



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:09 PM JST

PDB ID : 6JK8
EMDB ID : EMD-9838
Title : Cryo-EM structure of the full-length human IGF-1R in complex with insulin
Authors : Zhang, X.; Yu, D.; Wang, T.
Deposited on : 2019-02-27
Resolution : 4.70 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:

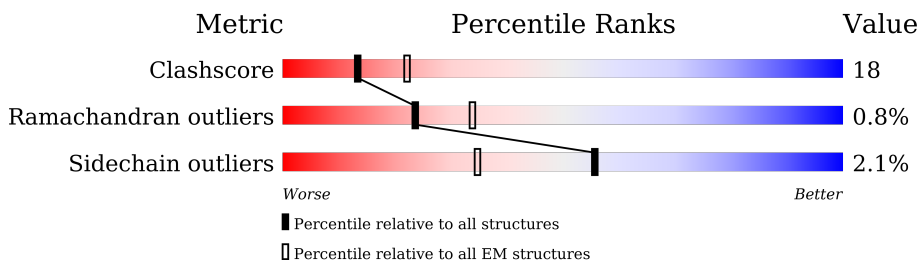
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al.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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1367	
1	B	1367	
2	C	110	
2	D	110	
3	E	2	
3	G	2	
3	H	2	
3	I	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	4	 A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a yellow segment on the left, a red segment in the middle, and an orange segment on the right. A vertical line is drawn at the 25% mark, and another vertical line is drawn at the 75% mark. The text '25%' is placed below the bar at the first vertical line, and '75%' is placed below the bar at the second vertical line. The text '75%' is also placed above the bar at the second vertical line.

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13666 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	823	Total	C	N	O	S	0	0
			6595	4166	1138	1241	50		
1	B	801	Total	C	N	O	S	1	0
			6450	4076	1119	1209	46		

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	21	Total	C	N	O	S	0	0
			163	99	25	35	4		
2	D	25	Total	C	N	O	S	1	0
			212	138	35	37	2		

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



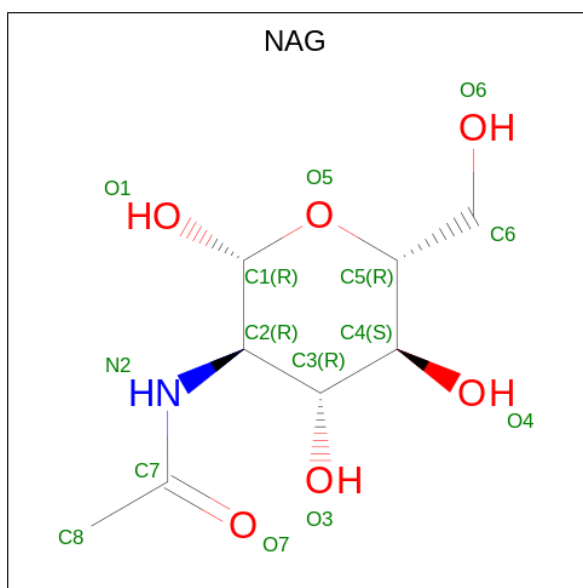
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-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		
4	F	4	50	28	2	20	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

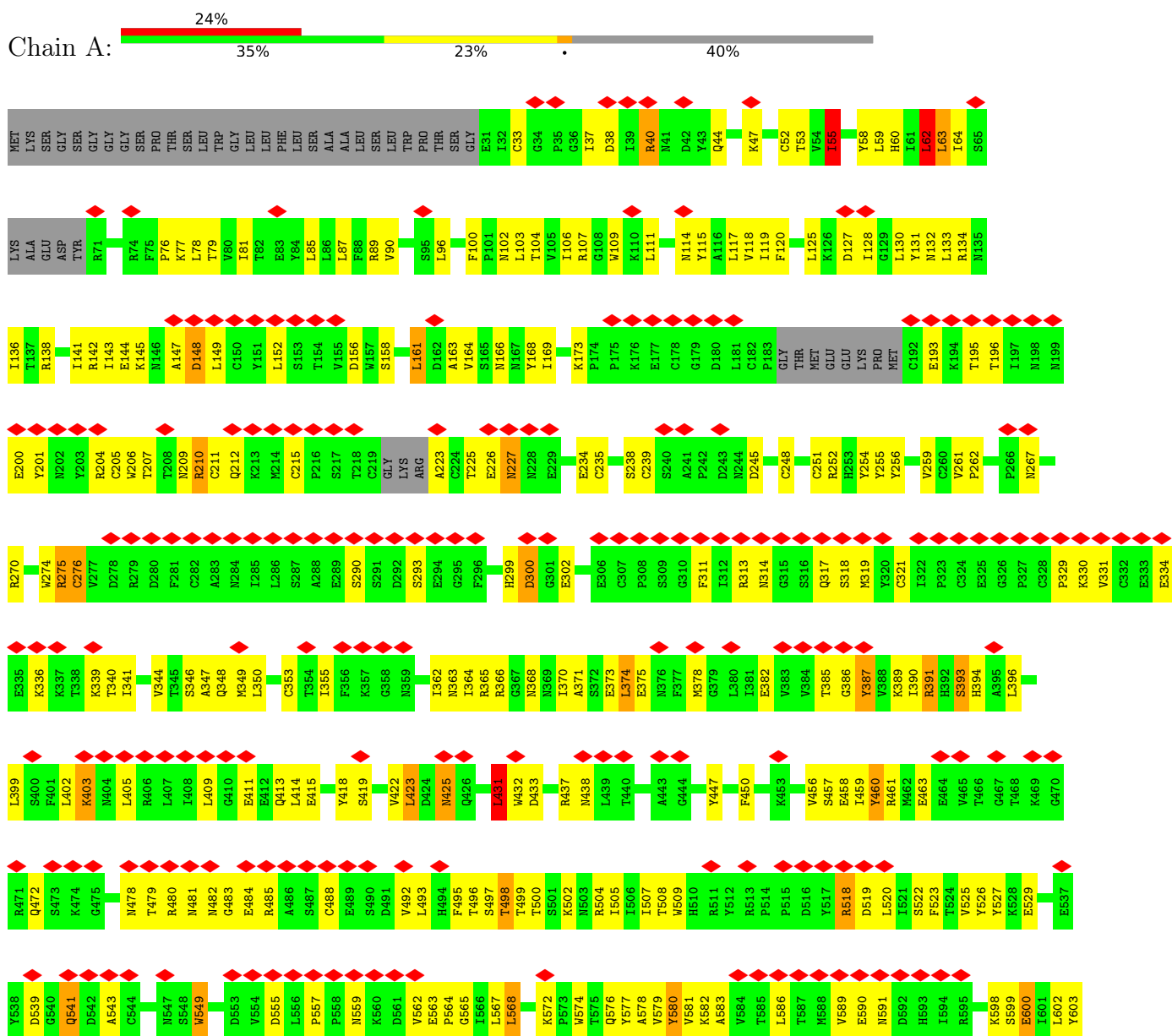


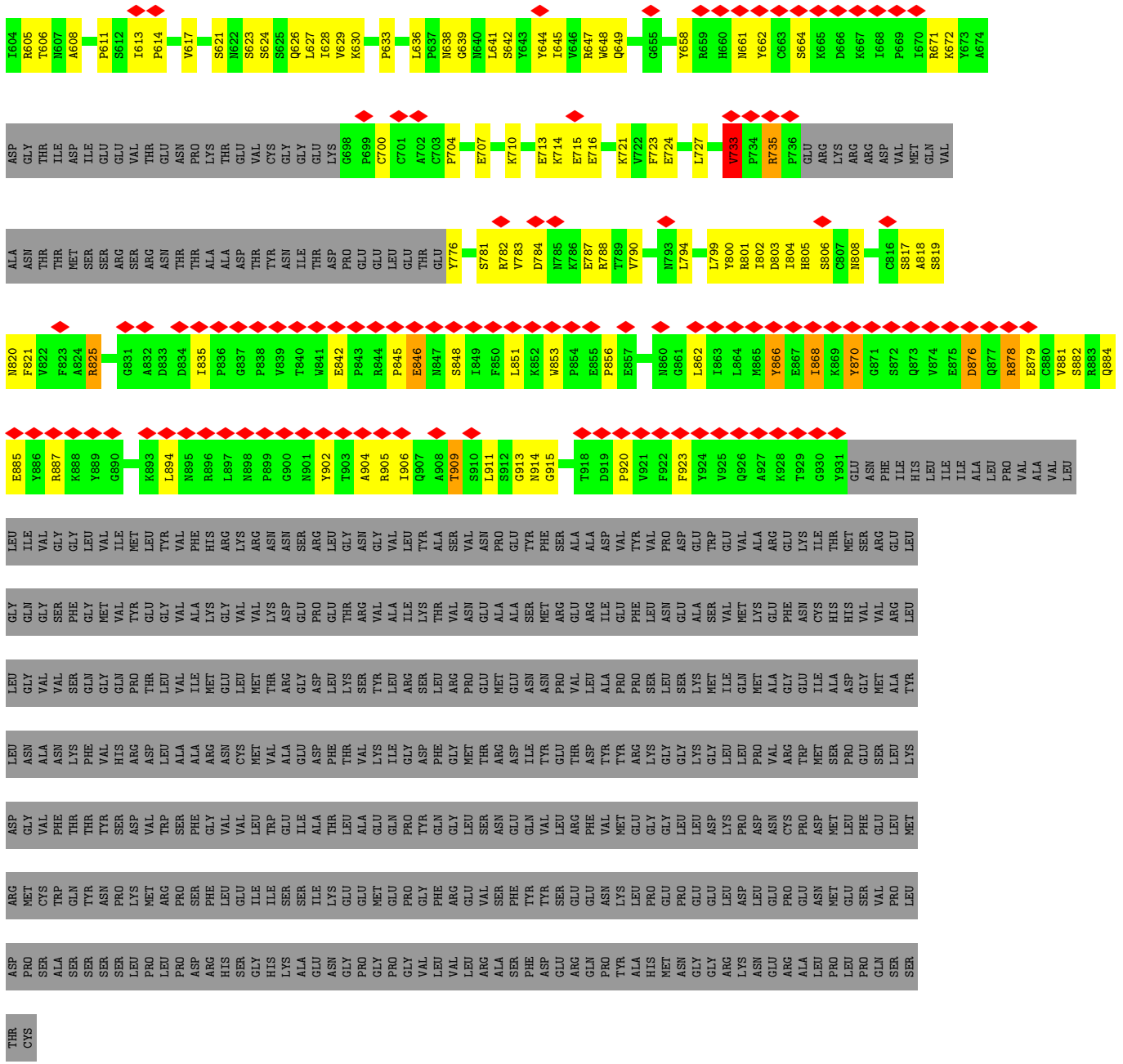
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	42	24	3	15	0
5	A	1	42	24	3	15	0
5	A	1	42	24	3	15	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0
5	B	1	42	24	3	15	0

3 Residue-property plots

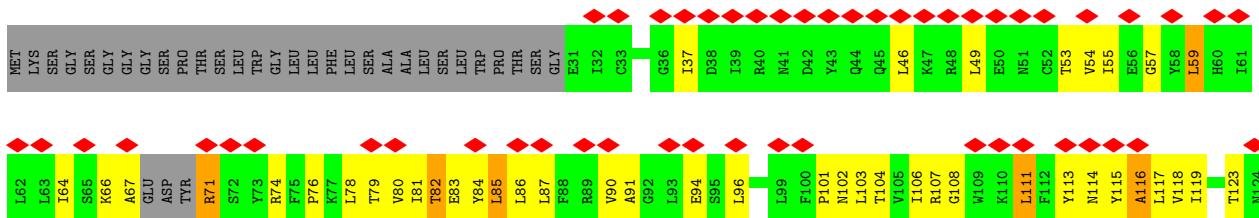
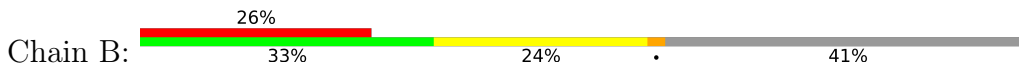
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

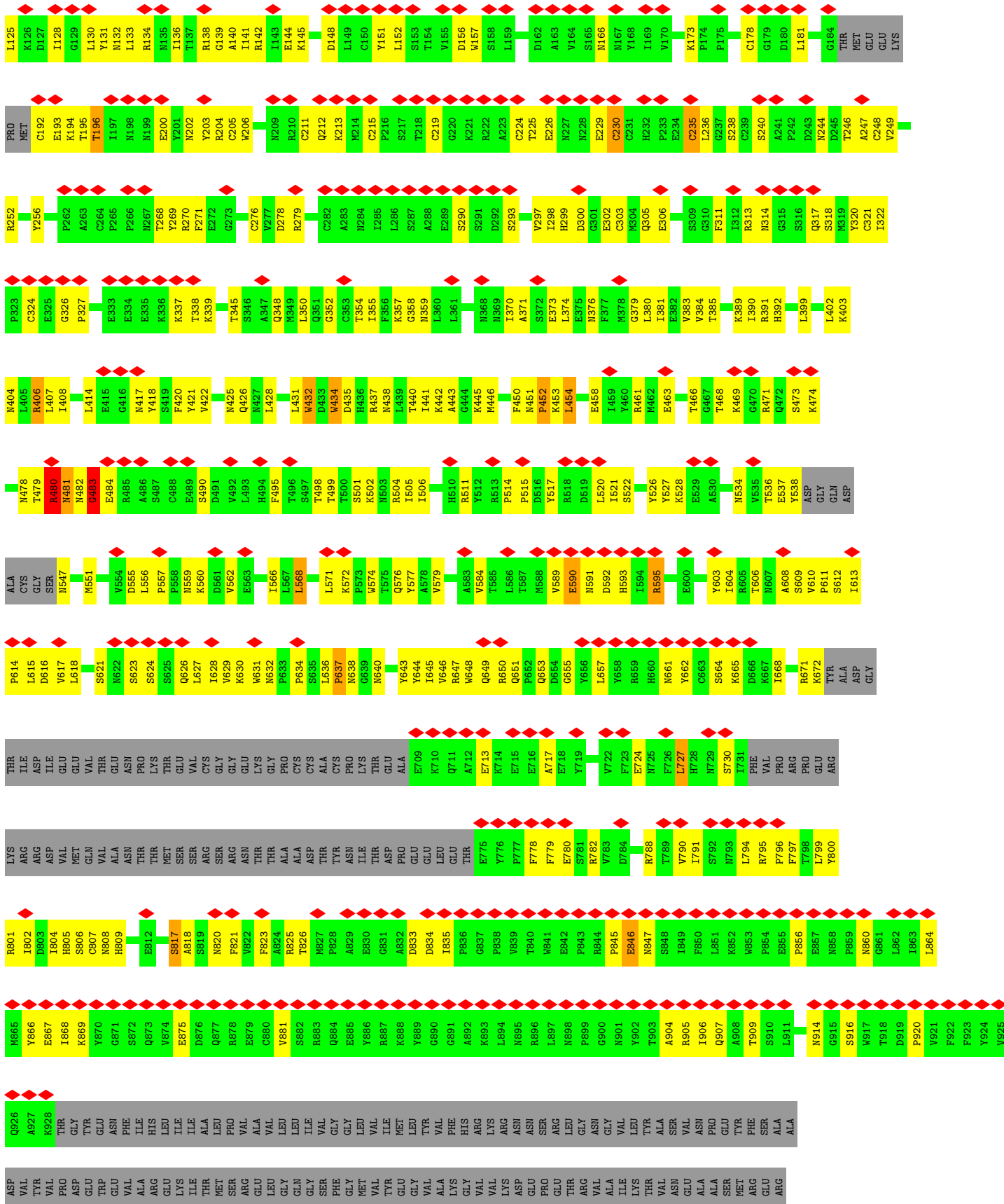
• Molecule 1: Insulin-like growth factor 1 receptor





