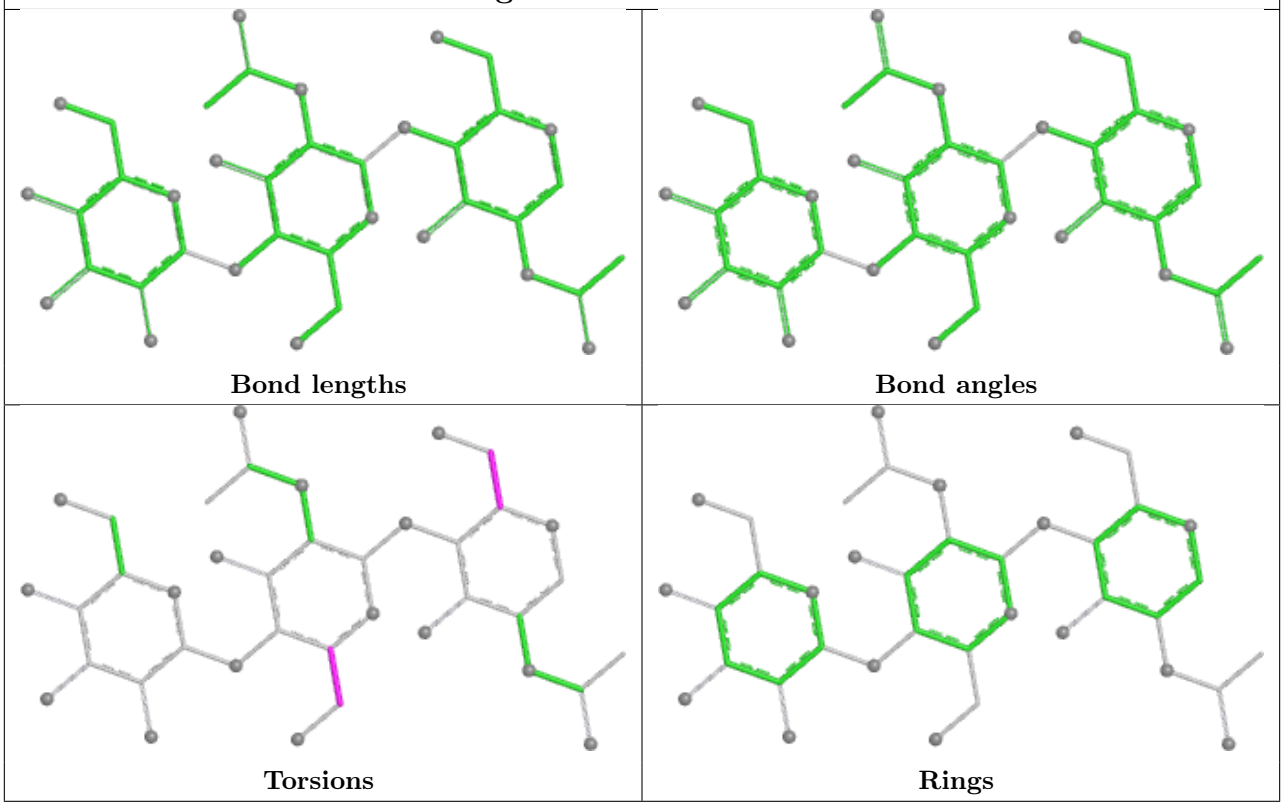
There are no ring outliers.

3 monomers are involved in 2 short contacts:

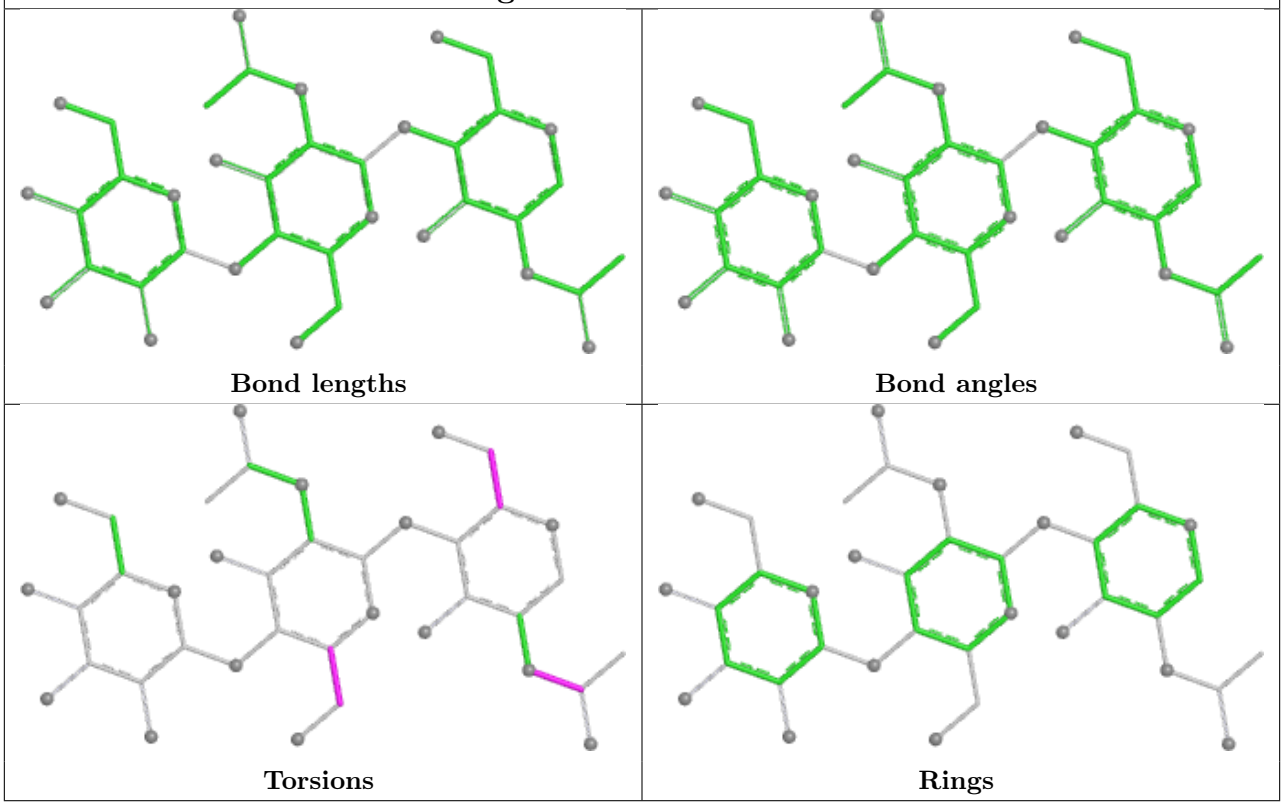
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	F	1	NAG	1	0
5	E	2	NAG	1	0

