

Oct 10, 2023 - 05:47 pm BST

PDB	ID	:	8AGB
EMDB 1	ID	:	EMD-15419
Ti	tle	:	Structure of yeast oligosaccharylransferase complex with lipid-linked oligosac- charide bound
Autho	ors	:	Ramirez, A.S.; de Capitani, M.; Pesciullesi, G.; Kowal, J.; Bloch, J.S.; Irobalieva B.N.; Aebi M.; Reymond, J.L.; Locher, K.P.
Deposited •	on	:	2022-07-19
Resoluti	on	:	3.00 Å(reported)
T 1.	•	. т	
1 11	IS 1S	a F	ull wwPDB EM validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.35.1

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 3.00 Å.

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



Metric	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of cha	ain
1	А	718	67%	22% · 11%
2	В	65	42% 11%	48%
3	С	86	6% 81%	17% •
4	D	130	8%	22% 15%
5	Е	476	6%	22% • 9%
6	F	285	68%	17% • 11%
7	G	430	71%	20% • 8%
8	Н	350	29% 5%	66%



Mol	Chain	Length		Quality of chain	
9	Ι	7	29%	57%	14%
10	J	3	33%	100%	
11	K	2	50%	100%	50%
12	L	11	27%	73%	9%



2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 17202 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 Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	642	Total 5165	C 3422	N 824	O 896	S 23	0	0

• Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4.

Mol	Chain	Residues		Atoms					Trace
2	В	34	Total	C 1CC	N	0	S	0	0
			258	100	38	50	4		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
В	37	ARG	-	expression tag	UNP Q99380	
В	38	THR	-	expression tag	UNP Q99380	
В	39	LEU	-	expression tag	UNP Q99380	
В	40	GLN	-	expression tag	UNP Q99380	
В	41	VAL	-	expression tag	UNP Q99380	
В	42	ASP	-	expression tag	UNP Q99380	
В	43	GLY	-	expression tag	UNP Q99380	
В	44	GLY	-	expression tag	UNP Q99380	
В	45	SER	-	expression tag	UNP Q99380	
В	46	GLY	-	expression tag	UNP Q99380	
В	47	GLY	-	expression tag	UNP Q99380	
В	48	SER	-	expression tag	UNP Q99380	
В	49	LEU	-	expression tag	UNP Q99380	
В	50	GLU	-	expression tag	UNP Q99380	
В	51	VAL	-	expression tag	UNP Q99380	
В	52	LEU	-	expression tag	UNP Q99380	
В	53	PHE	-	expression tag	UNP Q99380	
В	54	GLN	-	expression tag	UNP Q99380	
В	55	GLY	-	expression tag	UNP Q99380	
В	56	PRO	-	expression tag	UNP Q99380	



Chain	Residue	Modelled	Actual	Comment	Reference
В	57	THR	-	expression tag	UNP Q99380
В	58	GLU	-	expression tag	UNP Q99380
В	59	THR	-	expression tag	UNP Q99380
В	60	SER	-	expression tag	UNP Q99380
В	61	GLN	-	expression tag	UNP Q99380
В	62	VAL	-	expression tag	UNP Q99380
В	63	ALA	-	expression tag	UNP Q99380
В	64	PRO	-	expression tag	UNP Q99380
B	65	ALA	-	expression tag	UNP Q99380

• Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	85	Total 666	C 448	N 99	0 118	S 1	0	0

• Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	110	Total 899	C 606	N 142	0 145	S 6	0	0

• Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues		Atoms					Trace
5	Е	433	Total 3499	C 2273	N 559	O 660	S 7	0	0

• Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
6	F	255	Total 1914	C 1255	N 316	O 339	${S \over 4}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	285	THR	-	expression tag	UNP Q02795



Chain	Residue	Modelled	Actual	Comment	Reference
F	286	ILE	-	expression tag	UNP Q02795

• Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	394	Total 3201	C 2053	N 528	0 616	$\frac{S}{4}$	0	0

• Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Н	120	Total 973	C 662	N 147	O 159	${ m S}{ m 5}$	0	0

• Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyran ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns	AltConf	Trace	
9	Ι	7	Total	C 46	N 2	0	0	0

• Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxybeta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns	AltConf	Trace	
10	J	3	Total 39	C 22	N 2	0 15	0	0

• Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-



acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns	AltConf	Trace	
11	K	2	Total 28	C 16	N 2	O 10	0	0

• Molecule 12 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranos e-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose -(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ace tamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		AltConf	Trace
12	L	11	Total 127	C 70	N 2	O 55	0	0

• Molecule 13 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C₄₂H₈₀NO₈P).





Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf
12	Δ	1	Total	С	Ν	0	Р	0
10	A	1	52	42	1	8	1	0
12	В	1	Total	С	Ν	Ο	Р	0
10	D	1	52	42	1	8	1	0
12	F	1	Total	С	Ν	0	Р	0
10	Ľ	1	52	42	1	8	1	0
13	C	1	Total	С	N	0	Р	0
10	G	I	52	42	1	8	1	0

• Molecule 14 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues		Ato	oms			AltConf
14	Λ	1	Total	С	Ν	Ο	Р	0
14	A	1	42	32	1	8	1	0
14	F	1	Total	С	Ν	0	Р	0
14	Г	1	42	32	1	8	1	0

• Molecule 15 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	AltConf
15	А	1	Total Mn 1 1	0

• Molecule 16 is phosphono [(3 {R},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-6,10,1 4-trienyl] hydrogen phosphate (three-letter code: ELU) (formula: $C_{20}H_{38}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



ELU	
C2 C4 C5 C5	
CT CT CT	
c11 c11	
C13 C16 C17	
C (1)C (1)C (2)	