• Molecule 1: Insulin-like growth factor 1 receptor

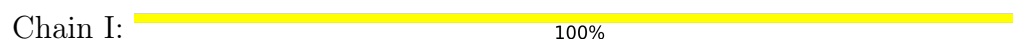




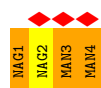
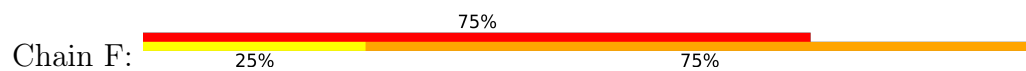
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301139	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	36496	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	219.2, 219.2, 219.2	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: NAG, MAN

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	0.49	3/6753 (0.0%)	0.92	21/9161 (0.2%)
1	B	0.46	0/6604	0.89	19/8951 (0.2%)
2	C	0.82	1/164 (0.6%)	1.19	0/220
2	D	0.90	1/218 (0.5%)	1.74	6/294 (2.0%)
All	All	0.49	5/13739 (0.0%)	0.93	46/18626 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	24
2	D	0	1
All	All	0	42

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	CYS	CA-CB	6.68	1.68	1.53
1	A	866	TYR	CD2-CE2	-6.11	1.30	1.39
2	C	19	TYR	CD2-CE2	-5.17	1.31	1.39
1	A	549	TRP	CB-CG	-5.03	1.41	1.50
1	A	387	TYR	CD2-CE2	-5.01	1.31	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	CYS	CA-CB-SG	11.93	135.47	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	LEU	CB-CG-CD2	-11.74	91.05	111.00
1	B	219	CYS	CA-CB-SG	-9.21	97.41	114.00
1	A	52	CYS	CA-CB-SG	8.31	128.95	114.00
1	B	235	CYS	CA-CB-SG	8.08	128.54	114.00
2	D	11	LEU	CA-CB-CG	7.89	133.46	115.30
1	B	59	LEU	CA-CB-CG	7.88	133.43	115.30
1	B	454	LEU	CA-CB-CG	7.55	132.66	115.30
1	A	300	ASP	CB-CG-OD1	7.42	124.98	118.30
1	B	111	LEU	CB-CG-CD1	7.33	123.47	111.00
2	D	4	GLN	CA-CB-CG	7.31	129.48	113.40
1	B	235	CYS	CB-CA-C	7.15	124.71	110.40
1	A	431	LEU	CA-CB-CG	6.91	131.18	115.30
1	B	402	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	230	CYS	CA-CB-SG	-6.51	102.28	114.00
1	A	276	CYS	N-CA-CB	-6.42	99.03	110.60
1	B	85	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	733	VAL	N-CA-C	-6.41	93.69	111.00
1	B	727	LEU	CB-CG-CD2	-6.18	100.49	111.00
1	A	374	LEU	CA-CB-CG	6.13	129.41	115.30
1	B	111	LEU	N-CA-CB	6.12	122.63	110.40
1	A	735	ARG	CA-CB-CG	6.06	126.74	113.40
1	A	55	ILE	CA-CB-CG1	6.03	122.45	111.00
1	A	62	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	62	LEU	CB-CG-CD2	-5.96	100.88	111.00
1	B	483	GLY	C-N-CA	5.90	136.45	121.70
1	B	590	GLU	C-N-CA	5.86	136.36	121.70
1	B	248	CYS	N-CA-CB	5.77	120.98	110.60
2	D	7	CYS	CA-CB-SG	5.65	124.17	114.00
1	A	396	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	484	GLU	CA-CB-CG	5.47	125.43	113.40
1	A	33	CYS	CA-CB-SG	-5.45	104.19	114.00
1	B	399	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	825	ARG	CA-CB-CG	5.41	125.31	113.40
2	D	26[A]	TYR	N-CA-CB	5.38	120.28	110.60
2	D	26[B]	TYR	N-CA-CB	5.38	120.28	110.60
1	A	498	THR	CA-CB-CG2	5.36	119.90	112.40
1	B	123	THR	C-N-CA	5.35	135.08	121.70
1	B	434	TRP	CB-CA-C	5.33	121.05	110.40
1	A	909	THR	N-CA-C	-5.29	96.73	111.00
1	A	423	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	391	ARG	CB-CG-CD	-5.15	98.20	111.60
1	A	825	ARG	CB-CG-CD	-5.05	98.46	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	ARG	C-N-CA	5.04	134.29	121.70
1	B	657	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	851	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASP	Peptide
1	A	227	ASN	Peptide
1	A	368	ASN	Peptide
1	A	393	SER	Peptide
1	A	425	ASN	Peptide
1	A	459	ILE	Peptide
1	A	541	GLN	Peptide
1	A	568	LEU	Peptide
1	A	600	GLU	Mainchain
1	A	62	LEU	Peptide
1	A	662	TYR	Peptide
1	A	700	CYS	Peptide
1	A	704	PRO	Peptide
1	A	845	PRO	Peptide
1	A	856	PRO	Peptide
1	A	870	TYR	Peptide
1	A	913	GLY	Peptide
1	B	113	TYR	Peptide
1	B	116	ALA	Peptide
1	B	196	THR	Peptide
1	B	271	PHE	Peptide
1	B	326	GLY	Peptide
1	B	406	ARG	Peptide
1	B	432	TRP	Peptide
1	B	483	GLY	Mainchain
1	B	495	PHE	Peptide
1	B	498	THR	Peptide
1	B	515	PRO	Peptide
1	B	521	ILE	Peptide
1	B	528	LYS	Peptide
1	B	536	THR	Peptide
1	B	555	ASP	Peptide
1	B	568	LEU	Peptide
1	B	589	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	595	ARG	Peptide
1	B	655	GLY	Peptide
1	B	788	ARG	Peptide
1	B	817	SER	Peptide
1	B	82	THR	Peptide
1	B	845	PRO	Peptide
1	B	846	GLU	Peptide
2	D	7	CYS	Mainchain

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	6595	0	6377	251	0
1	B	6450	0	6268	229	0
2	C	163	0	149	11	0
2	D	212	0	192	10	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	F	50	0	43	3	0
5	A	42	0	39	0	0
5	B	42	0	39	2	0
All	All	13666	0	13207	486	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 18.