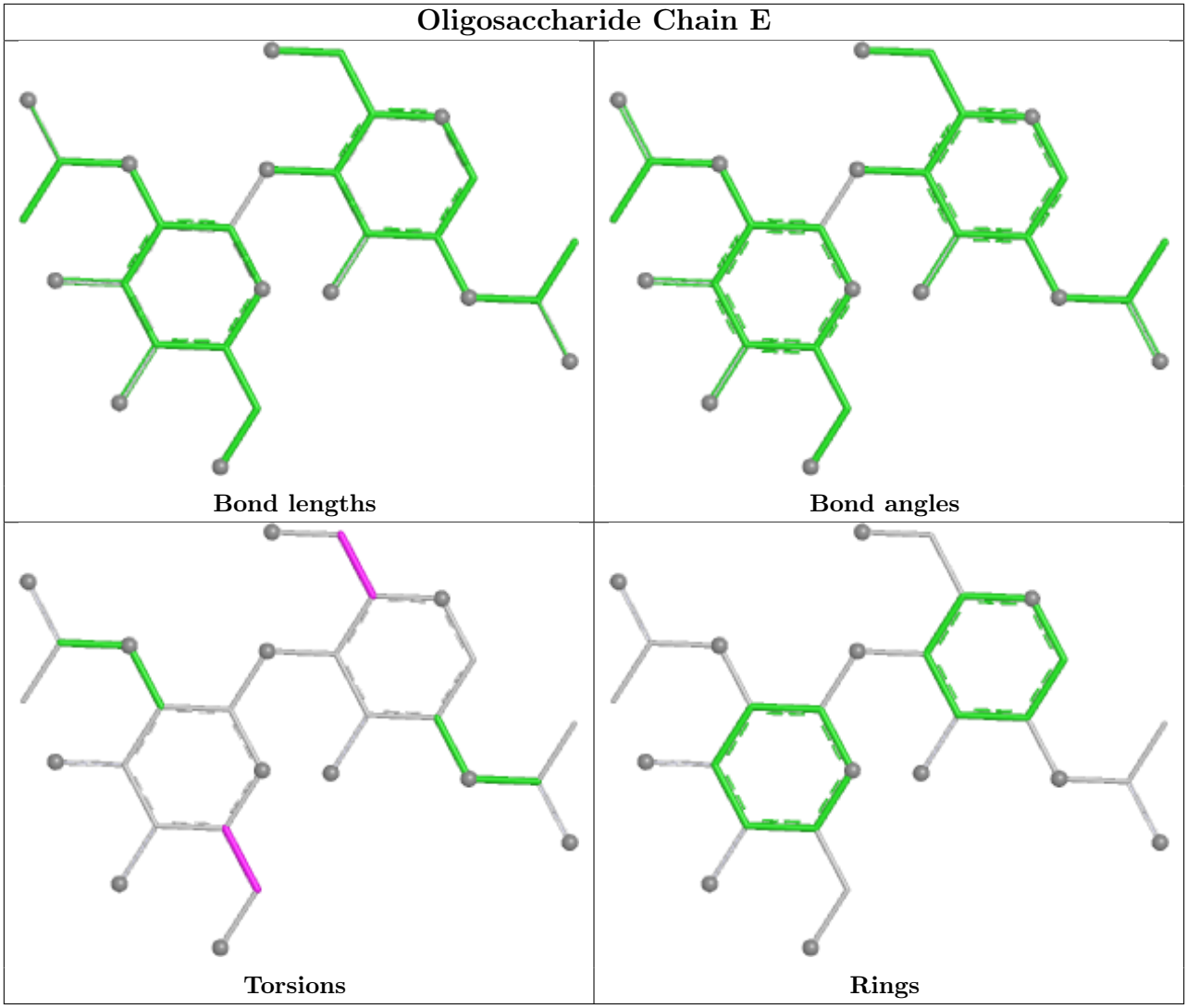
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain F