Mol	Chain	Residues	Atoms			AltConf	
16	А	1	Total 29	C 20	O 7	Р 2	0

• Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms			AltConf	
17	G	1	Total	С	Ν	Ο	0
11		1	14	8	1	5	0
17	С	1	Total	С	Ν	Ο	0
11	G	1	14	8	1	5	0



3 Residue-property plots (i)

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

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



• Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5









 $\label{eq:mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ \end{array}$



NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN6 MAN6

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



	33%			
Chain J:		100%		
NAG1 NAG2 BMA3				
• Molecu	le 11: 2-acetamido-2-	deoxy-beta-D-glucop	yranose-(1-4)-2-acetam	ido-2-deoxy-beta-D-glu
copyrano	se			

Chain K:	50%	100%	50%

 $\label{eq:constraint} \bullet \mbox{Molecule 12: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-2-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-2-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-2-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-2-glucopyranose-(1-4)-2-acetamido-2-glucopyranose-(1-4)-2-acetamido-2-glucopyranose-(1-4)-2-acetamido-2-glucopyranose-(1-4)-2-glucopyranose-(1-4)-2-glucopyranose-(1-4)-2-glucopyranose-(1-4)-2-gluc$

	27%		
Chain L:	18%	73%	9%
•	* *		
DG1 AG2 MA3 AN5 AN5 AN5 CC7	AN10 AN11 AN11		
IN MAN WIN	W W BI		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89566	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 $(e^-/\text{\AA}^2)$	64	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	Depositor
Maximum map value	2.243	Depositor
Minimum map value	-1.111	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.417	Depositor
Map size (Å)	326.40002, 326.40002, 326.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8500001, 0.8500001, 0.8500001	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: NDG, PTY, ELU, MAN, CPL, GLC, NAG, MN, BMA

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

Mal	Chain	Bond	lengths	Bond	angles
	Unam	Chain RMSZ $\# Z > 5$		RMSZ	# Z > 5
1	А	0.29	0/5316	0.45	0/7229
2	В	0.26	0/261	0.39	0/354
3	С	0.28	0/684	0.42	0/926
4	D	0.28	0/922	0.41	0/1243
5	Ε	0.28	0/3599	0.47	0/4897
6	F	0.28	0/1958	0.55	0/2666
7	G	0.28	0/3283	0.47	0/4459
8	Н	0.28	0/1001	0.41	0/1362
All	All	0.28	0/17024	0.46	0/23136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5165	0	5122	97	0
2	В	258	0	267	5	0
3	С	666	0	677	11	0
4	D	899	0	927	25	0
5	Е	3499	0	3383	61	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1914	0	1895	37	0
7	G	3201	0	3102	52	0
8	Н	973	0	998	12	0
9	Ι	83	0	70	2	0
10	J	39	0	34	0	0
11	Κ	28	0	25	0	0
12	L	127	0	105	3	0
13	А	52	0	80	3	0
13	В	52	0	80	1	0
13	Е	52	0	80	0	0
13	G	52	0	80	1	0
14	А	42	0	60	1	0
14	F	42	0	60	0	0
15	А	1	0	0	0	0
16	A	29	0	0	0	0
17	G	28	0	26	0	0
All	All	17202	0	17071	275	0

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

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:717:ARG:H	7:G:214:GLN:HE22	1.30	0.79
1:A:398:PHE:HB3	1:A:405:LEU:HD12	1.66	0.78
4:D:47:ILE:HG23	4:D:91:LEU:HD12	1.76	0.67
7:G:262:SER:HB3	7:G:364:LEU:HD23	1.77	0.67
1:A:110:ASP:OD1	1:A:111:ILE:N	2.27	0.66
1:A:466:SER:O	1:A:470:THR:HG23	1.94	0.66
1:A:134:THR:HB	1:A:143:GLY:HA2	1.79	0.64
6:F:156:LEU:HD21	6:F:158:LEU:HB3	1.81	0.63
4:D:102:PHE:HB3	4:D:103:PRO:HD2	1.81	0.62
1:A:136:GLU:OE2	1:A:184:LYS:NZ	2.32	0.62
1:A:688:GLN:HE22	7:G:104:GLU:HG2	1.64	0.62
2:B:31:THR:HG23	2:B:32:MET:HG2	1.80	0.62
6:F:253:TYR:HH	7:G:386:SER:HG	1.47	0.61
7:G:175:GLY:H	7:G:236:ASP:HB3	1.66	0.61
6:F:95:MET:HE1	6:F:120:ASP:H	1.66	0.61
7:G:159:LEU:HD12	7:G:190:PRO:HB2	1.84	0.60
5:E:69:ALA:HB1	5:E:112:ILE:HD12	1.83	0.60