All (486) 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:B:802:ILE:O	1:B:821:PHE:HA	1.55	1.04
1:A:492:VAL:HA	1:A:598:LYS:O	1.57	1.02
1:B:609:SER:O	1:B:808:ASN:ND2	1.96	0.99
1:B:640:ASN:HD21	5:B:1407:NAG:C1	1.74	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ALA:O	1:A:920:PRO:HA	1.63	0.98
1:A:579:VAL:O	1:A:602:LEU:HB3	1.69	0.93
1:A:254:TYR:HB2	1:A:261:VAL:O	1.71	0.91
1:B:115:TYR:HB2	1:B:140:ALA:HA	1.53	0.91
1:A:527:TYR:HA	1:A:578:ALA:O	1.71	0.90
1:B:196:THR:HA	1:B:200:GLU:O	1.71	0.89
1:A:802:ILE:O	1:A:821:PHE:HA	1.71	0.88
1:A:520:LEU:HB3	1:A:586:LEU:O	1.73	0.88
1:B:645:ILE:O	1:B:805:HIS:HB2	1.73	0.87
1:B:647:ARG:HA	1:B:779:PHE:O	1.77	0.85
1:A:507:ILE:O	1:A:565:GLY:HA2	1.79	0.82
1:A:645:ILE:O	1:A:804:ILE:HA	1.79	0.81
1:B:144:GLU:HG2	1:B:145:LYS:HG2	1.66	0.76
1:B:299:HIS:O	1:B:302:GLU:HB3	1.86	0.76
1:B:517:TYR:HB3	2:D:7:CYS:HB2	1.67	0.75
1:A:255:TYR:H	1:A:275:ARG:HA	1.52	0.74
1:A:576:GLN:HE21	1:A:603:TYR:HB3	1.52	0.74
1:A:647:ARG:O	1:A:802:ILE:HA	1.87	0.74
1:A:290:SER:H	1:A:293:SER:HB2	1.52	0.74
1:A:479:THR:HA	1:A:483:GLY:HA2	1.69	0.74
1:B:156:ASP:HB2	1:B:204:ARG:HE	1.54	0.72
1:B:37:ILE:HD11	1:B:59:LEU:HD22	1.70	0.72
1:B:905:ARG:HE	1:B:920:PRO:HG3	1.54	0.72
1:A:393:SER:H	1:A:425:ASN:HD22	1.39	0.71
1:A:735:ARG:NH1	2:D:15:LEU:O	2.24	0.71
1:A:493:LEU:H	1:A:599:SER:HA	1.56	0.70
1:B:640:ASN:ND2	5:B:1407:NAG:C1	2.52	0.69
1:A:629:VAL:O	1:A:788:ARG:HA	1.92	0.69
1:A:499:THR:O	1:A:505:ILE:HA	1.92	0.69
1:B:505:ILE:HG23	1:B:568:LEU:HB2	1.75	0.68
1:A:204:ARG:HB3	1:A:212:GLN:HB3	1.75	0.68
1:A:413:GLN:HG2	1:A:419:SER:HB2	1.74	0.68
1:A:59:LEU:HD12	1:A:85:LEU:HB2	1.76	0.67
1:A:518:ARG:NH1	1:A:519:ASP:OD1	2.28	0.67
1:B:514:PRO:O	2:D:5:HIS:NE2	2.28	0.67
1:B:833:ASP:HB3	1:B:860:ASN:H	1.58	0.67
1:A:848:SER:HA	1:A:894:LEU:O	1.93	0.67
1:A:371:ALA:HA	1:A:374:LEU:HG	1.77	0.67
1:A:902:TYR:HB3	1:A:923:PHE:O	1.95	0.66
1:B:102:ASN:HA	1:B:132:ASN:HD22	1.59	0.66
1:A:480:ARG:HD2	1:A:543:ALA:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HA	1:B:421:TYR:O	1.95	0.66
1:A:638:ASN:O	1:A:808:ASN:ND2	2.29	0.66
2:C:8:THR:OG1	2:D:4:GLN:NE2	2.25	0.65
1:B:268:THR:HA	1:B:278:ASP:HA	1.78	0.65
1:B:501:SER:HB2	1:B:504:ARG:H	1.61	0.65
1:A:239:CYS:HA	1:A:248:CYS:HA	1.78	0.65
1:B:142:ARG:NH2	1:B:144:GLU:OE1	2.30	0.65
1:B:79:THR:HB	1:B:249:VAL:HG13	1.79	0.65
1:B:297:VAL:O	1:B:303:CYS:HA	1.95	0.65
1:B:577:TYR:O	1:B:603:TYR:HA	1.97	0.65
1:B:804:ILE:H	1:B:820:ASN:H	1.44	0.65
1:B:114:ASN:HA	1:B:138:ARG:HA	1.77	0.65
1:B:206:TRP:HE1	1:B:213:LYS:H	1.43	0.65
1:B:354:THR:HA	1:B:381:ILE:HA	1.78	0.65
1:B:904:ALA:O	1:B:920:PRO:HA	1.96	0.65
1:A:196:THR:HA	1:A:200:GLU:O	1.97	0.64
1:B:290:SER:H	1:B:293:SER:HB2	1.60	0.64
1:A:721:LYS:HD2	1:B:520:LEU:HD22	1.77	0.64
1:A:649:GLN:O	1:A:800:TYR:HA	1.97	0.64
1:B:87:LEU:HB2	1:B:119:ILE:HG12	1.79	0.64
1:A:658:TYR:O	1:A:884:GLN:NE2	2.31	0.63
1:B:408:ILE:HB	1:B:441:ILE:HA	1.80	0.63
1:B:499:THR:HB	1:B:506:ILE:O	1.98	0.63
1:B:834:ASP:HB3	1:B:916:SER:H	1.64	0.63
1:A:234:GLU:HG3	1:A:262:PRO:HD3	1.80	0.63
1:B:314:ASN:HB3	1:B:318:SER:HB2	1.81	0.62
1:A:245:ASP:HB3	1:A:259:VAL:HA	1.80	0.62
1:A:87:LEU:HD12	1:A:119:ILE:HG12	1.81	0.62
1:B:440:THR:HA	1:B:466:THR:HG23	1.80	0.62
1:B:646:VAL:O	1:B:780:GLU:HA	1.99	0.62
1:A:504:ARG:HA	1:A:568:LEU:O	1.99	0.62
1:A:414:LEU:HB2	1:A:418:TYR:HB2	1.81	0.62
1:B:649:GLN:HB3	1:B:801:ARG:HB3	1.81	0.62
1:A:251:CYS:HB2	1:A:255:TYR:HB2	1.81	0.62
1:A:520:LEU:HD12	1:A:586:LEU:HB2	1.81	0.62
1:B:313:ARG:HE	1:B:317:GLN:HA	1.64	0.61
1:B:478:ASN:ND2	1:B:481:ASN:OD1	2.32	0.61
1:B:608:ALA:HB2	1:B:809:HIS:CE1	2.34	0.61
1:B:506:ILE:HA	1:B:566:ILE:O	2.01	0.61
1:B:791:ILE:HG22	1:B:794:LEU:HD11	1.81	0.61
1:A:868:ILE:O	1:A:878:ARG:HA	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:THR:HA	1:B:108:GLY:H	1.64	0.61
1:B:478:ASN:OD1	1:B:482:ASN:ND2	2.34	0.61
1:B:490:SER:HA	1:B:595:ARG:HD3	1.82	0.61
1:B:537:GLU:O	1:B:547:ASN:ND2	2.33	0.61
1:A:478:ASN:OD1	1:A:478:ASN:N	2.34	0.61
1:A:311:PHE:HB3	1:A:321:CYS:HB3	1.82	0.61
1:A:559:ASN:HB2	1:A:562:VAL:HG22	1.83	0.61
1:B:576:GLN:HG2	1:B:603:TYR:HB3	1.83	0.61
1:A:520:LEU:CB	1:A:586:LEU:O	2.47	0.61
1:A:644:TYR:HB2	1:A:783:VAL:O	2.01	0.60
1:B:505:ILE:HG22	1:B:571:LEU:HD21	1.83	0.60
1:A:644:TYR:O	1:A:782:ARG:HA	2.01	0.60
1:B:192:CYS:SG	1:B:193:GLU:N	2.73	0.60
1:B:66:LYS:H	1:B:91:ALA:HB3	1.66	0.60
1:B:373:GLU:O	1:B:376:ASN:HB3	2.00	0.60
2:C:2:ILE:HG23	2:C:3:VAL:HG23	1.84	0.60
1:B:134:ARG:NH1	1:B:215:CYS:SG	2.75	0.60
1:B:173:LYS:HE2	1:B:178:CYS:HA	1.84	0.60
1:A:256:TYR:O	1:A:259:VAL:HB	2.02	0.60
1:A:133:LEU:HD21	1:A:136:ILE:HD11	1.84	0.59
1:A:399:LEU:HD13	1:A:402:LEU:HD12	1.84	0.59
1:B:629:VAL:HG13	1:B:631:TRP:HZ3	1.67	0.59
1:A:143:ILE:H	1:A:169:ILE:HG13	1.68	0.59
1:B:442:LYS:O	1:B:471:ARG:NH1	2.34	0.59
1:A:134:ARG:NH1	1:A:215:CYS:SG	2.76	0.59
1:B:81:ILE:HD13	1:B:103:LEU:HD13	1.84	0.59
1:B:480:ARG:O	1:B:482:ASN:N	2.35	0.59
1:A:119:ILE:HD12	1:A:143:ILE:HG12	1.83	0.59
1:A:107:ARG:HD2	1:A:274:TRP:HB3	1.85	0.59
1:A:613:ILE:HG22	1:A:818:ALA:HB3	1.84	0.59
1:A:735:ARG:H	2:C:2:ILE:HD11	1.67	0.59
1:A:256:TYR:HB2	1:A:276:CYS:HB3	1.85	0.58
1:A:340:THR:HG23	1:A:363:ASN:HD21	1.68	0.58
1:A:628:ILE:HG22	1:A:790:VAL:HG22	1.85	0.58
1:A:914:ASN:OD1	1:A:914:ASN:N	2.32	0.58
1:A:142:ARG:HG2	1:A:168:TYR:HB3	1.84	0.58
1:B:404:ASN:H	1:B:437:ARG:HH22	1.51	0.58
1:B:608:ALA:HB2	1:B:809:HIS:NE2	2.19	0.58
1:B:662:TYR:HA	1:B:665:LYS:HB2	1.86	0.58
1:B:256:TYR:HB2	1:B:276:CYS:HB2	1.86	0.57
1:B:379:GLY:O	1:B:404:ASN:ND2	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ARG:HH11	1:B:672:LYS:H	1.52	0.57
1:A:103:LEU:HD11	1:A:106:ILE:HD11	1.86	0.57
1:A:37:ILE:HB	1:A:59:LEU:HA	1.85	0.57
1:A:128:ILE:HD13	1:A:152:LEU:HD13	1.87	0.57
1:A:614:PRO:O	1:A:820:ASN:ND2	2.36	0.57
1:B:355:ILE:HA	1:B:383:VAL:HB	1.87	0.57
1:B:502:LYS:HB2	1:B:609:SER:HB3	1.86	0.57
1:A:163:ALA:HB1	1:A:166:ASN:HB2	1.87	0.57
1:A:504:ARG:HB3	1:A:567:LEU:HD11	1.86	0.57
1:B:354:THR:HG23	1:B:355:ILE:HG13	1.87	0.57
1:B:435:ASP:OD2	1:B:461:ARG:NH1	2.35	0.57
1:A:78:LEU:HD11	1:A:81:ILE:HD11	1.86	0.56
1:B:94:GLU:HA	1:B:125:LEU:HA	1.87	0.56
1:B:269:TYR:OH	1:B:279:ARG:NH2	2.39	0.56
1:A:55:ILE:HG13	1:A:81:ILE:HD12	1.88	0.56
1:A:735:ARG:NH2	2:C:19:TYR:OH	2.39	0.56
1:B:106:ILE:HB	1:B:136:ILE:HD13	1.88	0.56
1:A:385:THR:HG22	1:A:409:LEU:HD12	1.87	0.56
1:A:481:ASN:OD1	1:A:482:ASN:N	2.38	0.56
1:B:202:ASN:HB3	1:B:204:ARG:HH12	1.71	0.56
1:A:572:LYS:HD3	1:A:636:LEU:HD21	1.87	0.56
1:A:437:ARG:HE	1:A:438:ASN:H	1.54	0.55
1:A:803:ASP:HB3	1:A:819:SER:HB2	1.88	0.55
1:B:724:GLU:HA	1:B:727:LEU:HD12	1.87	0.55
1:A:87:LEU:HD11	1:A:96:LEU:HD21	1.88	0.55
1:A:497:SER:OG	1:A:508:THR:OG1	2.22	0.55
1:B:194:LYS:HB3	1:B:203:TYR:HD1	1.71	0.55
1:B:311:PHE:HB3	1:B:321:CYS:HB3	1.88	0.55
1:A:40:ARG:HH21	1:A:62:LEU:HD21	1.72	0.55
1:A:518:ARG:NH2	1:A:589:VAL:O	2.40	0.55
1:A:909:THR:HG23	1:A:914:ASN:HA	1.88	0.55
1:B:53:THR:HA	1:B:78:LEU:HA	1.88	0.55
1:A:40:ARG:HB3	1:A:62:LEU:HG	1.87	0.55
1:A:81:ILE:HB	1:A:106:ILE:HG23	1.89	0.55
1:A:870:TYR:O	1:A:876:ASP:C	2.44	0.55
1:B:612:SER:O	1:B:806:SER:OG	2.20	0.55
1:B:909:THR:HA	1:B:914:ASN:HA	1.89	0.55
1:A:431:LEU:HG	1:A:433:ASP:H	1.71	0.55
1:A:314:ASN:ND2	1:A:317:GLN:OE1	2.40	0.55
1:A:195:THR:O	1:A:201:TYR:HA	2.06	0.54
1:A:868:ILE:HG23	1:A:906:ILE:HB	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:O	1:B:119:ILE:HA	2.07	0.54
1:B:358:GLY:H	1:B:385:THR:HG1	1.51	0.54
1:B:425:ASN:HB3	1:B:428:LEU:HD23	1.89	0.54
1:A:38:ASP:HA	1:A:60:HIS:HB2	1.90	0.54
1:B:236:LEU:HB2	1:B:252:ARG:HB3	1.89	0.54
1:B:538:TYR:HA	1:B:547:ASN:HD22	1.72	0.54
1:B:668:ILE:HB	1:B:864:LEU:HD23	1.89	0.54
1:B:81:ILE:HB	1:B:106:ILE:HG12	1.89	0.54
1:B:205:CYS:HA	1:B:211:CYS:HA	1.90	0.54
1:A:733:VAL:HG23	2:C:19:TYR:HD1	1.73	0.54
1:B:511:ARG:HH22	1:B:560:LYS:HB3	1.72	0.54
1:B:615:LEU:HB2	1:B:632:ASN:HB2	1.90	0.54
1:A:270:ARG:HB2	1:A:302:GLU:HG2	1.89	0.53
1:A:365:ARG:HH11	1:A:715:GLU:HG2	1.73	0.53
1:A:508:THR:HB	1:A:563:GLU:HG3	1.90	0.53
1:B:644:TYR:O	1:B:782:ARG:HA	2.08	0.53
1:B:799:LEU:HD11	1:B:823:PHE:HB3	1.90	0.53
1:A:399:LEU:HD11	1:A:432:TRP:HE3	1.72	0.53
1:A:582:LYS:HE2	1:A:598:LYS:HE2	1.88	0.53
1:B:795:ARG:N	1:B:800:TYR:OH	2.36	0.53
1:A:339:LYS:HG2	1:A:350:LEU:HD21	1.89	0.53
1:A:111:LEU:HD11	1:A:138:ARG:HG2	1.90	0.53
1:A:347:ALA:HA	1:A:350:LEU:HD23	1.90	0.53
1:B:270:ARG:NH2	1:B:300:ASP:O	2.41	0.53
1:A:362:ILE:HD12	1:A:390:ILE:HG13	1.89	0.53
1:A:87:LEU:HD21	1:A:96:LEU:HD11	1.90	0.53
1:A:234:GLU:O	1:A:252:ARG:N	2.42	0.53
1:B:67:ALA:O	1:B:71:ARG:N	2.42	0.53
1:B:627:LEU:HG	1:B:826:THR:HG22	1.90	0.53
2:C:17:GLU:HG2	2:C:20:CYS:HB2	1.90	0.53
1:B:104:THR:HA	1:B:133:LEU:HA	1.91	0.53
1:B:311:PHE:HA	1:B:322:ILE:O	2.08	0.53
1:A:364:ILE:H	1:A:393:SER:HA	1.72	0.53
1:B:613:ILE:HG22	1:B:818:ALA:HB3	1.91	0.52
1:A:375:GLU:OE1	1:A:403:LYS:NZ	2.42	0.52
1:B:618:LEU:HB2	1:B:630:LYS:HE3	1.91	0.52
1:A:79:THR:O	1:A:104:THR:N	2.36	0.52
1:B:76:PRO:O	1:B:102:ASN:ND2	2.32	0.52
1:A:111:LEU:HD21	1:A:138:ARG:HB3	1.90	0.52
1:A:103:LEU:HD12	1:A:130:LEU:HG	1.92	0.52
1:B:614:PRO:HG3	1:B:806:SER:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:LYS:N	1:B:577:TYR:OH	2.38	0.52
1:B:621:SER:OG	1:B:623:SER:O	2.27	0.52
1:B:151:TYR:OH	1:B:181:LEU:O	2.24	0.52
1:B:610:VAL:HG13	1:B:817:SER:HB2	1.91	0.52
1:A:707:GLU:HA	1:A:710:LYS:HB2	1.92	0.52
1:A:846:GLU:O	1:A:848:SER:N	2.43	0.52
1:A:539:ASP:HB3	1:A:549:TRP:CE2	2.44	0.51
2:D:8:GLY:H	2:D:11:LEU:HB2	1.76	0.51
1:A:314:ASN:HB3	1:A:317:GLN:HB2	1.91	0.51
1:A:649:GLN:NE2	1:A:776:TYR:O	2.42	0.51
1:A:713:GLU:HA	1:A:716:GLU:HG3	1.92	0.51
1:B:576:GLN:HA	1:B:604:ILE:O	2.10	0.51
1:A:614:PRO:HG3	1:A:806:SER:HB2	1.93	0.51
1:B:867:GLU:N	1:B:907:GLN:O	2.44	0.51
1:A:866:TYR:HB2	1:A:906:ILE:HD11	1.92	0.51
1:B:645:ILE:O	1:B:805:HIS:CB	2.51	0.51
2:C:12:SER:H	2:C:15:GLN:HE21	1.59	0.51
1:B:647:ARG:HB3	1:B:778:PHE:HB3	1.93	0.51
1:A:238:SER:OG	1:A:239:CYS:N	2.43	0.51
1:A:735:ARG:HG3	2:C:16:LEU:HG	1.93	0.51
1:A:225:THR:HG23	1:A:227:ASN:H	1.76	0.50
1:B:81:ILE:O	1:B:107:ARG:N	2.44	0.50
1:B:240:SER:HB2	1:B:247:ALA:HB1	1.92	0.50
1:B:406:ARG:HH12	1:B:437:ARG:HH21	1.59	0.50
1:B:556:LEU:HD12	1:B:557:PRO:HD2	1.93	0.50
1:A:55:ILE:HD11	1:A:59:LEU:HB2	1.93	0.50
1:B:517:TYR:HB2	2:D:5:HIS:HB3	1.93	0.50
1:A:870:TYR:O	1:A:876:ASP:O	2.29	0.50
1:B:645:ILE:HD11	1:B:780:GLU:HG2	1.93	0.50
1:B:106:ILE:HD12	1:B:116:ALA:HB1	1.94	0.50
1:B:653:GLN:OE1	1:B:825:ARG:NH1	2.39	0.50
1:B:835:ILE:HD13	1:B:856:PRO:HD3	1.92	0.50
1:A:207:THR:HG21	1:A:210:ARG:HE	1.76	0.50
1:A:136:ILE:HB	1:A:161:LEU:HB3	1.94	0.50
1:B:866:TYR:HB2	1:B:881:VAL:HB	1.94	0.50
1:A:365:ARG:NH1	1:A:366:ARG:HH12	2.10	0.50
1:A:386:GLY:HA2	1:A:411:GLU:H	1.76	0.50
1:A:313:ARG:NH2	1:A:318:SER:O	2.44	0.50
1:A:557:PRO:HD3	1:A:564:PRO:HB3	1.93	0.50
1:B:148:ASP:HA	1:B:173:LYS:HD2	1.92	0.50
1:B:403:LYS:HD3	1:B:437:ARG:HH12	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:LYS:HG2	1:B:875:GLU:HB3	1.92	0.50
1:A:649:GLN:HB3	1:A:801:ARG:HB3	1.93	0.49
2:D:12:VAL:O	2:D:16:TYR:HB2	2.12	0.49
1:A:120:PHE:CD1	1:A:144:GLU:HG3	2.47	0.49
1:A:362:ILE:O	1:A:393:SER:OG	2.30	0.49
1:B:305:GLN:HG2	1:B:306:GLU:HG3	1.93	0.49
1:B:650:ARG:HD2	1:B:795:ARG:HD3	1.94	0.49
1:A:339:LYS:NZ	1:A:349:MET:SD	2.74	0.49
1:B:57:GLY:N	1:B:82:THR:OG1	2.44	0.49
1:B:612:SER:HB2	1:B:636:LEU:H	1.78	0.49
1:A:193:GLU:O	1:A:204:ARG:N	2.46	0.49
1:A:463:GLU:OE1	1:A:472:GLN:NE2	2.46	0.49
1:B:441:ILE:HG13	1:B:468:THR:HG21	1.95	0.49
4:F:2:NAG:H5	4:F:3:MAN:H3	1.94	0.49
1:A:507:ILE:O	1:A:565:GLY:CA	2.56	0.49
1:A:721:LYS:NZ	1:B:517:TYR:O	2.46	0.49
1:B:115:TYR:N	1:B:139:GLY:O	2.44	0.49
1:B:634:PRO:HG2	1:B:637:PRO:HA	1.94	0.49
1:A:341:ILE:HD11	1:A:362:ILE:HG23	1.95	0.49
1:B:406:ARG:HH22	1:B:437:ARG:HH21	1.61	0.49
1:A:63:LEU:HD22	1:A:89:ARG:HG2	1.95	0.48
1:A:539:ASP:HB3	1:A:549:TRP:NE1	2.28	0.48
1:A:733:VAL:HG23	2:C:19:TYR:CD1	2.48	0.48
1:B:55:ILE:O	1:B:82:THR:OG1	2.23	0.48
1:A:450:PHE:H	1:A:481:ASN:ND2	2.12	0.48
1:A:456:VAL:HG23	1:A:482:ASN:HB3	1.95	0.48
1:B:103:LEU:HD23	1:B:130:LEU:HD13	1.94	0.48
1:B:224:CYS:HA	1:B:230:CYS:HA	1.94	0.48
1:B:420:PHE:HB3	1:B:446:MET:HG3	1.96	0.48
1:A:523:PHE:HA	1:A:583:ALA:HA	1.94	0.48
1:B:628:ILE:HG22	1:B:790:VAL:HG22	1.96	0.48
1:A:500:THR:HA	1:A:505:ILE:HG12	1.94	0.48
1:A:671:ARG:HH22	1:A:799:LEU:HB2	1.78	0.48
1:B:517:TYR:N	2:D:5:HIS:HD2	2.12	0.48
1:B:616:ASP:HB2	1:B:632:ASN:HD21	1.79	0.48
1:A:209:ASN:HB2	1:A:210:ARG:HD3	1.96	0.48
1:A:498:THR:OG1	4:F:4:MAN:O4	2.27	0.48
1:B:226:GLU:OE1	1:B:238:SER:OG	2.32	0.47
1:A:339:LYS:NZ	1:A:346:SER:O	2.47	0.47
1:B:371:ALA:HA	1:B:374:LEU:HB2	1.96	0.47
1:A:299:HIS:CE1	1:A:321:CYS:HB2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:HB2	1:B:469:LYS:HB3	1.96	0.47
1:A:402:LEU:HB3	1:A:405:LEU:HD22	1.97	0.47
1:B:152:LEU:O	1:B:157:TRP:NE1	2.43	0.47
1:B:298:ILE:HA	1:B:302:GLU:O	2.13	0.47
1:A:109:TRP:O	1:A:138:ARG:NH1	2.47	0.47
1:B:118:VAL:HG13	1:B:142:ARG:HB3	1.95	0.47
1:B:406:ARG:NE	1:B:438:ASN:O	2.48	0.47
1:A:254:TYR:HA	1:A:275:ARG:HA	1.95	0.47
1:A:580:TYR:CD2	1:A:602:LEU:HB2	2.49	0.47
1:A:76:PRO:O	1:A:102:ASN:ND2	2.33	0.47
1:B:225:THR:N	1:B:229:GLU:O	2.38	0.47
1:A:64:ILE:HB	1:A:90:VAL:HG22	1.97	0.47
1:A:508:THR:HG22	1:A:565:GLY:HA3	1.97	0.47
1:A:40:ARG:NH2	2:D:26[A]:TYR:OH	2.48	0.47
1:A:608:ALA:N	4:F:1:NAG:O6	2.46	0.47
1:B:337:LYS:O	1:B:359:ASN:N	2.42	0.47
1:B:479:THR:OG1	1:B:480:ARG:NH1	2.46	0.47
1:A:334:GLU:OE2	1:A:336:LYS:NZ	2.48	0.46
1:A:485:ARG:HG3	1:A:590:GLU:HB3	1.97	0.46
1:B:96:LEU:HD12	1:B:128:ILE:HA	1.97	0.46
1:B:499:THR:O	1:B:505:ILE:HA	2.16	0.46
1:B:612:SER:N	1:B:636:LEU:HB2	2.31	0.46
1:B:425:ASN:N	1:B:451:ASN:OD1	2.48	0.46
1:A:38:ASP:N	1:A:38:ASP:OD1	2.49	0.46
1:A:53:THR:O	1:A:79:THR:OG1	2.32	0.46
1:A:125:LEU:N	1:A:148:ASP:OD2	2.40	0.46
1:A:495:PHE:CE2	1:A:498:THR:HG23	2.51	0.46
1:A:806:SER:N	1:A:817:SER:OG	2.39	0.46
1:B:443:ALA:HA	1:B:471:ARG:HH22	1.81	0.46
1:B:650:ARG:HG2	1:B:800:TYR:HE1	1.81	0.46
1:A:671:ARG:HH21	1:A:825:ARG:HE	1.62	0.46
1:B:451:ASN:HB3	1:B:454:LEU:HD21	1.98	0.46
1:B:610:VAL:HA	1:B:611:PRO:HD3	1.55	0.46
1:B:647:ARG:HE	1:B:805:HIS:HE1	1.62	0.46
1:A:102:ASN:HA	1:A:132:ASN:ND2	2.30	0.46
1:A:390:ILE:HD13	1:A:422:VAL:HG12	1.98	0.46
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.74	0.46
1:A:784:ASP:OD1	1:A:784:ASP:N	2.46	0.46
1:B:54:VAL:HG22	1:B:80:VAL:HB	1.98	0.46
1:B:314:ASN:HB2	1:B:320:TYR:HB2	1.97	0.46
1:A:131:TYR:HA	1:A:206:TRP:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:N	1:A:58:TYR:O	2.46	0.46
1:A:223:ALA:HB2	1:A:252:ARG:HH21	1.81	0.46
1:B:338:THR:HA	1:B:359:ASN:HB2	1.98	0.46
1:B:417:ASN:O	1:B:445:LYS:NZ	2.43	0.46
1:B:115:TYR:HB3	1:B:141:ILE:HG12	1.99	0.45
1:A:478:ASN:OD1	1:A:481:ASN:ND2	2.48	0.45
1:A:671:ARG:NH2	1:A:799:LEU:HB2	2.31	0.45
1:B:390:ILE:HB	1:B:422:VAL:HG13	1.97	0.45
1:B:636:LEU:HB3	1:B:638:ASN:ND2	2.31	0.45
1:A:526:TYR:O	1:A:579:VAL:HA	2.16	0.45
1:B:339:LYS:HG2	1:B:350:LEU:HD11	1.99	0.45
1:B:868:ILE:HG12	1:B:906:ILE:HG12	1.98	0.45
1:A:574:TRP:N	1:A:606:THR:OG1	2.50	0.45
1:A:884:GLN:HG3	1:A:887:ARG:HH21	1.81	0.45
1:A:639:GLY:HA3	1:A:808:ASN:HD22	1.82	0.45
1:B:651:GLN:HG2	1:B:801:ARG:HB2	1.98	0.45
1:A:418:TYR:CZ	1:A:447:TYR:HB2	2.52	0.45
1:A:457:SER:OG	1:A:458:GLU:N	2.48	0.45
1:B:559:ASN:HB3	1:B:562:VAL:HG22	1.99	0.45
1:A:330:LYS:HD3	1:A:353:CYS:HA	1.99	0.45
1:A:866:TYR:CE2	1:A:881:VAL:HB	2.52	0.45
1:B:434:TRP:HH2	1:B:534:ASN:HB2	1.82	0.45
1:A:385:THR:HA	1:A:409:LEU:HB2	1.99	0.45
1:A:522:SER:HA	1:A:555:ASP:HA	1.97	0.45
1:B:499:THR:CB	1:B:506:ILE:O	2.65	0.45
1:B:195:THR:HG22	1:B:204:ARG:HG3	1.99	0.45
1:B:115:TYR:HE2	1:B:166:ASN:HB2	1.81	0.44
1:A:259:VAL:HG12	1:A:261:VAL:HB	1.99	0.44
1:B:84:TYR:HE2	1:B:86:LEU:HD12	1.82	0.44
1:A:235:CYS:HA	1:A:251:CYS:HA	2.00	0.44
1:A:523:PHE:HB3	1:A:581:VAL:HG13	1.98	0.44
1:A:661:ASN:O	1:A:664:SER:OG	2.31	0.44
1:A:40:ARG:NH2	1:A:62:LEU:HD21	2.31	0.44
1:A:387:TYR:CE2	1:A:389:LYS:HE2	2.52	0.44
1:A:496:THR:H	1:A:509:TRP:HA	1.83	0.44
1:B:502:LYS:HE2	1:B:609:SER:HB2	1.97	0.44
1:B:643:TYR:O	1:B:807:CYS:HB2	2.17	0.44
1:B:661:ASN:HB3	1:B:664:SER:HB2	1.99	0.44
1:A:389:LYS:HD3	1:A:391:ARG:NH1	2.33	0.44
1:A:672:LYS:H	1:A:825:ARG:HH11	1.65	0.44
1:B:235:CYS:O	1:B:252:ARG:NE	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:HA	1:A:132:ASN:HD22	1.82	0.44
1:A:145:LYS:NZ	1:A:724:GLU:OE1	2.46	0.44
1:A:835:ILE:HD11	1:A:853:TRP:HB2	2.00	0.44
1:A:636:LEU:HD23	1:A:636:LEU:HA	1.86	0.44
1:B:103:LEU:HD11	1:B:106:ILE:HG13	2.00	0.44
1:A:205:CYS:HA	1:A:211:CYS:HA	1.99	0.44
1:B:426:GLN:HA	1:B:452:PRO:HD2	2.00	0.44
1:B:867:GLU:HB2	1:B:907:GLN:HB3	2.00	0.43
1:A:156:ASP:HB2	1:A:195:THR:HG21	1.99	0.43
1:B:108:GLY:HA3	1:B:111:LEU:HD12	1.99	0.43
1:B:646:VAL:HG23	1:B:648:TRP:HZ3	1.83	0.43
1:B:650:ARG:HA	1:B:800:TYR:CD1	2.53	0.43
1:A:37:ILE:O	1:A:60:HIS:N	2.51	0.43
1:A:125:LEU:HD23	1:A:149:LEU:HD22	2.01	0.43
1:A:862:LEU:O	1:A:911:LEU:N	2.49	0.43
1:B:357:LYS:HD2	1:B:385:THR:HG21	2.00	0.43
1:A:522:SER:OG	1:A:523:PHE:N	2.51	0.43
1:A:611:PRO:HB2	1:A:817:SER:HB3	1.99	0.43
1:B:404:ASN:H	1:B:437:ARG:NH2	2.14	0.43
1:B:616:ASP:HB2	1:B:632:ASN:ND2	2.34	0.43
1:A:414:LEU:HB3	1:A:415:GLU:H	1.67	0.43
1:A:723:PHE:CE2	1:A:727:LEU:HD12	2.53	0.43
1:B:244:ASN:ND2	1:B:246:THR:OG1	2.52	0.43
1:A:460:TYR:HD1	1:A:460:TYR:HA	1.66	0.43
1:A:529:GLU:HA	1:A:577:TYR:CD1	2.54	0.43
1:A:621:SER:HA	1:A:627:LEU:HA	2.01	0.43
1:B:403:LYS:HG2	1:B:432:TRP:CZ2	2.54	0.43
1:B:406:ARG:HB2	1:B:407:LEU:HG	2.00	0.43
1:B:591:ASN:O	1:B:593:HIS:N	2.51	0.43
1:B:797:PHE:N	1:B:826:THR:OG1	2.47	0.43
1:A:225:THR:OG1	1:A:226:GLU:N	2.52	0.43
1:A:331:VAL:HG22	1:A:355:ILE:HD12	2.00	0.43
1:A:461:ARG:HD2	1:A:488:CYS:SG	2.59	0.43
1:A:623:SER:HB3	1:A:626:GLN:HB2	2.01	0.43
1:B:345:THR:HA	1:B:348:GLN:HB3	2.00	0.43
1:A:902:TYR:CE2	1:A:904:ALA:HB2	2.54	0.43
1:B:527:TYR:HB2	1:B:579:VAL:HG22	2.01	0.43
1:B:473:SER:OG	1:B:474:LYS:N	2.50	0.42
1:B:799:LEU:HA	1:B:825:ARG:HA	2.01	0.42
1:A:529:GLU:HA	1:A:577:TYR:HD1	1.84	0.42
1:A:882:SER:H	1:A:885:GLU:HB3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:SER:HB2	1:B:796:PRO:HB3	2.01	0.42
1:B:713:GLU:O	1:B:717:ALA:HB2	2.19	0.42
1:A:114:ASN:HB3	1:A:344:VAL:HG12	2.01	0.42
1:A:382:GLU:HA	1:A:405:LEU:HA	2.01	0.42
1:A:633:PRO:HD3	1:A:787:GLU:HG2	2.00	0.42
1:B:111:LEU:HB2	1:B:138:ARG:HB3	2.00	0.42
1:B:206:TRP:CD1	1:B:212:GLN:HA	2.54	0.42
1:B:431:LEU:HD23	1:B:458:GLU:HG2	2.02	0.42
1:B:833:ASP:OD1	1:B:833:ASP:N	2.47	0.42
1:A:103:LEU:HB3	1:A:130:LEU:HD12	2.00	0.42
1:A:329:PRO:HB2	1:A:355:ILE:HG13	2.01	0.42
2:D:6:LEU:HD23	2:D:14:ALA:HB1	2.01	0.42
1:A:391:ARG:CZ	1:B:590:GLU:HG3	2.49	0.42
1:A:617:VAL:HA	1:A:630:LYS:O	2.20	0.42
1:B:64:ILE:HB	1:B:90:VAL:HA	2.01	0.42
1:A:254:TYR:HD1	1:A:276:CYS:HB2	1.85	0.42
1:A:525:VAL:HA	1:A:580:TYR:O	2.20	0.42
1:A:641:LEU:HA	1:A:808:ASN:HA	2.01	0.42
1:A:44:GLN:O	1:A:47:LYS:HB2	2.20	0.42
1:A:127:ASP:N	1:A:127:ASP:OD1	2.51	0.42
1:A:370:ILE:O	1:A:373:GLU:N	2.52	0.42
1:A:805:HIS:ND1	1:A:817:SER:O	2.36	0.42
1:B:131:TYR:HA	1:B:206:TRP:CG	2.55	0.42
1:B:352:GLY:HA2	1:B:380:LEU:HD22	2.02	0.42
1:B:380:LEU:HA	1:B:404:ASN:HD22	1.84	0.42
1:A:879:GLU:HB2	1:A:894:LEU:HD21	2.01	0.42
1:B:391:ARG:HG2	1:B:392:HIS:CD2	2.55	0.42
1:A:574:TRP:CE2	1:A:605:ARG:HD3	2.55	0.41
1:B:414:LEU:HB3	1:B:418:TYR:HB2	2.02	0.41
1:B:53:THR:HG23	1:B:54:VAL:HG23	2.02	0.41
1:A:196:THR:HG22	1:A:201:TYR:HB3	2.01	0.41
1:A:623:SER:OG	1:A:624:SER:N	2.54	0.41
1:A:648:TRP:HH2	1:A:781:SER:HG	1.66	0.41
1:B:202:ASN:HB3	1:B:204:ARG:NH1	2.35	0.41
2:C:1:GLY:N	2:C:4:GLU:OE2	2.35	0.41
1:B:628:ILE:H	1:B:628:ILE:HG13	1.63	0.41
1:A:96:LEU:O	1:A:100:PHE:N	2.39	0.41
1:B:608:ALA:CB	1:B:809:HIS:CE1	3.02	0.41
1:B:59:LEU:HD12	1:B:85:LEU:HD12	2.03	0.41
1:B:623:SER:H	1:B:626:GLN:HB2	1.86	0.41
1:A:714:LYS:HE2	1:B:584:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:N	1:B:140:ALA:O	2.54	0.41
1:B:522:SER:HB3	1:B:584:VAL:HB	2.03	0.41
1:B:574:TRP:N	1:B:606:THR:OG1	2.54	0.41
1:A:53:THR:O	1:A:79:THR:N	2.48	0.41
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.82	0.41
1:B:526:TYR:CD1	1:B:551:MET:HG2	2.56	0.41
1:B:730:SER:O	1:B:730:SER:OG	2.37	0.41
1:A:115:TYR:CD1	1:A:142:ARG:HG3	2.55	0.41
1:A:119:ILE:HB	1:A:143:ILE:HG23	2.03	0.41
1:A:387:TYR:CE2	1:A:389:LYS:HB2	2.55	0.41
1:A:390:ILE:HB	1:A:422:VAL:HA	2.03	0.41
1:B:76:PRO:HA	1:B:101:PRO:HD2	2.03	0.41
1:B:236:LEU:HD22	1:B:252:ARG:HA	2.03	0.41
1:B:453:LYS:HD2	1:B:453:LYS:HA	1.87	0.41
1:B:617:VAL:HG22	1:B:631:TRP:HB3	2.02	0.41
1:A:44:GLN:O	1:A:47:LYS:CB	2.68	0.41
1:A:158:SER:HA	1:A:164:VAL:HG22	2.03	0.41
1:A:147:ALA:HA	1:A:173:LYS:N	2.36	0.40
1:A:254:TYR:CE1	1:A:270:ARG:HG2	2.56	0.40
1:A:364:ILE:O	1:A:394:HIS:N	2.51	0.40
1:A:580:TYR:HD2	1:A:600:GLU:O	2.04	0.40
1:A:642:SER:H	1:A:808:ASN:HA	1.86	0.40
1:B:450:PHE:HA	1:B:481:ASN:HB2	2.03	0.40
1:A:120:PHE:HD1	1:A:144:GLU:HG3	1.84	0.40
1:A:485:ARG:HD3	1:A:591:ASN:O	2.21	0.40
1:B:46:LEU:HD12	1:B:49:LEU:HD12	2.04	0.40
1:B:384:VAL:HG23	1:B:408:ILE:HA	2.03	0.40
2:C:3:VAL:O	2:C:7:CYS:HB2	2.21	0.40
1:A:117:LEU:HD23	1:A:141:ILE:HG23	2.04	0.40
1:A:909:THR:HA	1:A:915:GLY:N	2.36	0.40
1:A:391:ARG:HH11	1:A:391:ARG:HD2	1.76	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	811/1367 (59%)	687 (85%)	121 (15%)	3 (0%)	34	72
1	B	790/1367 (58%)	682 (86%)	98 (12%)	10 (1%)	12	48
2	C	19/110 (17%)	15 (79%)	4 (21%)	0	100	100
2	D	24/110 (22%)	18 (75%)	6 (25%)	0	100	100
All	All	1644/2954 (56%)	1402 (85%)	229 (14%)	13 (1%)	24	60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	846	GLU
1	A	876	ASP
1	B	83	GLU
1	B	481	ASN
1	B	592	ASP
1	B	484	GLU
1	A	541	GLN
1	B	846	GLU
1	B	452	PRO
1	B	847	ASN
1	B	327	PRO
1	B	483	GLY
1	B	637	PRO