5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
7	NAG	B	1001	2	14,14,15	0.18	0	17,19,21	0.41	0
7	NAG	A	1005	1	14,14,15	0.17	0	17,19,21	0.43	0
6	BMA	A	1001	-	11,11,12	0.54	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	1004	1	14,14,15	0.28	0	17,19,21	0.46	0
7	NAG	A	1003	1	14,14,15	0.19	0	17,19,21	0.47	0
7	NAG	B	1003	2	14,14,15	0.22	0	17,19,21	0.53	0
7	NAG	B	1002	2	14,14,15	0.16	0	17,19,21	0.42	0
7	NAG	A	1002	1	14,14,15	0.53	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
7	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
6	BMA	A	1001	-	-	0/2/19/22	0/1/1/1
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
7	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1005	NAG	C4-C5-C6-O6
7	A	1002	NAG	O5-C5-C6-O6
7	A	1005	NAG	O5-C5-C6-O6
7	A	1002	NAG	C4-C5-C6-O6
7	B	1002	NAG	C4-C5-C6-O6
7	A	1002	NAG	C8-C7-N2-C2
7	A	1002	NAG	O7-C7-N2-C2
7	B	1002	NAG	O5-C5-C6-O6
7	B	1001	NAG	C4-C5-C6-O6
7	B	1001	NAG	O5-C5-C6-O6

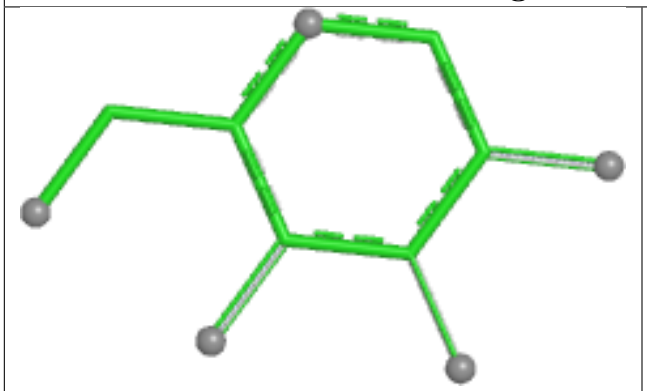
There are no ring outliers.

3 monomers are involved in 3 short contacts:

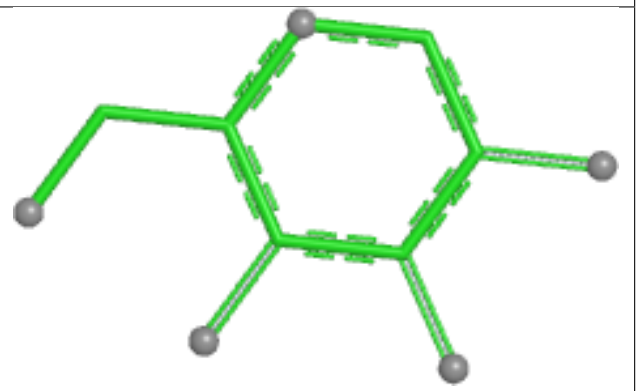
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	BMA	1	0
7	A	1004	NAG	1	0
7	B	1002	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

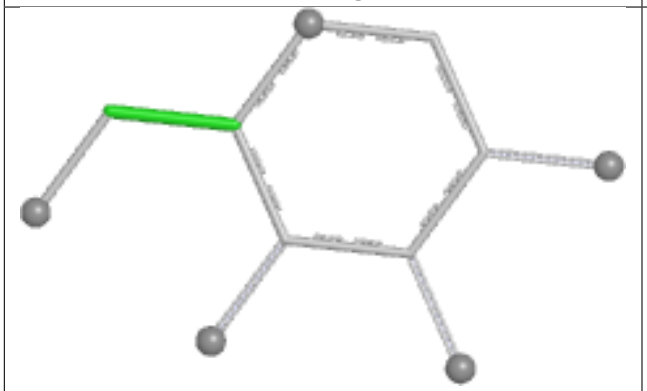
Ligand BMA A 1001



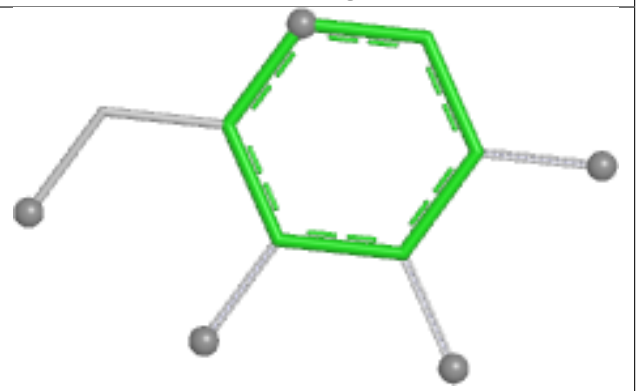
Bond lengths



Bond angles



Torsions



Rings

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.

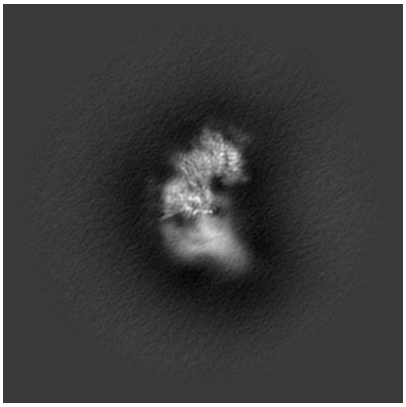
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24791. These allow visual inspection of the internal detail of the map and identification of artifacts.