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
4:D:49:THR:OG1	6:F:215:TRP:NE1	2.35	0.59	
6:F:199:ILE:O	6:F:203:ILE:HG12	2.03	0.59	
6:F:51:ASP:O	6:F:153:ARG:NH2	2.36	0.59	
5:E:411:ASP:OD1	5:E:449:LYS:NZ	2.35	0.58	
6:F:30:PHE:N	6:F:108:SER:HG	2.01	0.58	
5:E:177:LEU:HD12	5:E:222:ILE:HD13	1.85	0.58	
6:F:75:SER:OG	6:F:76:THR:N	2.35	0.58	
6:F:246:GLU:HG3	7:G:407:ILE:HD11	1.85	0.57	
1:A:32:ARG:NE	1:A:160:SER:OG	2.37	0.57	
1:A:186:GLN:HE22	1:A:383:ASP:HB3	1.70	0.56	
7:G:303:GLU:N	7:G:303:GLU:OE1	2.38	0.56	
5:E:290:VAL:HG23	5:E:324:ARG:HG2	1.86	0.56	
5:E:41:ASP:HA	5:E:178:ILE:O	2.05	0.56	
1:A:573:PHE:O	1:A:676:MET:HA	2.05	0.56	
5:E:226:HIS:CE1	5:E:228:ALA:HB3	2.41	0.55	
7:G:126:LEU:O	7:G:129:LEU:N	2.38	0.55	
1:A:574:GLY:HA3	1:A:579:PHE:HB3	1.88	0.55	
5:E:252:GLU:OE1	5:E:303:TYR:OH	2.24	0.55	
5:E:71:GLU:N	5:E:71:GLU:OE2	2.36	0.55	
8:H:266:PHE:N	8:H:269:GLU:OE2	2.35	0.55	
7:G:70:ASP:HB2	7:G:75:LEU:HD13	1.88	0.55	
5:E:38:ARG:NH1	5:E:161:ASN:OD1	2.39	0.54	
5:E:144:TYR:HB3	5:E:145:PRO:HD3	1.89	0.54	
1:A:685:ASP:OD1	1:A:685:ASP:N	2.39	0.54	
6:F:33:THR:HB	6:F:112:TYR:HB2	1.90	0.54	
1:A:695:VAL:O	1:A:699:THR:HG23	2.07	0.54	
1:A:254:PRO:HD3	13:G:503:CPL:H132	1.90	0.53	
2:B:1:MET:HG2	2:B:2:ILE:H	1.73	0.53	
7:G:376:ARG:HG2	7:G:377:HIS:H	1.73	0.53	
7:G:192:LEU:HG	7:G:193:ASN:H	1.73	0.53	
5:E:81:PHE:CE2	5:E:94:SER:HB2	2.44	0.53	
7:G:26:THR:HG23	7:G:78:ASN:HB2	1.91	0.53	
6:F:253:TYR:OH	7:G:386:SER:OG	2.21	0.52	
7:G:150:GLU:HG2	7:G:175:GLY:HA2	1.91	0.52	
7:G:31:ASP:OD2	7:G:84:THR:HG23	2.09	0.52	
1:A:8:VAL:O	1:A:11:VAL:HG12	2.09	0.52	
1:A:138:LYS:HE3	1:A:423:LYS:HG2	1.91	0.52	
6:F:30:PHE:N	6:F:108:SER:O	2.43	0.52	
7:G:333:ASP:CG	7:G:334:SER:H	2.13	0.52	
3:C:60:TYR:CE2	5:E:465:PHE:HB2	2.45	0.52	
5:E:160:THR:OG1	5:E:161:ASN:N	2.42	0.52	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
6:F:146:LYS:HE3	6:F:149:GLU:HB2	1.92	0.52	
3:C:61:THR:O	3:C:65:VAL:HG23	2.11	0.51	
4:D:45:LYS:O	4:D:49:THR:HG23	2.11	0.51	
5:E:185:GLU:HG3	5:E:186:TYR:N	2.24	0.51	
7:G:302:GLU:OE1	7:G:302:GLU:N	2.42	0.51	
4:D:24:GLN:OE1	4:D:24:GLN:N	2.42	0.51	
4:D:32:ARG:HA	4:D:35:PHE:CE2	2.45	0.51	
5:E:317:GLU:O	5:E:320:HIS:HB2	2.10	0.51	
1:A:212:VAL:HA	1:A:215:THR:HG22	1.91	0.51	
7:G:187:GLN:HE21	7:G:224:LEU:HD21	1.75	0.51	
3:C:31:CYS:O	3:C:34:ILE:HG12	2.10	0.51	
4:D:80:GLY:O	4:D:83:ILE:HG22	2.11	0.51	
4:D:34:TYR:O	4:D:38:ILE:HG23	2.11	0.51	
7:G:152:VAL:HG13	7:G:171:ASP:HB3	1.91	0.50	
3:C:57:LEU:O	3:C:61:THR:HG23	2.10	0.50	
5:E:53:ILE:HG22	5:E:55:ILE:H	1.76	0.50	
1:A:580:GLY:O	1:A:585:ASN:ND2	2.43	0.50	
4:D:72:PHE:HE2	7:G:389:ILE:HD13	1.75	0.50	
7:G:410:VAL:O	7:G:414:VAL:HG22	2.12	0.50	
5:E:310:LEU:O	5:E:326:ARG:NH1	2.45	0.50	
1:A:451:VAL:HG22	8:H:317:ALA:HB2	1.94	0.50	
7:G:371:ASP:OD2	7:G:373:LYS:HE2	2.12	0.50	
1:A:366:LEU:HD22	1:A:417:ALA:HB1	1.93	0.50	
1:A:370:PHE:O	1:A:374:VAL:HG23	2.12	0.49	
6:F:160:LEU:HB3	6:F:162:PHE:CD1	2.47	0.49	
1:A:528:ASP:O	1:A:529:ARG:HD3	2.13	0.49	
5:E:349:LEU:HD12	5:E:361:ALA:HB2	1.94	0.49	
1:A:51:ASN:O	1:A:55:THR:HG22	2.13	0.49	
1:A:471:ARG:HH11	2:B:8:ASN:ND2	2.11	0.49	
2:B:19:MET:O	2:B:23:VAL:HG23	2.13	0.49	
8:H:256:TYR:HD2	8:H:268:ILE:HD13	1.78	0.49	
1:A:221:HIS:CE1	1:A:387:PHE:HB2	2.48	0.49	
1:A:600:GLU:OE1	1:A:600:GLU:N	2.34	0.49	
1:A:190:SER:OG	4:D:113:GLU:OE2	2.31	0.49	
1:A:452:SER:O	1:A:456:ILE:HG13	2.13	0.49	
7:G:89:ASN:O	7:G:93:GLN:HG2	2.12	0.49	
7:G:30:TYR:CZ	7:G:58:ASP:HB2	2.48	0.48	
6:F:38:ARG:HB2	6:F:116:LEU:HB3	1.94	0.48	
5:E:196:GLY:HA2	5:E:205:PHE:HB3	1.94	0.48	
7:G:109:ILE:HB	7:G:229:LEU:HD12	1.96	0.48	