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	734/1204 (61%)	709 (97%)	25 (3%)	37	61
1	B	718/1204 (60%)	713 (99%)	5 (1%)	84	90
2	C	20/88 (23%)	19 (95%)	1 (5%)	24	51
2	D	22/88 (25%)	22 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1494/2584 (58%)	1463 (98%)	31 (2%)	56 72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	55	ILE
1	A	63	LEU
1	A	77	LYS
1	A	118	VAL
1	A	161	LEU
1	A	210	ARG
1	A	267	ASN
1	A	275	ARG
1	A	300	ASP
1	A	319	MET
1	A	348	GLN
1	A	378	MET
1	A	403	LYS
1	A	423	LEU
1	A	431	LEU
1	A	460	TYR
1	A	502	LYS
1	A	518	ARG
1	A	580	TYR
1	A	733	VAL
1	A	842	GLU
1	A	868	ILE
1	A	878	ARG
1	A	905	ARG
1	B	71	ARG
1	B	74	ARG
1	B	324	CYS
1	B	370	ILE
1	B	480	ARG
2	C	19	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	394	HIS
1	A	425	ASN
1	A	576	GLN
1	A	651	GLN
1	A	847	ASN
1	B	132	ASN
1	B	253	HIS
1	B	284	ASN
1	B	478	ASN
1	B	481	ASN
1	B	482	ASN
1	B	547	ASN
1	B	632	ASN
1	B	640	ASN
1	B	725	ASN
2	C	15	GLN
2	D	4	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](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.20	3 (17%)
4	NAG	F	1	1,4	14,14,15	1.39	1 (7%)	17,19,21	0.76	0
4	NAG	F	2	4	14,14,15	0.51	0	17,19,21	0.61	0
4	MAN	F	3	4	11,11,12	1.80	1 (9%)	15,15,17	1.30	2 (13%)
4	MAN	F	4	4	11,11,12	0.89	0	15,15,17	1.10	2 (13%)
3	NAG	G	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	H	1	1,3	14,14,15	0.58	0	17,19,21	0.58	0
3	NAG	H	2	3	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
3	NAG	I	1	1,3	14,14,15	1.06	1 (7%)	17,19,21	1.06	1 (5%)
3	NAG	I	2	3	14,14,15	0.43	0	17,19,21	0.61	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	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	MAN	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	MAN	C1-C2	5.69	1.65	1.52
4	F	1	NAG	O5-C1	-4.99	1.35	1.43
3	E	2	NAG	C1-C2	4.57	1.59	1.52
3	I	1	NAG	O5-C1	-3.68	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.77	1.39	1.43
3	H	2	NAG	C1-C2	2.59	1.56	1.52
3	G	1	NAG	C1-C2	2.32	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C4-C3-C2	2.92	115.29	111.02
4	F	3	MAN	C1-O5-C5	2.85	116.05	112.19
3	E	2	NAG	C1-O5-C5	2.67	115.81	112.19
3	I	1	NAG	O4-C4-C3	-2.60	104.34	110.35
3	E	2	NAG	O5-C5-C4	-2.57	104.58	110.83
4	F	4	MAN	C1-O5-C5	2.39	115.43	112.19
3	E	1	NAG	O4-C4-C5	2.35	115.13	109.30
4	F	3	MAN	O2-C2-C3	-2.11	105.91	110.14
4	F	4	MAN	O2-C2-C3	-2.07	106.00	110.14
3	I	2	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