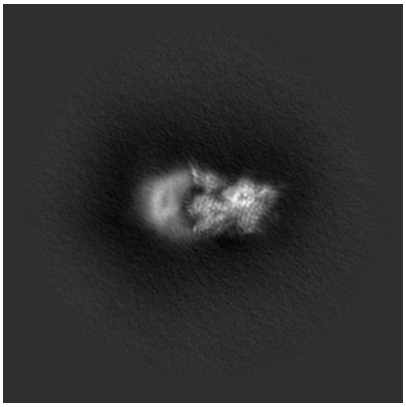
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

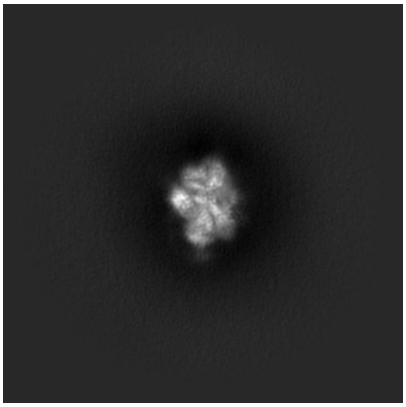
6.1.1 Primary map



X



Y

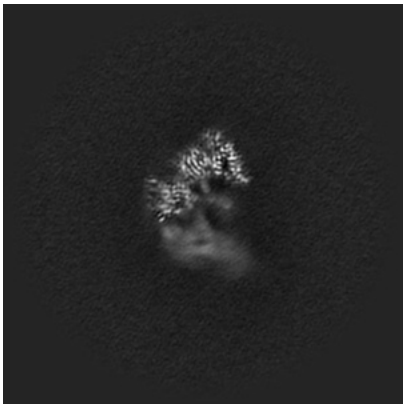


Z

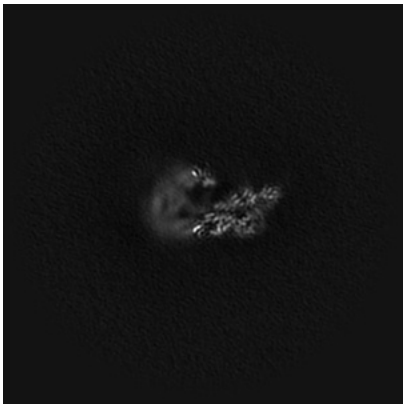
The images above show the map projected in three orthogonal directions.

6.2 Central slices

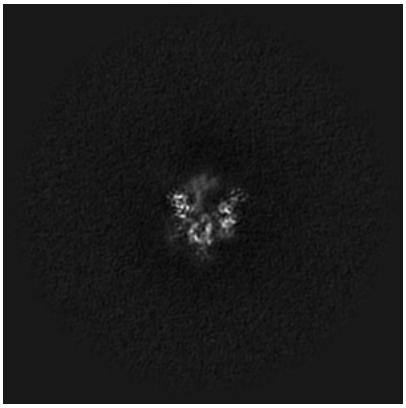
6.2.1 Primary map



X Index: 200



Y Index: 200

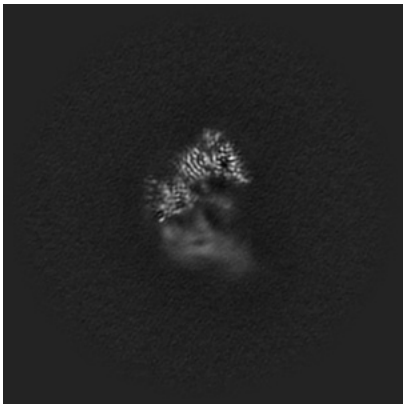


Z Index: 200

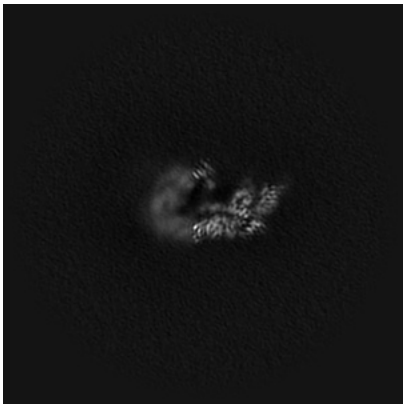
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

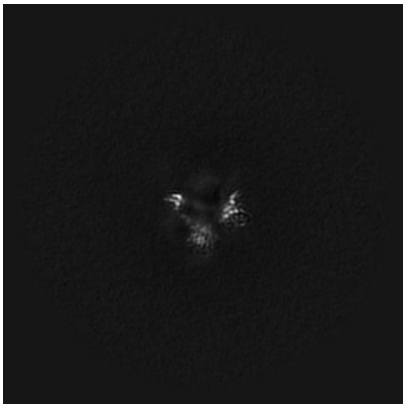
6.3.1 Primary map



X Index: 201



Y Index: 205

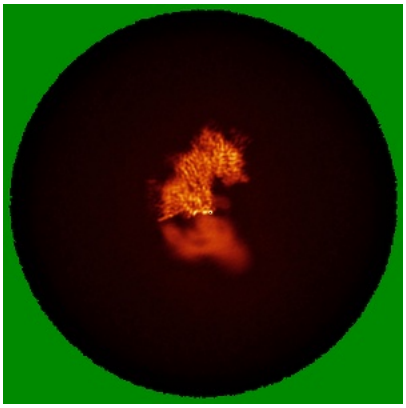


Z Index: 192

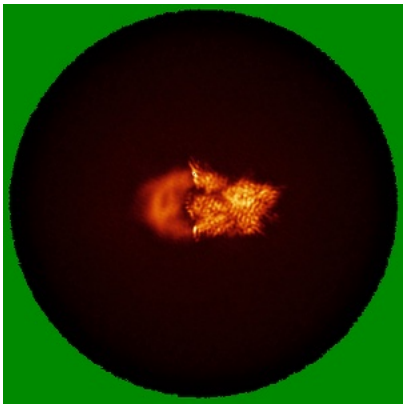
The images above show the largest variance slices of the map in three orthogonal directions.