1:A:7:CYS:SG	1:A:8:VAL:N	2.86	0.48	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:263:SER:O	1:A:267:MET:HG2	2.13	0.48
6:F:67:ILE:HG13	6:F:69:VAL:HG22	1.95	0.48
1:A:171:ALA:HB2	1:A:208:TRP:HB2	1.94	0.48
6:F:36:LYS:O	6:F:37:SER:HB2	2.12	0.48
1:A:293:LYS:NZ	4:D:22:ASP:HB3	2.28	0.48
6:F:81:GLN:O	6:F:81:GLN:HG3	2.13	0.48
1:A:121:LEU:HD22	13:A:801:CPL:H263	1.95	0.48
1:A:545:ILE:HD11	9:I:2:NAG:H82	1.96	0.48
7:G:32:GLN:HE21	7:G:36:PRO:HB3	1.79	0.48
1:A:268:ALA:O	1:A:272:VAL:HG23	2.13	0.47
1:A:615:ARG:HH22	1:A:619:ARG:HH11	1.61	0.47
5:E:369:PRO:HD2	5:E:372:THR:HG21	1.96	0.47
7:G:32:GLN:NE2	7:G:36:PRO:HB3	2.29	0.47
1:A:504:ARG:O	1:A:529:ARG:NH1	2.47	0.47
5:E:449:LYS:HB3	5:E:450:PRO:HD3	1.96	0.47
1:A:378:PHE:HE1	14:A:802:PTY:H111	1.79	0.47
1:A:595:GLU:HG3	1:A:602:ILE:O	2.15	0.47
1:A:628:LEU:O	1:A:632:MET:HB2	2.14	0.47
4:D:68:ILE:HG13	4:D:70:ASP:H	1.80	0.47
4:D:72:PHE:CE2	7:G:389:ILE:HD13	2.49	0.47
5:E:31:TRP:CE3	5:E:55:ILE:HG12	2.50	0.47
6:F:226:ILE:HG12	7:G:415:THR:HG23	1.97	0.47
5:E:288:VAL:HB	5:E:329:ILE:HB	1.97	0.47
12:L:1:NDG:H6C1	12:L:2:NAG:HN2	1.79	0.47
8:H:294:LEU:O	8:H:298:LEU:HB2	2.14	0.47
5:E:384:PRO:HB2	5:E:441:TYR:CE1	2.50	0.47
5:E:408:SER:OG	5:E:409:TYR:N	2.48	0.47
8:H:284:VAL:O	8:H:288:VAL:HG23	2.15	0.46
7:G:412:SER:O	7:G:416:THR:HG23	2.15	0.46
1:A:202:PHE:HA	1:A:205:VAL:HG13	1.97	0.46
3:C:14:LYS:HE2	3:C:14:LYS:HB3	1.66	0.46
5:E:270:ARG:O	5:E:274:MET:HG3	2.15	0.46
6:F:202:LEU:O	6:F:206:ILE:HG12	2.15	0.46
5:E:240:ILE:HG21	5:E:363:ILE:HD13	1.97	0.46
1:A:72:ASP:OD1	1:A:72:ASP:N	2.32	0.46
7:G:59:ILE:HB	7:G:89:ASN:HB3	1.98	0.46
1:A:516:TRP:CE3	1:A:516:TRP:HA	2.50	0.46
1:A:710:LYS:HA	1:A:710:LYS:HD3	1.80	0.46
5:E:447:PHE:O	5:E:451:LEU:HD13	2.15	0.46
6:F:200:PHE:O	6:F:204:ILE:HG13	2.16	0.46
1:A:289:ILE:HD12	1:A:293:LYS:HG3	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:409:LEU:O	1:A:413:ILE:HG13	2.16	0.46
7:G:258:PHE:O	7:G:260:GLU:HG2	2.15	0.46
6:F:45:GLU:N	6:F:157:GLN:O	2.35	0.46
5:E:119:PHE:HE1	5:E:131:LEU:HD21	1.81	0.45
5:E:213:ARG:HG3	5:E:214:PHE:HD2	1.81	0.45
1:A:171:ALA:O	1:A:174:LEU:N	2.50	0.45
7:G:125:PHE:O	7:G:128:GLU:HB2	2.16	0.45
1:A:81:VAL:O	1:A:83:GLY:N	2.46	0.45
1:A:274:GLY:O	1:A:278:ILE:HG12	2.16	0.45
1:A:248:VAL:HB	4:D:82:ILE:HG21	1.99	0.45
1:A:493:ILE:HD13	1:A:577:ILE:HD12	1.98	0.45
1:A:556:LYS:O	1:A:560:ILE:HG13	2.16	0.45
6:F:39:VAL:HG23	6:F:162:PHE:CE2	2.51	0.45
7:G:163:VAL:HG11	7:G:191:ILE:HD13	1.96	0.45
1:A:156:TYR:CE1	1:A:172:ILE:HG21	2.51	0.45
4:D:53:PHE:CD2	6:F:211:LEU:HB2	2.52	0.45
5:E:44:ASN:ND2	5:E:44:ASN:H	2.13	0.45
5:E:303:TYR:CE2	5:E:340:GLY:HA3	2.51	0.45
1:A:291:THR:HG23	1:A:292:ALA:H	1.81	0.45
3:C:43:ALA:HB2	3:C:63:LEU:HB3	1.99	0.45
1:A:157:ILE:O	1:A:161:VAL:HG23	2.16	0.45
1:A:497:ARG:NH2	5:E:309:GLY:HA3	2.32	0.45
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.84	0.45
5:E:56:LYS:HG2	5:E:57:ASN:N	2.31	0.45
5:E:297:GLU:OE2	5:E:297:GLU:N	2.50	0.45
6:F:45:GLU:O	6:F:157:GLN:HB3	2.17	0.45
7:G:327:LEU:HB3	7:G:339:TYR:HB3	1.98	0.45
1:A:401:VAL:HG12	1:A:402:MET:HG2	1.98	0.45
1:A:622:GLU:HG3	1:A:626:ASN:ND2	2.32	0.45
4:D:43:LYS:O	4:D:47:ILE:HG13	2.17	0.45
7:G:140:ILE:HD11	7:G:179:ALA:HB2	1.99	0.45
13:B:101:CPL:H412	13:B:101:CPL:H441	1.73	0.45
5:E:385:GLU:HG2	5:E:414:LYS:O	2.17	0.45
4:D:32:ARG:HA	4:D:35:PHE:CD2	2.52	0.44
6:F:107:LEU:HD22	6:F:107:LEU:HA	1.82	0.44
7:G:376:ARG:HD2	7:G:377:HIS:O	2.18	0.44
1:A:11:VAL:O	1:A:15:ILE:HG12	2.17	0.44
1:A:672:SER:OG	1:A:673:GLU:N	2.50	0.44
1:A:686:ASP:OD2	1:A:690:ARG:NE	2.50	0.44
7:G:46:ASP:HA	7:G:49:GLN:HG2	1.99	0.44
1:A:523:ILE:O	1:A:527:ALA:HB3	2.18	0.44