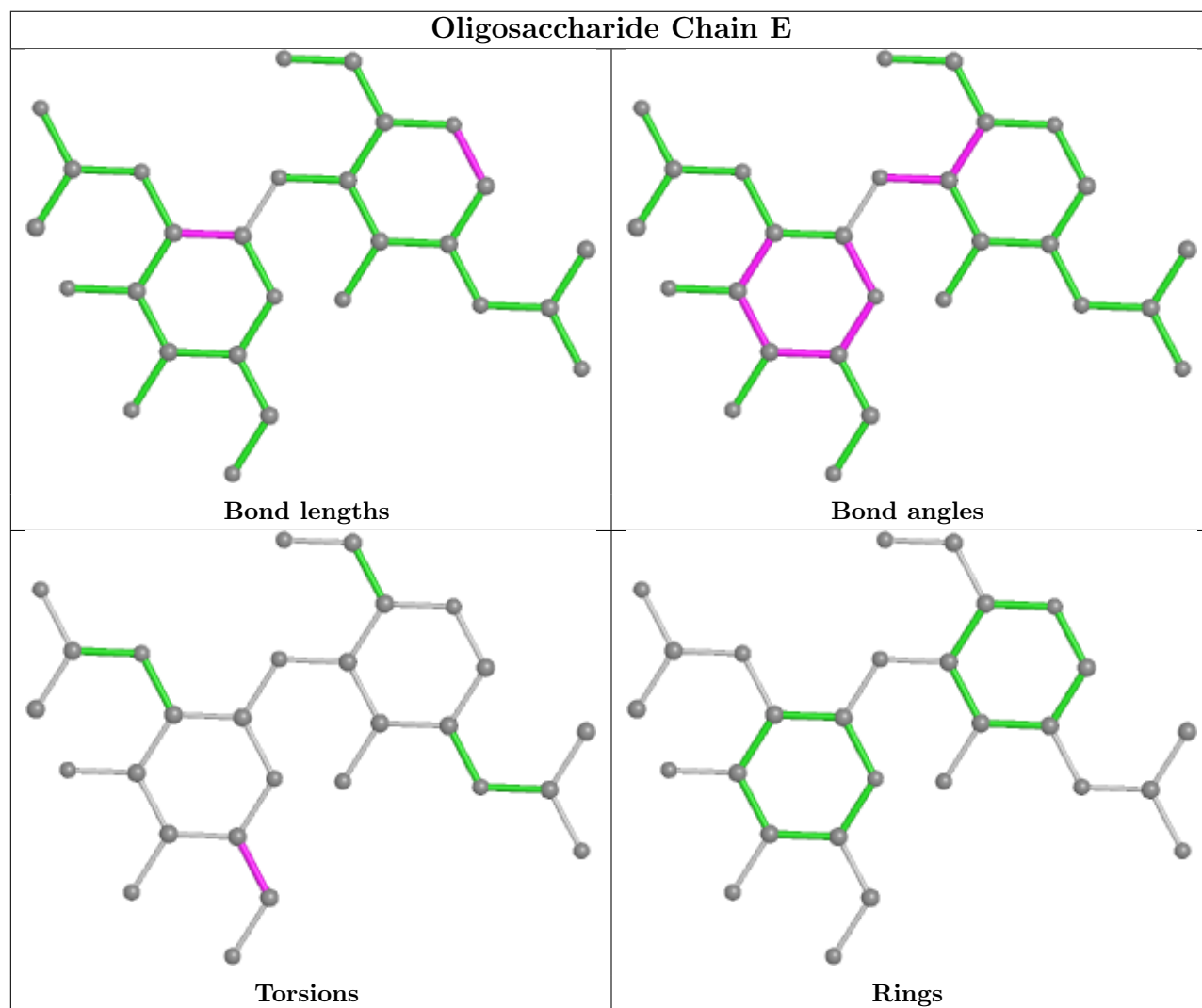
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	F	3	MAN	C4-C5-C6-O6
4	F	3	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