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

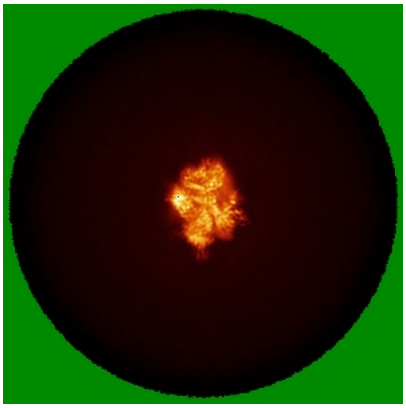
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1529. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

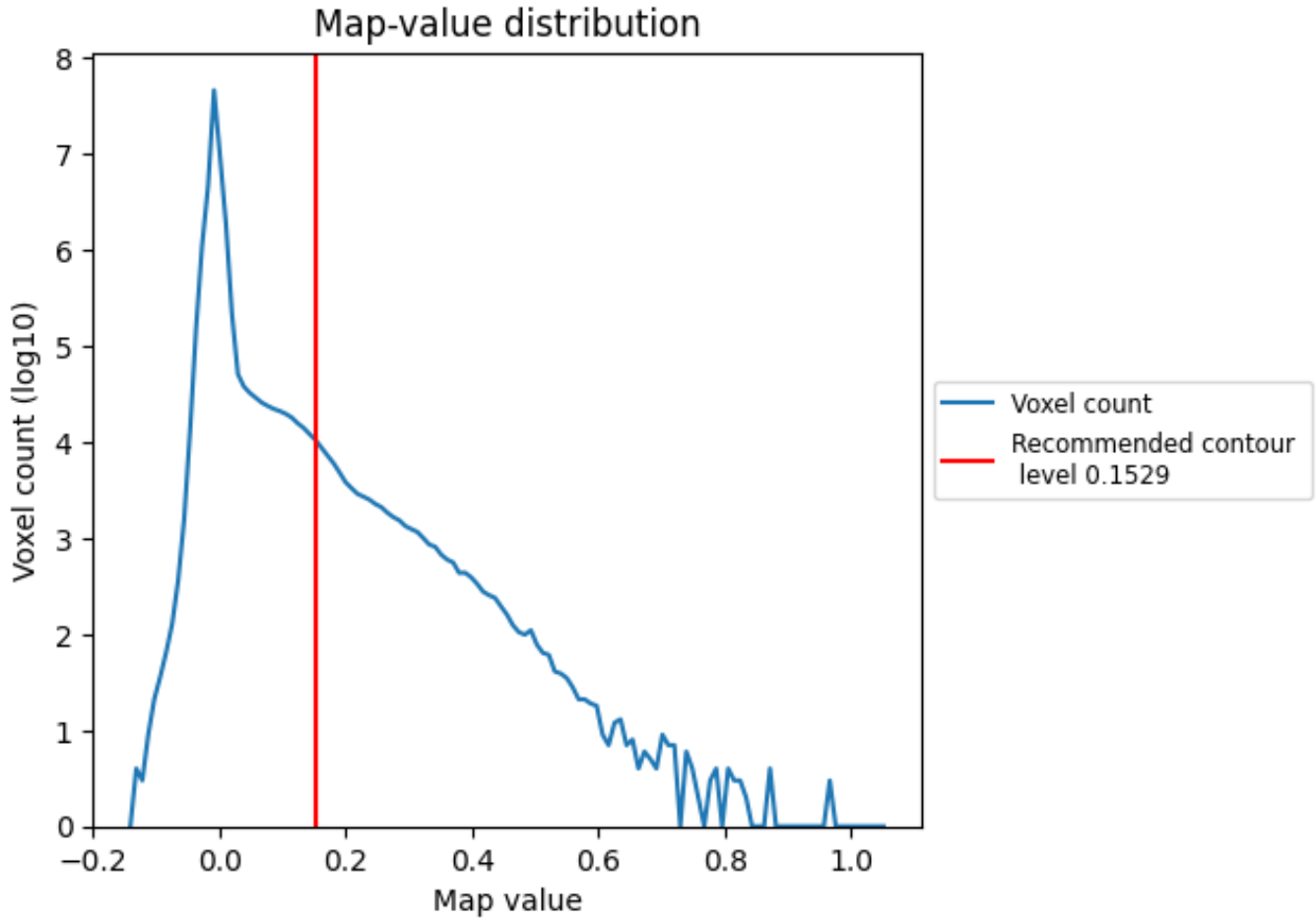
6.6 Mask visualisation (i)