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:E:276:GLN:HG3	5:E:280:GLN:CD	2.37	0.44
1:A:656:THR:OG1	1:A:659:ASP:OD1	2.35	0.44
1:A:411:PRO:O	1:A:415:VAL:HG23	2.17	0.44
1:A:471:ARG:HH11	2:B:8:ASN:HD22	1.66	0.44
4:D:28:LYS:O	4:D:32:ARG:HG3	2.18	0.44
5:E:166:SER:OG	5:E:167:ALA:N	2.50	0.44
5:E:352:SER:HB2	5:E:358:LYS:HB3	2.00	0.44
1:A:548:LYS:HB2	1:A:594:SER:HB2	2.00	0.44
7:G:155:SER:HB2	7:G:170:GLU:O	2.17	0.44
5:E:469:THR:O	5:E:469:THR:HG22	2.18	0.43
6:F:30:PHE:N	6:F:108:SER:OG	2.50	0.43
5:E:242:LEU:HD23	5:E:345:LEU:HD11	2.00	0.43
1:A:273:PHE:O	1:A:277:GLN:HG2	2.19	0.43
1:A:506:ASN:ND2	5:E:334:ASN:H	2.15	0.43
3:C:76:VAL:HG13	3:C:86:VAL:HG21	2.00	0.43
5:E:123:ILE:HG23	5:E:127:GLU:HB2	2.00	0.43
6:F:221:ALA:HA	7:G:416:THR:HG21	1.99	0.43
7:G:34:THR:HG23	7:G:35:GLU:H	1.84	0.43
4:D:28:LYS:HB3	4:D:32:ARG:NH1	2.33	0.43
13:A:801:CPL:H441	13:A:801:CPL:H472	1.82	0.43
6:F:133:PRO:HB3	6:F:159:ASN:OD1	2.19	0.43
1:A:353:PRO:HB3	8:H:240:ILE:HD12	2.01	0.43
1:A:638:PRO:HA	1:A:646:ALA:HB2	1.99	0.43
5:E:124:SER:OG	5:E:127:GLU:HG2	2.19	0.43
5:E:273:LEU:O	5:E:277:ILE:HG12	2.19	0.43
7:G:316:LEU:HB3	7:G:323:TYR:HB2	2.00	0.43
1:A:277:GLN:HE21	1:A:277:GLN:HB3	1.65	0.43
5:E:35:ASP:OD1	5:E:36:TYR:N	2.51	0.43
1:A:631:LYS:HD2	1:A:661:PRO:HG2	2.01	0.43
1:A:59:VAL:HG21	1:A:111:ILE:HD13	2.01	0.43
1:A:139:ASP:OD1	1:A:140:ALA:N	2.50	0.43
1:A:378:PHE:CE2	1:A:389:ILE:HG21	2.54	0.43
5:E:41:ASP:HB3	5:E:48:SER:OG	2.18	0.43
7:G:264:ILE:HD11	7:G:364:LEU:HD13	2.00	0.43
1:A:353:PRO:HG3	8:H:240:ILE:HB	2.01	0.43
6:F:133:PRO:HB2	6:F:157:GLN:HG3	2.01	0.43
1:A:367:ILE:HG13	8:H:232:ILE:HD12	2.01	0.42
3:C:47:VAL:HA	3:C:56:LYS:HE3	2.01	0.42
4:D:109:ARG:O	4:D:113:GLU:HG3	2.19	0.42
1:A:186:GLN:HE22	1:A:383:ASP:CB	2.32	0.42
1:A:20:ILE:HG21	1:A:144:LEU:HD22	2.01	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:717:ARG:H	7:G:214:GLN:NE2	2.06	0.42
3:C:80:ASN:HD21	3:C:86:VAL:H	1.67	0.42
5:E:205:PHE:CD1	5:E:205:PHE:N	2.88	0.42
6:F:140:LEU:HD12	6:F:151:LEU:HB3	2.00	0.42
7:G:275:ASP:OD1	7:G:277:THR:OG1	2.29	0.42
7:G:399:ILE:O	7:G:402:VAL:HG12	2.19	0.42
7:G:73:GLN:HE21	7:G:73:GLN:HB2	1.59	0.42
8:H:258:LEU:HD13	8:H:266:PHE:CZ	2.54	0.42
4:D:73:PRO:HA	12:L:8:GLC:O3	2.19	0.42
5:E:111:GLU:HG2	5:E:113:ARG:HH22	1.84	0.42
1:A:278:ILE:HG12	1:A:278:ILE:H	1.72	0.42
5:E:453:ILE:O	5:E:457:ILE:HG13	2.20	0.42
8:H:324:PHE:O	8:H:328:THR:HG23	2.19	0.42
1:A:562:LYS:HB3	1:A:562:LYS:HE2	1.70	0.42
5:E:37:LYS:HB2	5:E:52:GLU:HB3	2.01	0.42
6:F:159:ASN:O	6:F:160:LEU:HD23	2.20	0.42
6:F:227:PRO:HB2	6:F:231:THR:HG23	2.02	0.42
1:A:168:GLU:O	1:A:172:ILE:HG22	2.19	0.42
1:A:157:ILE:HG21	1:A:470:THR:HB	2.02	0.42
4:D:22:ASP:N	4:D:22:ASP:OD1	2.52	0.42
5:E:470:LEU:HD12	5:E:470:LEU:HA	1.83	0.42
4:D:127:HIS:HD2	6:F:252:TYR:OH	2.03	0.41
12:L:11:MAN:O4	12:L:11:MAN:O6	2.37	0.41
1:A:289:ILE:HG21	4:D:26:THR:HG22	2.03	0.41
1:A:447:ALA:HB2	8:H:310:ALA:HB1	2.01	0.41
5:E:183:PHE:HB3	5:E:222:ILE:HD11	2.02	0.41
1:A:157:ILE:HD12	1:A:470:THR:HG21	2.02	0.41
1:A:555:GLU:O	1:A:559:GLU:HG2	2.20	0.41
5:E:156:LEU:O	5:E:223:VAL:HA	2.20	0.41
1:A:33:LEU:HD13	13:A:801:CPL:H132	2.02	0.41
1:A:50:PHE:HE2	1:A:86:LEU:HD13	1.86	0.41
5:E:414:LYS:HB2	5:E:414:LYS:HE2	1.89	0.41
7:G:389:ILE:HG22	7:G:391:ASN:H	1.85	0.41
1:A:627:SER:O	1:A:631:LYS:HG2	2.20	0.41
3:C:3:TYR:HD1	5:E:393:ASP:HB3	1.85	0.41
5:E:134:LYS:HB3	5:E:134:LYS:HE3	1.80	0.41
6:F:99:PRO:HB2	6:F:110:TYR:HB3	2.02	0.41
7:G:39:GLU:H	7:G:39:GLU:HG2	1.70	0.41
8:H:339:PRO:O	8:H:341:PRO:HD3	2.21	0.41
5:E:70:PHE:HD2	5:E:75:PHE:HD2	1.70	0.41
7:G:330:SER:HB3	7:G:340:THR:HG22	2.02	0.41