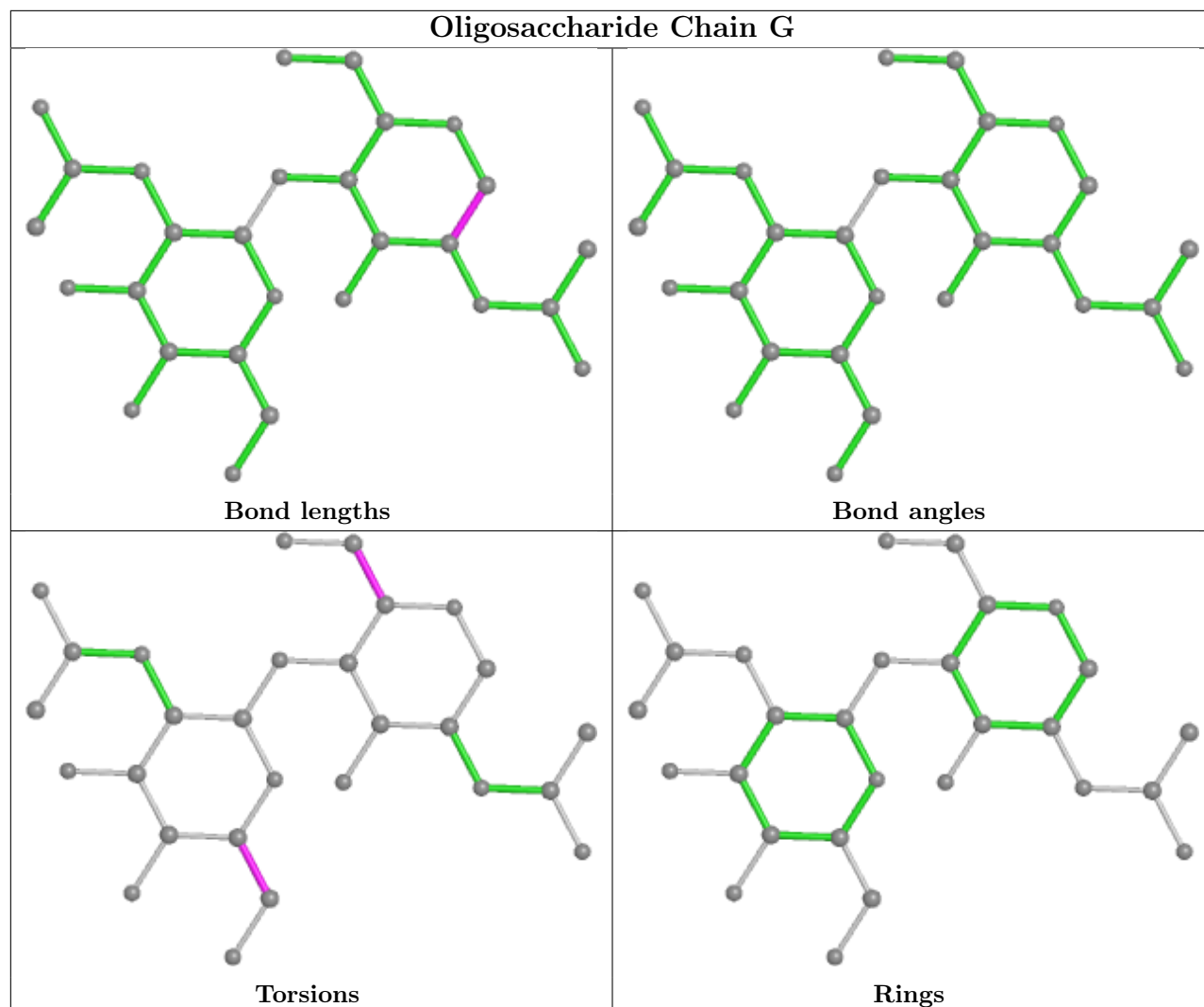
There are no ring outliers.

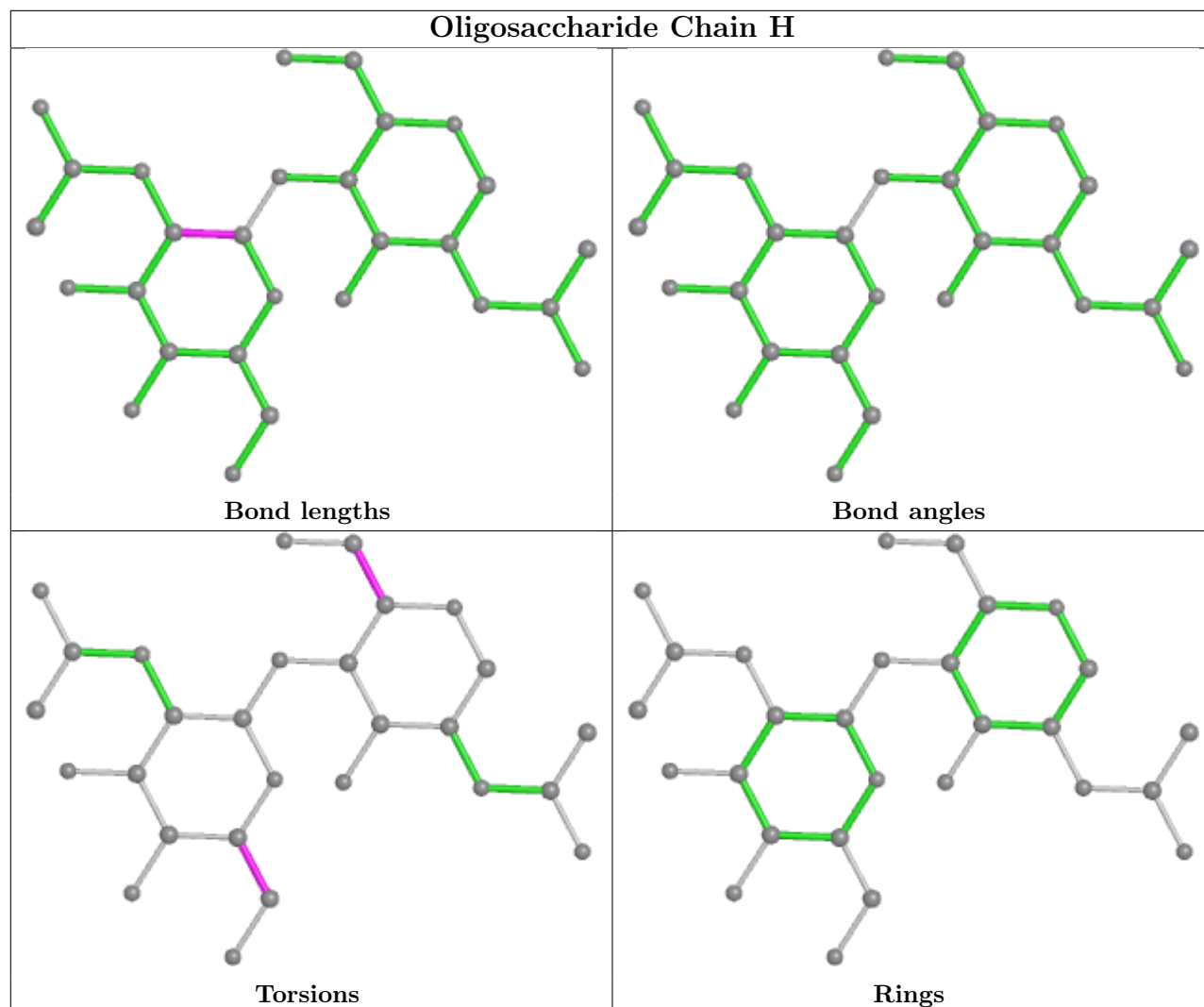
4 monomers are involved in 3 short contacts:

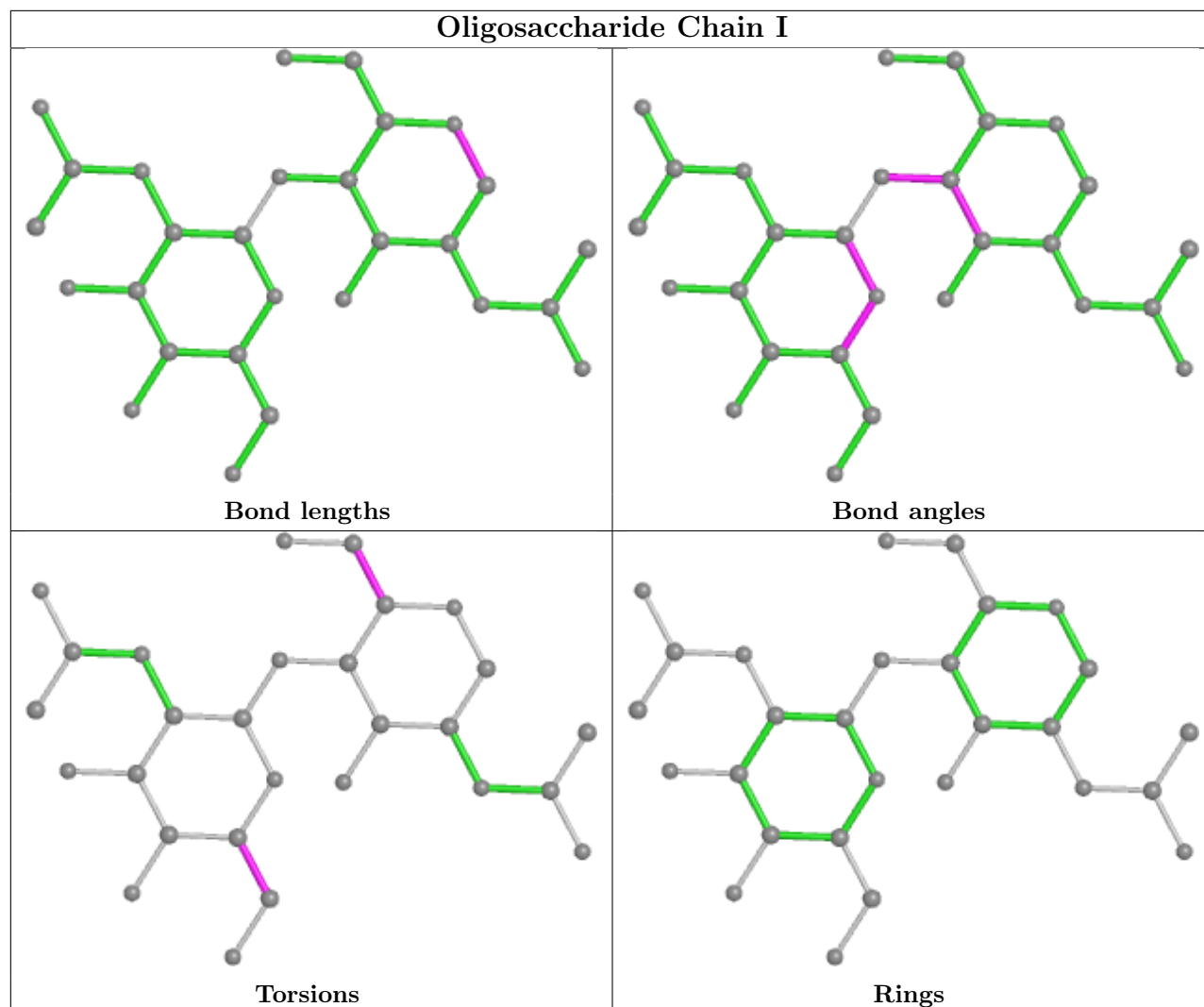
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	F	2	NAG	1	0
4	F	3	MAN	1	0
4	F	4	MAN	1	0

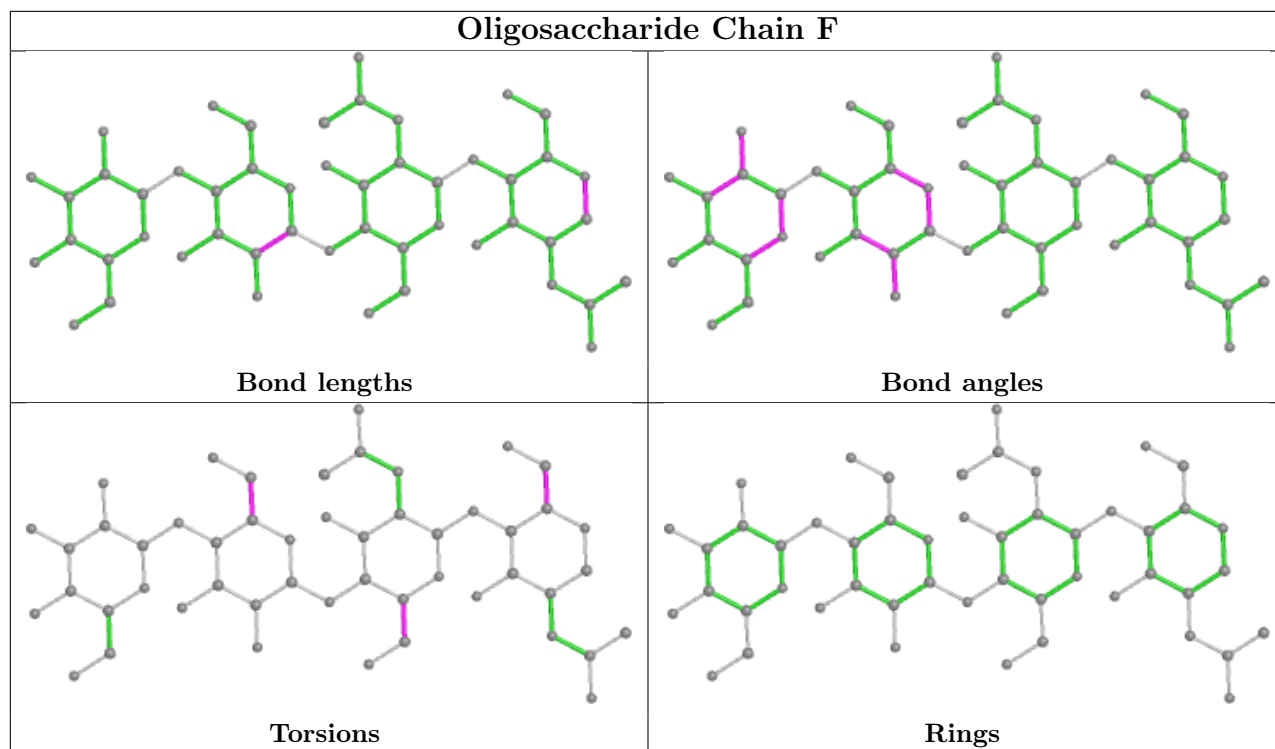
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

6 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$
5	NAG	B	1407	-	14,14,15	0.42	0	17,19,21	0.71	1 (5%)
5	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
5	NAG	B	1401	1	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
5	NAG	B	1404	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	A	1401	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
5	NAG	A	1404	1	14,14,15	0.30	0	17,19,21	0.65	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
5	NAG	B	1407	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1409	NAG	C2-N2-C7	3.13	127.36	122.90
5	B	1401	NAG	C2-N2-C7	3.11	127.33	122.90
5	A	1401	NAG	C2-N2-C7	3.04	127.23	122.90
5	B	1407	NAG	C1-O5-C5	2.46	115.53	112.19
5	B	1404	NAG	C1-O5-C5	2.29	115.29	112.19
5	A	1404	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1404	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1409	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	A	1409	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1401	NAG	C3-C2-N2-C7
5	A	1409	NAG	C3-C2-N2-C7
5	B	1401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1407	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

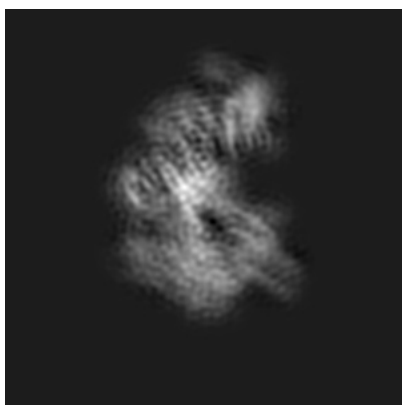
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9838. These allow visual inspection of the internal detail of the map and identification of artifacts.