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

7 Map analysis

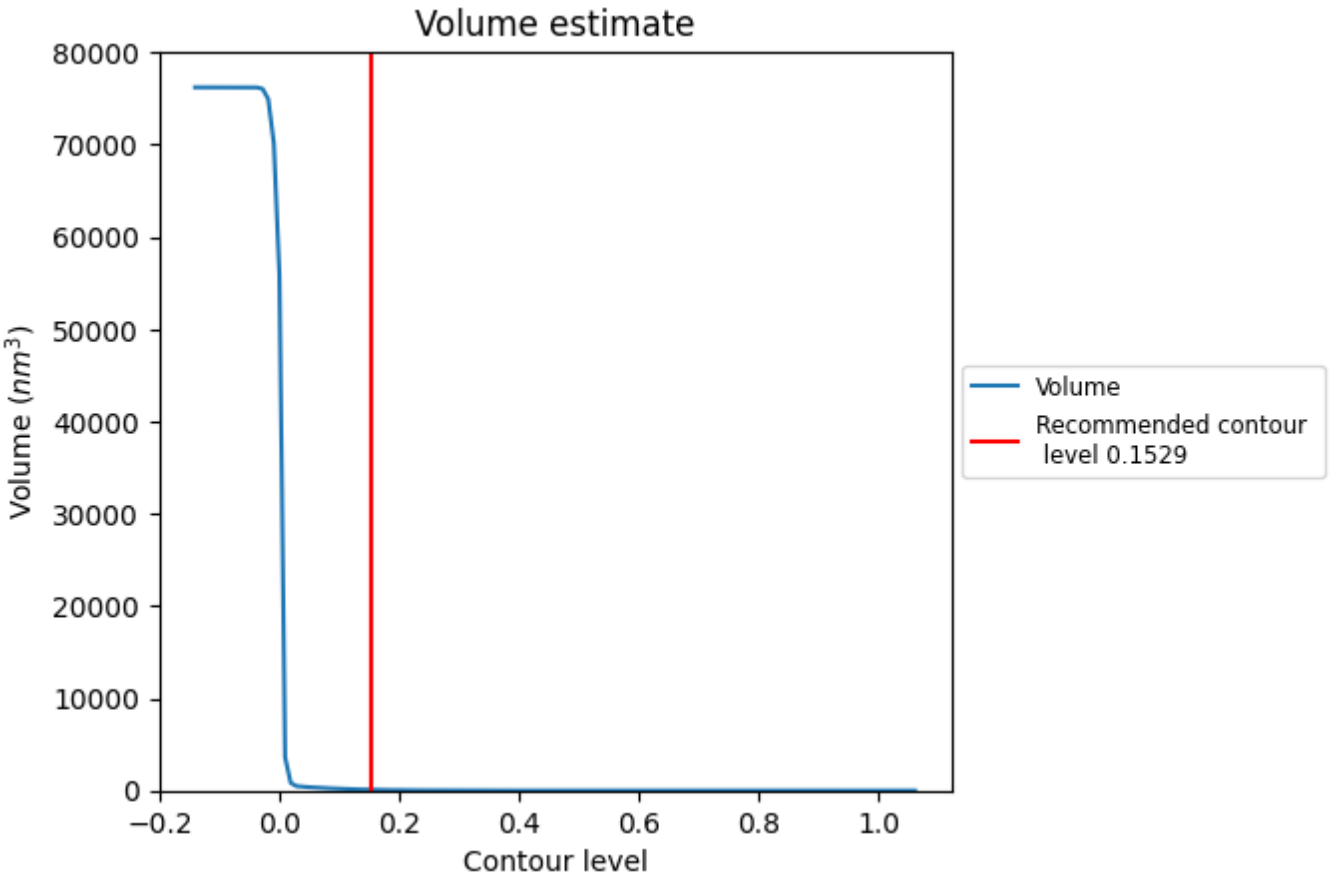
This section contains the results of statistical analysis of the map.

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.