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:587:PHE:O	1:A:591:ILE:HG13	2.21	0.40	
1:A:709:ILE:HG21	7:G:135:PRO:HG3	2.03	0.40	
5:E:361:ALA:O	5:E:436:LEU:HA	2.21	0.40	
5:E:407:LYS:HB3	5:E:407:LYS:HE2	1.92	0.40	
1:A:538:TRP:CZ3	1:A:539:ASN:HB2	2.55	0.40	
1:A:110:ASP:O	1:A:114:VAL:HG23	2.20	0.40	
1:A:135:LYS:HG2	1:A:135:LYS:O	2.21	0.40	
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.92	0.40	
5:E:37:LYS:HB3	5:E:37:LYS:HE3	1.71	0.40	
6:F:184:ILE:HD11	9:I:6:MAN:H3	2.04	0.40	
4:D:87:GLN:HE21	4:D:91:LEU:CD2	2.35	0.40	
6:F:79:PRO:HG3	6:F:140:LEU:HB3	2.04	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	Perce	entiles
1	А	634/718~(88%)	602~(95%)	32~(5%)	0	100	100
2	В	32/65~(49%)	31~(97%)	1 (3%)	0	100	100
3	С	83/86~(96%)	75~(90%)	8 (10%)	0	100	100
4	D	108/130~(83%)	104 (96%)	4 (4%)	0	100	100
5	Е	427/476~(90%)	404 (95%)	23~(5%)	0	100	100
6	F	253/285~(89%)	233~(92%)	17 (7%)	3 (1%)	13	48
7	G	392/430~(91%)	373~(95%)	19 (5%)	0	100	100
8	Н	116/350~(33%)	106 (91%)	10 (9%)	0	100	100
All	All	2045/2540 (80%)	1928 (94%)	114 (6%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
6	F	40	MET
6	F	37	SER
6	F	41	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	542/613~(88%)	514 (95%)	28~(5%)	23 59
2	В	31/55~(56%)	31 (100%)	0	100 100
3	С	74/75~(99%)	74 (100%)	0	100 100
4	D	99/115~(86%)	97~(98%)	2(2%)	55 83
5	Ε	389/426~(91%)	371~(95%)	18 (5%)	27 64
6	F	193/248~(78%)	175 (91%)	18 (9%)	9 33
7	G	359/392~(92%)	343~(96%)	16 (4%)	27 64
8	Н	104/316~(33%)	100 (96%)	4 (4%)	33 69
All	All	1791/2240 (80%)	1705 (95%)	86 (5%)	29 62