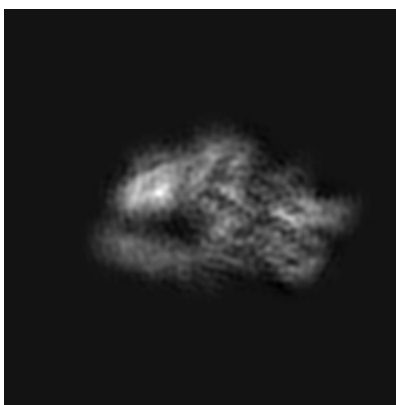
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

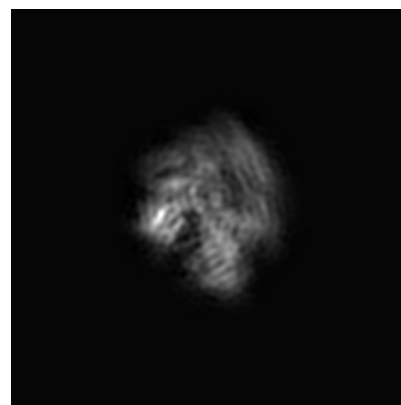
6.1.1 Primary map



X



Y

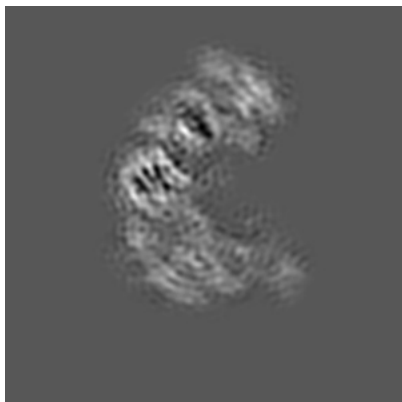


Z

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

6.2 Central slices [i](#)

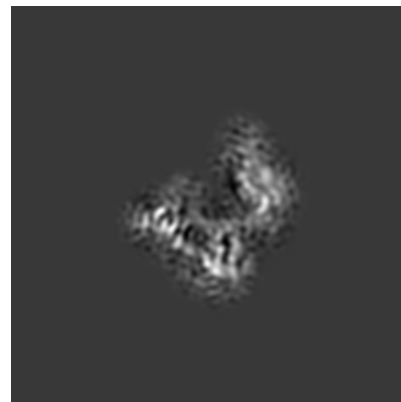
6.2.1 Primary map



X Index: 80



Y Index: 80

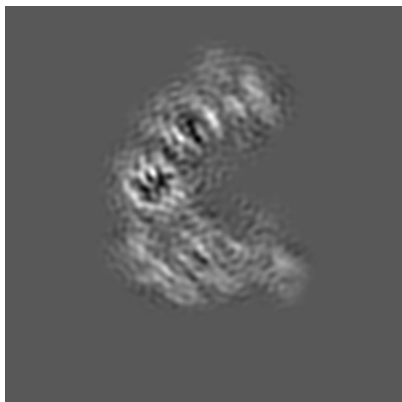


Z Index: 80

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

6.3 Largest variance slices [i](#)

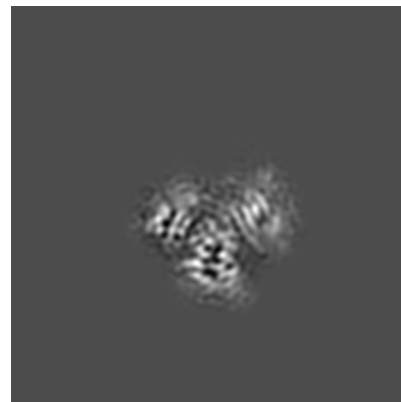
6.3.1 Primary map



X Index: 82



Y Index: 76

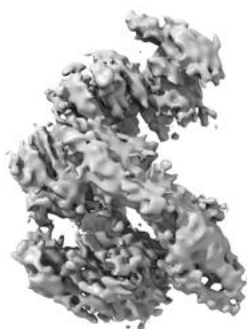


Z Index: 90

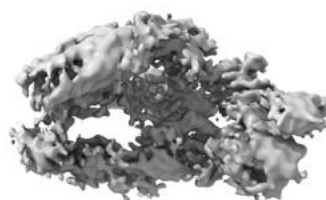
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

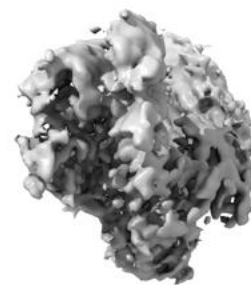
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

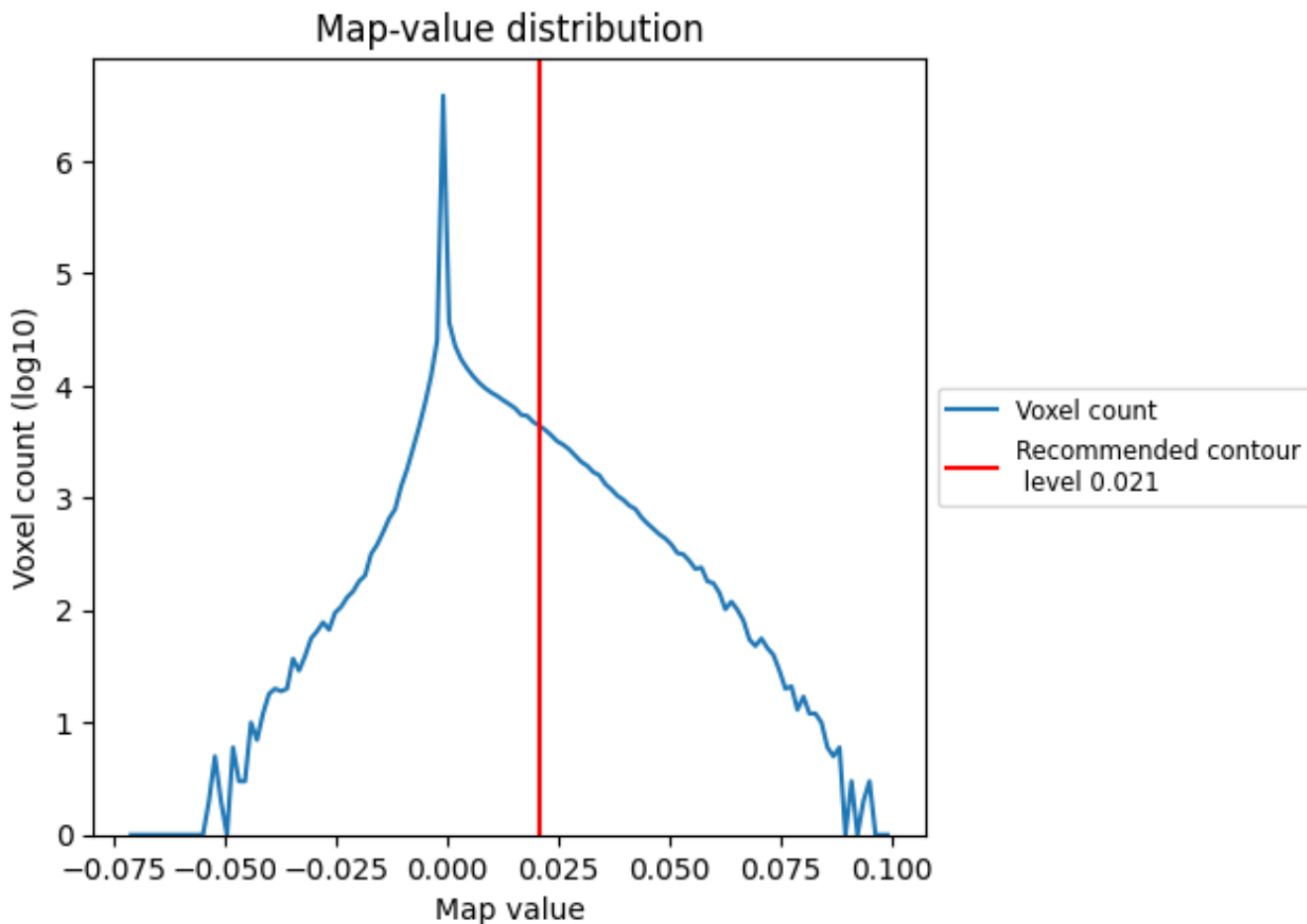
6.5 Mask visualisation

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

7 Map analysis [i](#)

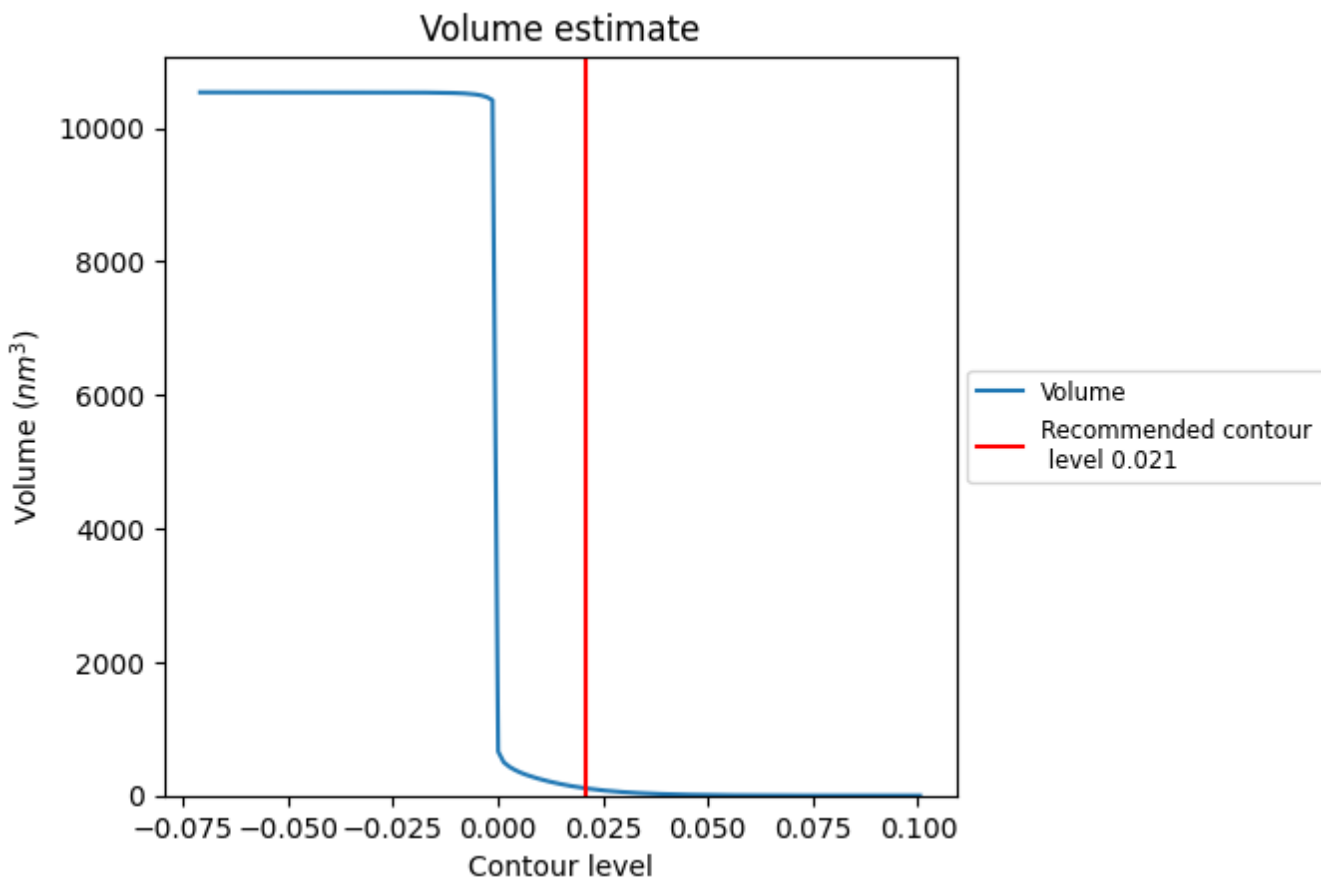
This section contains the results of statistical analysis of the map.

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.