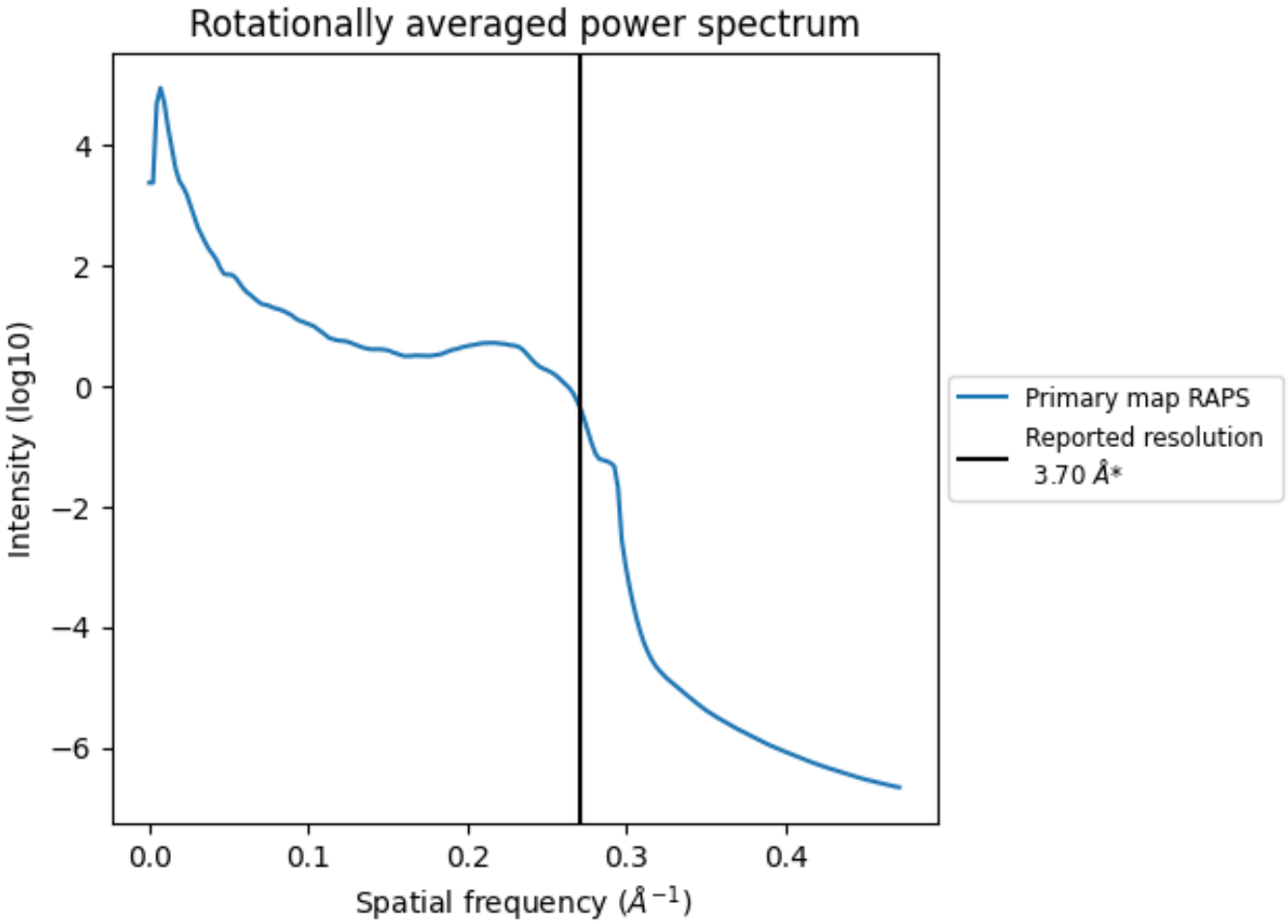
7.2 Volume estimate



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 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 0.270 Å^{-1}

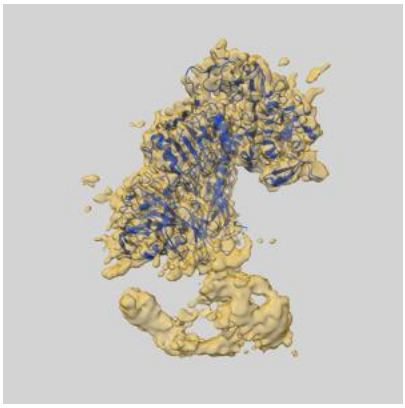
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

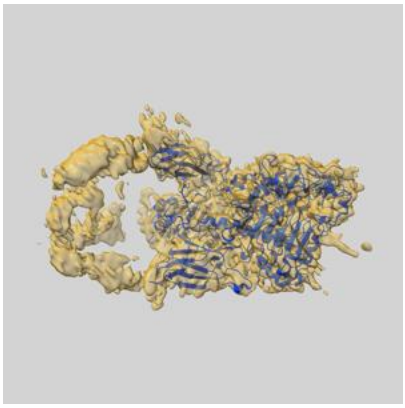
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24791 and PDB model 7S0Q. Per-residue inclusion information can be found in section 3 on page 8.

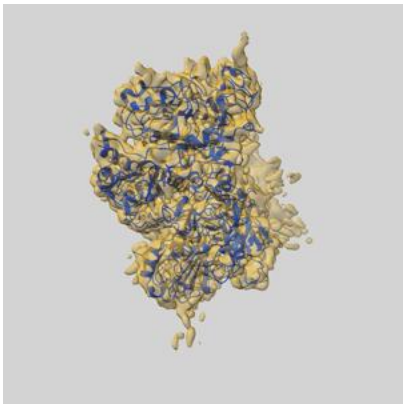
9.1 Map-model overlay



X



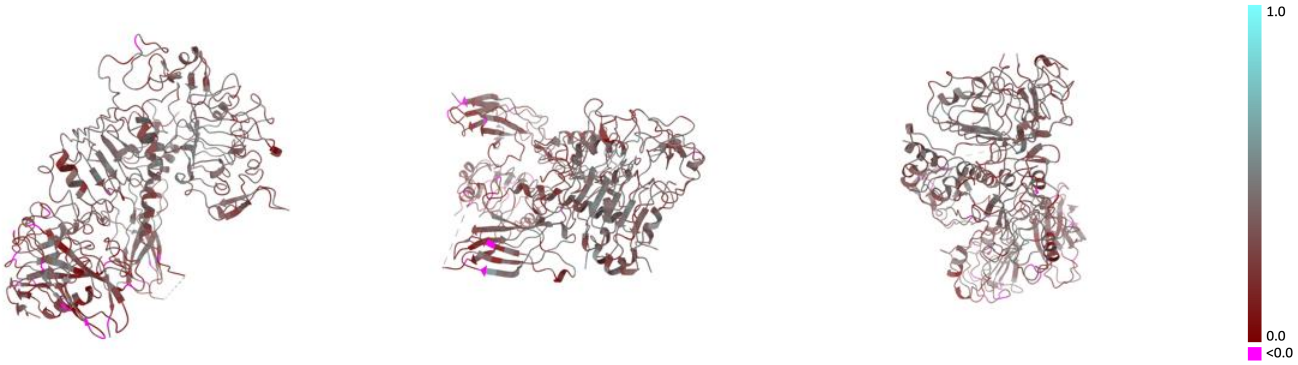
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1529 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.