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	45	GLU
1	А	48	PRO
1	А	160	SER
1	А	170	ILE
1	А	203	TYR
1	А	205	VAL
1	А	255	PHE
1	А	262	ARG
1	А	283	ASP
1	А	294	PHE
1	А	354	VAL
1	А	365	PHE
1	А	378	PHE



Mol	Chain	Res	Type
1	А	379	LEU
1	А	381	LEU
1	А	391	TYR
1	А	395	CYS
1	А	416	SER
1	А	446	LEU
1	А	542	HIS
1	А	543	ILE
1	А	572	ILE
1	А	587	PHE
1	А	594	SER
1	А	617	ASP
1	А	671	THR
1	А	691	THR
1	А	716	LEU
4	D	50	PHE
4	D	128	PHE
5	Е	44	ASN
5	Е	58	ILE
5	Е	79	SER
5	Е	82	SER
5	Е	123	ILE
5	Е	124	SER
5	Е	148	VAL
5	Е	170	THR
5	Е	185	GLU
5	Е	204	GLU
5	Е	205	PHE
5	Е	216	SER
5	Е	243	SER
5	Е	252	GLU
5	E	350	HIS
5	Е	379	LEU
5	Е	380	SER
5	Е	467	LEU
6	F	33	THR
6	F	36	LYS
6	F	38	ARG
6	F	39	VAL
6	F	40	MET
6	F	78	LYS
6	F	80	PHE



Mol	Chain	Res	Type
6	F	100	GLU
6	F	102	LYS
6	F	103	ASP
6	F	107	LEU
6	F	118	LYS
6	F	119	LEU
6	F	140	LEU
6	F	146	LYS
6	F	151	LEU
6	F	159	ASN
6	F	175	PHE
7	G	60	ASN
7	G	66	VAL
7	G	67	ASP
7	G	68	LEU
7	G	73	GLN
7	G	136	LYS
7	G	140	ILE
7	G	141	ARG
7	G	145	SER
7	G	154	SER
7	G	202	SER
7	G	244	ASP
7	G	318	GLN
7	G	348	ASP
7	G	362	ILE
7	G	391	ASN
8	Н	293	PHE
8	Н	297	HIS
8	Н	309	ASP
8	Н	324	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	186	GLN
1	А	266	HIS
1	А	277	GLN
1	А	506	ASN
1	А	542	HIS
1	А	626	ASN
1	А	653	GLN



Mol	Chain	Res	Type
1	А	688	GLN
2	В	6	GLN
2	В	8	ASN
3	С	21	HIS
3	С	25	GLN
3	С	80	ASN
4	D	61	GLN
4	D	87	GLN
4	D	122	HIS
4	D	127	HIS
5	Е	44	ASN
5	Е	93	ASN
5	Е	118	GLN
5	Е	217	ASN
5	Е	226	HIS
5	Е	367	ASN
5	Е	416	HIS
5	Е	425	ASN
6	F	90	ASN
6	F	104	ASN
6	F	125	GLN
6	F	150	ASN
6	F	166	HIS
6	F	217	ASN
7	G	73	GLN
7	G	108	ASN
7	G	157	HIS
7	G	214	GLN
7	G	226	ASN
7	G	242	ASN
7	G	243	GLN
7	G	246	ASN
7	G	271	HIS
7	G	273	HIS
7	G	318	GLN
7	G	391	ASN
8	Н	238	ASN
8	Н	260	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

23 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).

Mal	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		les
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
9	NAG	Ι	1	9,1	14,14,15	0.44	0	$17,\!19,\!21$	0.46	0
9	NAG	Ι	2	9	14,14,15	0.22	0	$17,\!19,\!21$	0.46	0
9	BMA	Ι	3	9	11,11,12	0.44	0	$15,\!15,\!17$	0.79	0
9	MAN	Ι	4	9	11,11,12	0.65	0	$15,\!15,\!17$	1.17	2 (13%)
9	MAN	Ι	5	9	11,11,12	0.68	0	$15,\!15,\!17$	1.00	1 (6%)
9	MAN	Ι	6	9	11,11,12	0.67	0	$15,\!15,\!17$	0.87	1 (6%)
9	MAN	Ι	7	9	11,11,12	0.69	0	$15,\!15,\!17$	0.91	1 (6%)
10	NAG	J	1	5,10	14,14,15	0.25	0	17,19,21	0.39	0
10	NAG	J	2	10	14,14,15	0.18	0	17,19,21	0.48	0
10	BMA	J	3	10	11,11,12	0.60	0	$15,\!15,\!17$	0.75	0
11	NAG	К	1	5,11	14,14,15	0.76	1 (7%)	$17,\!19,\!21$	1.03	1(5%)
11	NAG	K	2	11	14,14,15	0.22	0	$17,\!19,\!21$	0.50	0
12	NDG	L	1	16,12	14,14,15	0.25	0	$17,\!19,\!21$	0.42	0
12	MAN	L	10	12	11,11,12	1.08	2 (18%)	$15,\!15,\!17$	1.33	2 (13%)
12	MAN	L	11	12	11,11,12	0.87	1 (9%)	$15,\!15,\!17$	1.32	2 (13%)
12	NAG	L	2	12	14,14,15	0.26	0	17,19,21	0.51	0
12	BMA	L	3	12	11,11,12	0.52	0	$15,\!15,\!17$	0.69	0
12	MAN	L	4	12	11,11,12	0.67	0	$15,\!15,\!17$	1.28	2 (13%)
12	MAN	L	5	12	11,11,12	0.90	1 (9%)	$15,\!15,\!17$	1.02	1 (6%)
12	MAN	L	6	12	11,11,12	0.64	0	$15,\!15,\!17$	0.92	1 (6%)
12	GLC	L	7	12	11,11,12	0.61	0	$15,\!15,\!17$	0.87	1 (6%)
12	GLC	L	8	12	11,11,12	0.60	0	$15,\!15,\!17$	0.83	0
12	GLC	L	9	12	11,11,12	0.64	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
9	NAG	Ι	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	Ι	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Ι	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Ι	4	9	-	2/2/19/22	0/1/1/1
9	MAN	Ι	5	9	-	0/2/19/22	0/1/1/1
9	MAN	Ι	6	9	-	0/2/19/22	0/1/1/1
9	MAN	Ι	7	9	-	0/2/19/22	0/1/1/1
10	NAG	J	1	5,10	-	2/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	2/2/19/22	0/1/1/1
11	NAG	K	1	5,11	-	4/6/23/26	0/1/1/1
11	NAG	К	2	11	-	3/6/23/26	0/1/1/1
12	NDG	L	1	16,12	-	2/6/23/26	0/1/1/1
12	MAN	L	10	12	-	2/2/19/22	0/1/1/1
12	MAN	L	11	12	-	1/2/19/22	1/1/1/1
12	NAG	L	2	12	-	1/6/23/26	0/1/1/1
12	BMA	L	3	12	-	0/2/19/22	0/1/1/1
12	MAN	L	4	12	-	2/2/19/22	0/1/1/1
12	MAN	L	5	12	_	0/2/19/22	0/1/1/1
12	MAN	L	6	12	-	0/2/19/22	0/1/1/1
12	GLC	L	7	12	-	0/2/19/22	0/1/1/1
12	GLC	L	8	12	_	0/2/19/22	0/1/1/1
12	GLC	L	9	12	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	10	MAN	C1-C2	2.76	1.58	1.52
11	Κ	1	NAG	O5-C1	2.51	1.47	1.43
12	L	5	MAN	O5-C1	-2.13	1.40	1.43
12	L	11	MAN	C1-C2	2.06	1.56	1.52
12	L	10	MAN	C2-C3	2.04	1.55	1.52