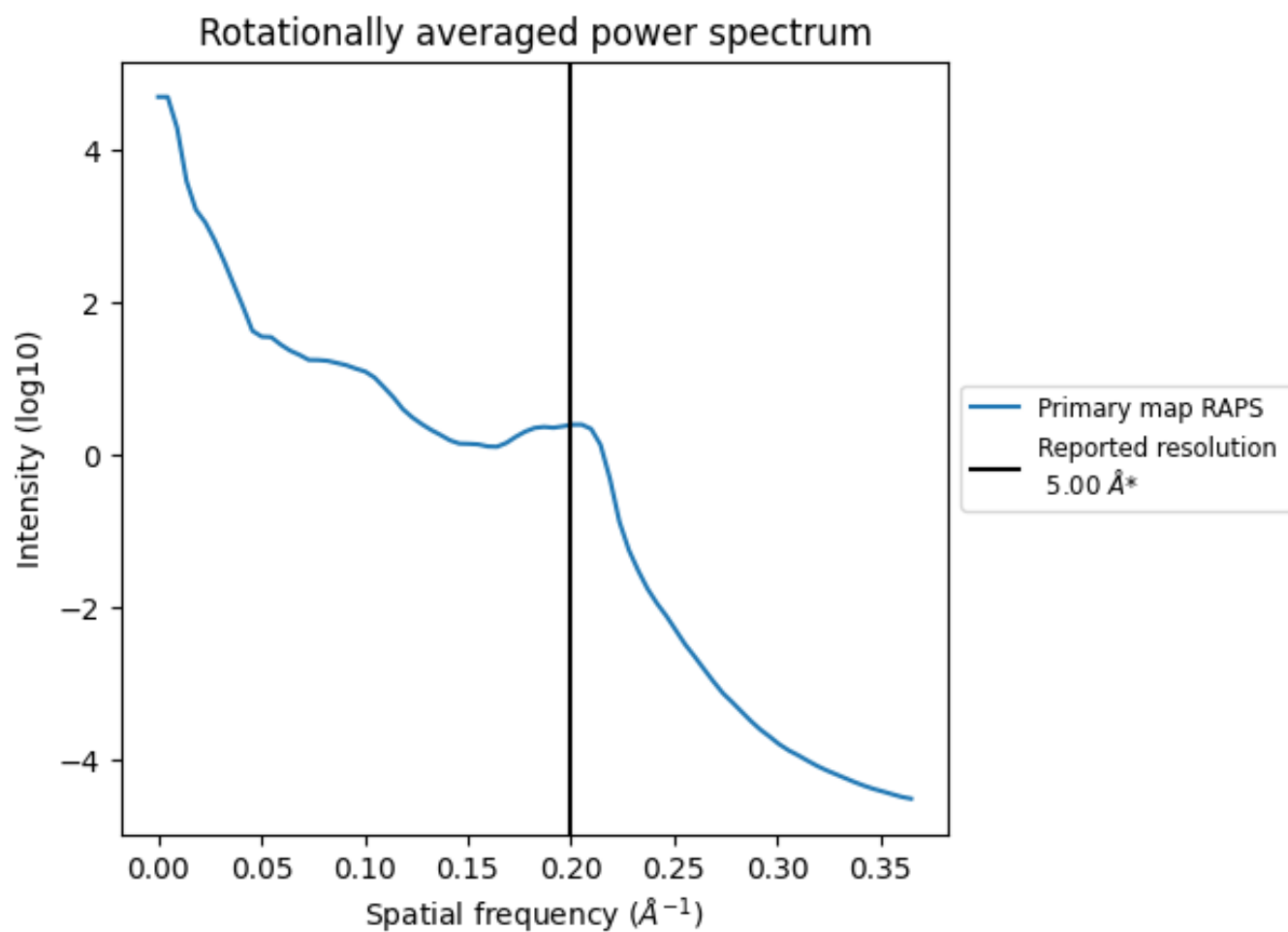
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 98 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](#)

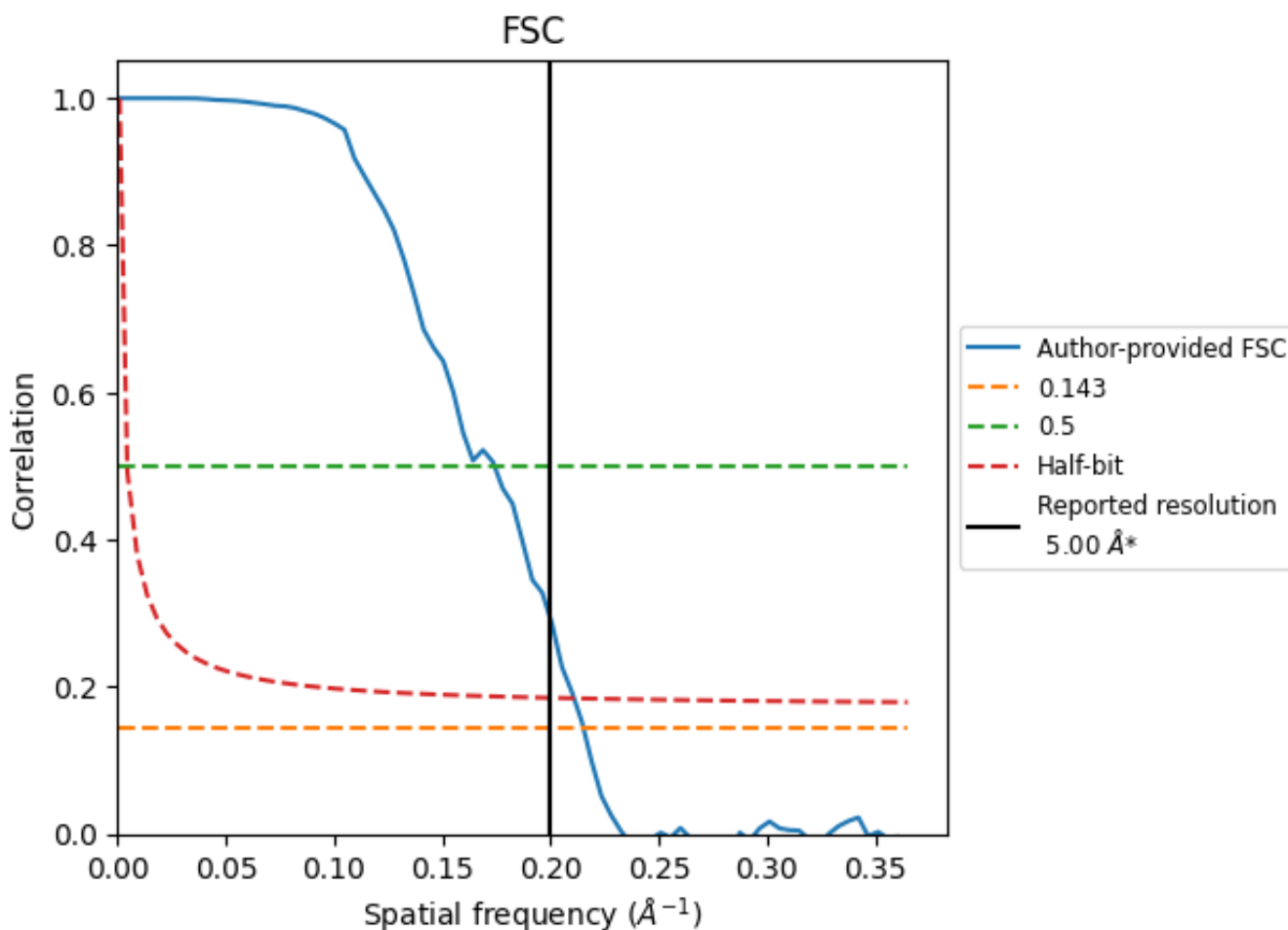


*Reported resolution corresponds to spatial frequency of 0.200\AA^{-1}

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

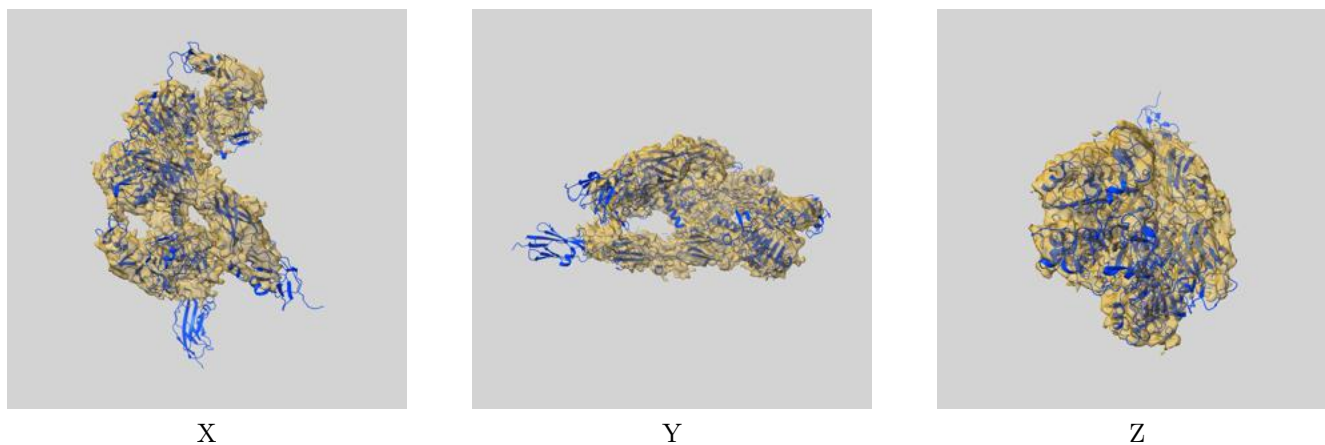
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.65	5.74	4.74
Unmasked-calculated*	-	-	-

*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-9838 and PDB model 6JK8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



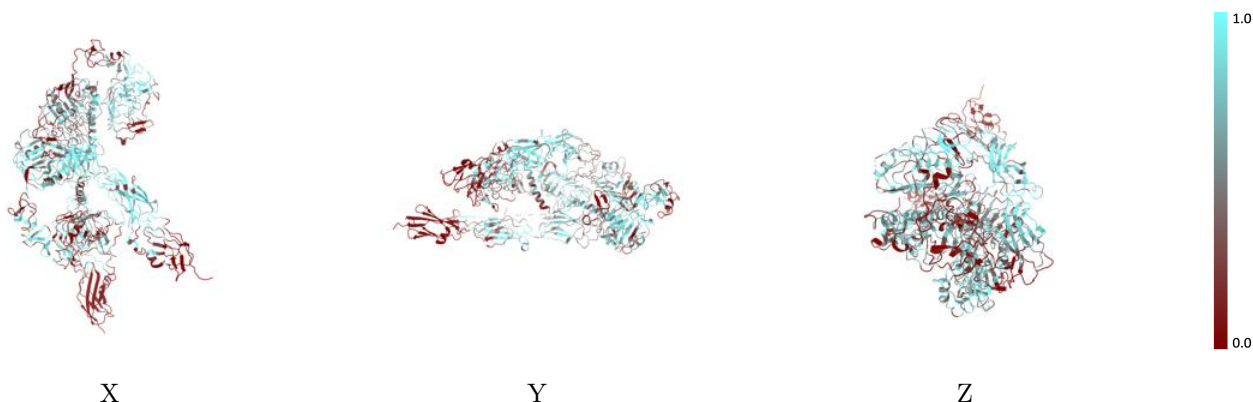
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



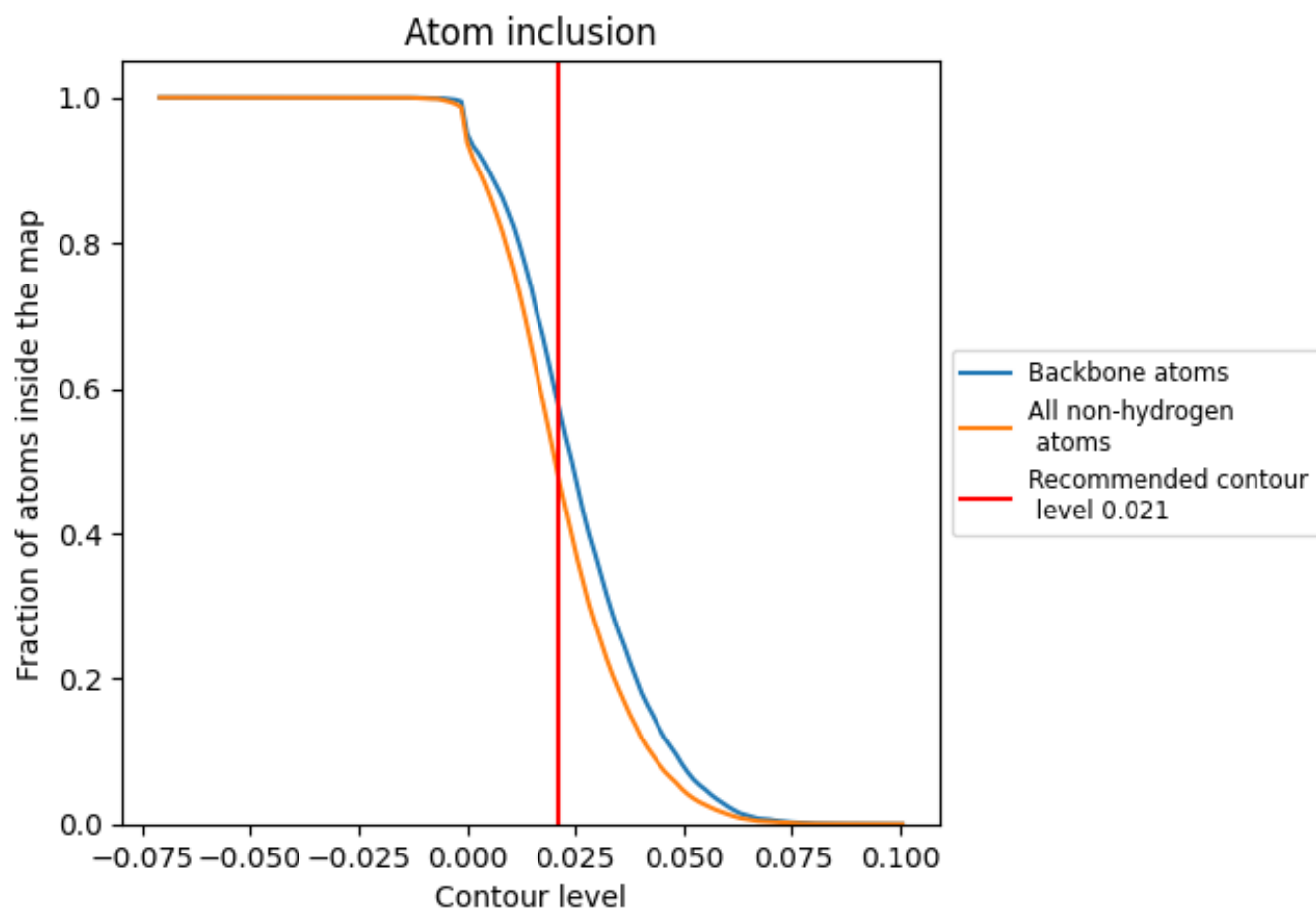
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.021).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 48% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4805	 0.1220
A	 0.5071	 0.1330
B	 0.4571	 0.1100
C	 0.3727	 0.1010
D	 0.4337	 0.1620
E	 0.9286	 0.3520
F	 0.3000	 0.1020
G	 0.2143	 -0.0360
H	 0.4286	 0.1470
I	 0.7500	 0.2880