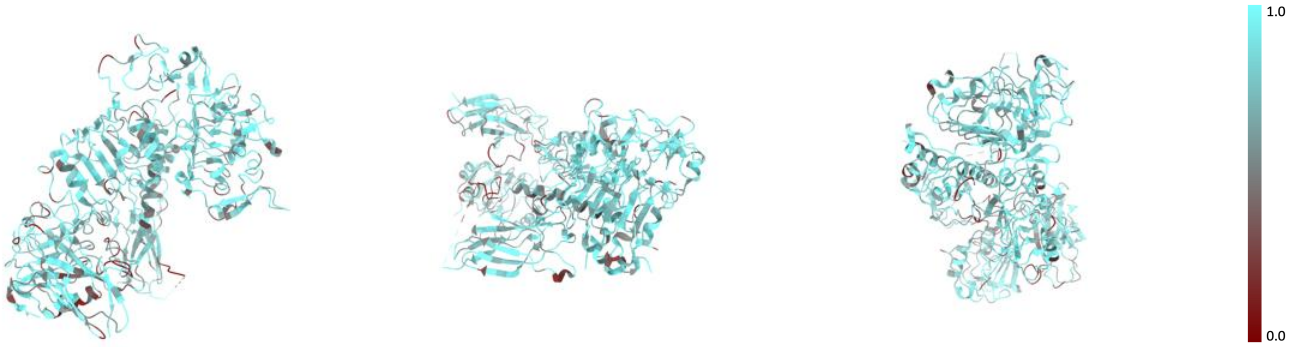
9.2 Q-score mapped to coordinate model (i)



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.

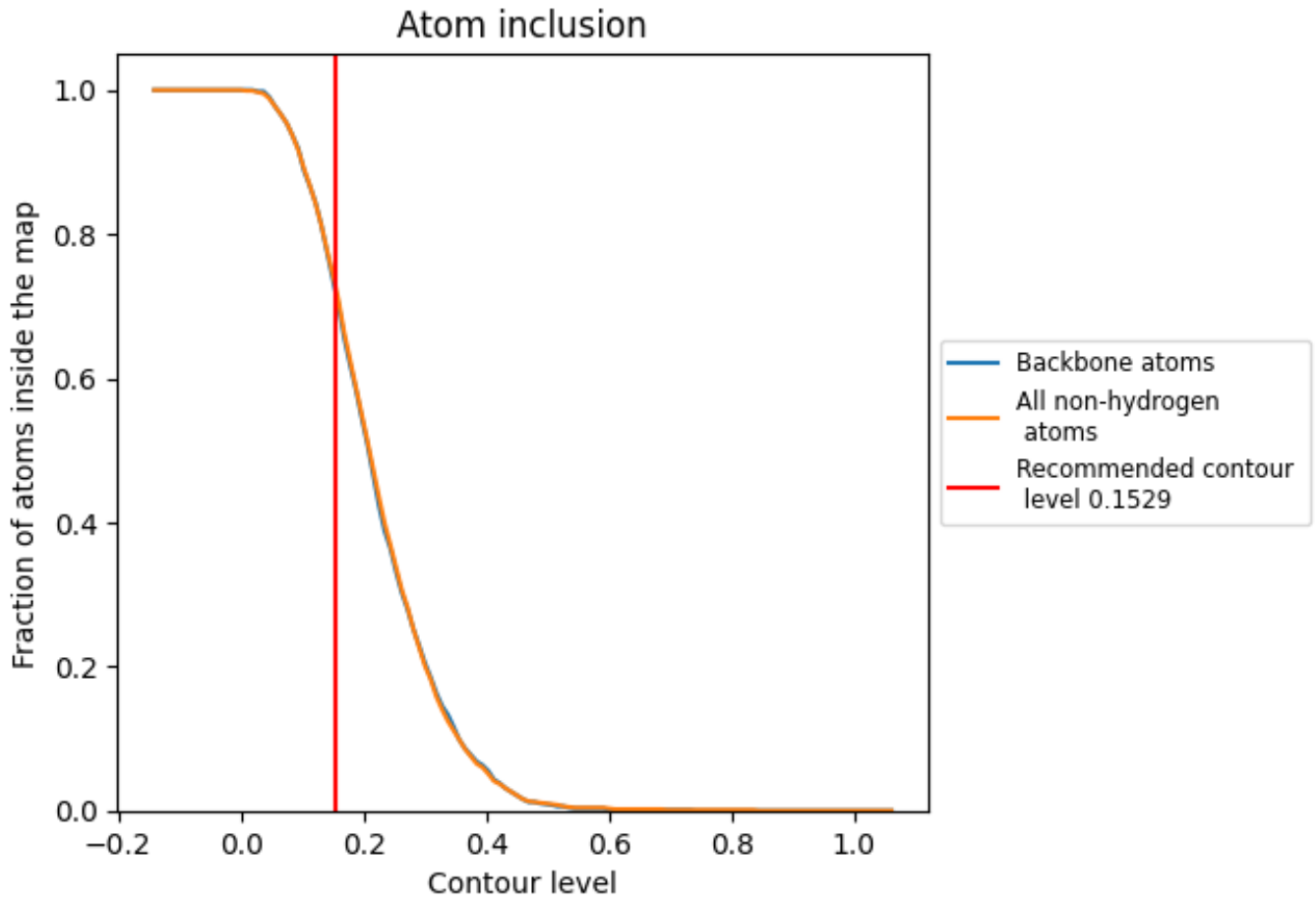
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1529).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.1529) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.3280
A	0.7620	0.3420
B	0.7210	0.2950
C	0.7440	0.4380
D	0.7270	0.3550
E	0.5710	0.4480
F	0.4100	0.3490