All (15) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
11	Κ	1	NAG	C1-O5-C5	3.90	117.48	112.19
12	L	11	MAN	C1-O5-C5	3.37	116.76	112.19
12	L	4	MAN	O2-C2-C3	-3.20	103.73	110.14
9	Ι	4	MAN	O2-C2-C3	-3.20	103.73	110.14
12	L	5	MAN	O2-C2-C3	-3.13	103.88	110.14
12	L	10	MAN	C1-C2-C3	3.05	113.41	109.67
12	L	4	MAN	C1-O5-C5	2.95	116.19	112.19
9	Ι	5	MAN	O2-C2-C3	-2.67	104.79	110.14
9	Ι	4	MAN	C1-O5-C5	2.49	115.57	112.19
12	L	11	MAN	O2-C2-C3	-2.25	105.63	110.14
12	L	6	MAN	O2-C2-C3	-2.23	105.67	110.14
12	L	7	GLC	C1-C2-C3	2.22	112.40	109.67
9	Ι	6	MAN	O2-C2-C3	-2.22	105.70	110.14
9	Ι	7	MAN	O2-C2-C3	-2.19	105.75	110.14
12	L	10	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

All	(30)) torsion	outliers	are	listed	below:	
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Mol	Chain	Res	Type	Atoms
12	L	4	MAN	C4-C5-C6-O6
9	Ι	2	NAG	O5-C5-C6-O6
12	L	1	NDG	O5-C5-C6-O6
12	L	4	MAN	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
9	Ι	3	BMA	C4-C5-C6-O6
9	Ι	4	MAN	O5-C5-C6-O6
9	Ι	2	NAG	C4-C5-C6-O6
12	L	1	NDG	C4-C5-C6-O6
9	Ι	4	MAN	C4-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6
9	Ι	1	NAG	C8-C7-N2-C2
9	Ι	1	NAG	O7-C7-N2-C2
11	Κ	1	NAG	C8-C7-N2-C2
11	Κ	1	NAG	O7-C7-N2-C2
11	Κ	1	NAG	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
9	Ι	3	BMA	O5-C5-C6-O6
12	L	9	GLC	O5-C5-C6-O6
12	L	11	MAN	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
11	Κ	2	NAG	C4-C5-C6-O6
10	J	3	BMA	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
11	Κ	2	NAG	O5-C5-C6-O6
12	L	10	MAN	C4-C5-C6-O6
11	Κ	2	NAG	C3-C2-N2-C7
12	L	10	MAN	O5-C5-C6-O6
11	Κ	1	NAG	C4-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
12	L	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	11	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Ι	2	NAG	1	0
12	L	11	MAN	1	0
12	L	8	GLC	1	0
12	L	2	NAG	1	0
9	Ι	6	MAN	1	0
12	L	1	NDG	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)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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).

Mal	Tuno	Chain	Dog	Link	Bo	Bond lengths			Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
17	NAG	G	502	7	14,14,15	1.18	1 (7%)	17,19,21	1.09	2 (11%)	
14	PTY	А	802	-	41,41,49	0.93	4 (9%)	44,46,54	1.07	2 (4%)	
13	CPL	В	101	-	51,51,51	1.28	6 (11%)	$57,\!59,\!59$	1.02	2 (3%)	
16	ELU	А	804	15,12	26,28,28	0.74	0	33,37,37	1.45	7 (21%)	
14	PTY	F	301	-	41,41,49	0.94	4 (9%)	44,46,54	1.07	2 (4%)	
13	CPL	А	801	-	51,51,51	1.27	5 (9%)	57,59,59	0.89	1 (1%)	



Mal	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec Link		Dog	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2									
13	CPL	Е	501	-	51,51,51	0.37	0	$57,\!59,\!59$	0.34	0									
17	NAG	G	501	7	14,14,15	0.70	1 (7%)	17,19,21	1.02	1 (5%)									
13	CPL	G	503	-	51,51,51	1.28	6 (11%)	57,59,59	1.06	3 (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
17	NAG	G	502	7	-	1/6/23/26	0/1/1/1
14	PTY	А	802	-	-	23/45/45/53	-
13	CPL	В	101	-	-	16/55/55/55	-
16	ELU	А	804	15,12	-	15/31/31/31	-
14	PTY	F	301	-	-	23/45/45/53	-
13	CPL	А	801	-	-	16/55/55/55	-
13	CPL	Е	501	-	-	27/55/55/55	-
17	NAG	G	501	7	-	2/6/23/26	0/1/1/1
13	CPL	G	503	-	-	22/55/55/55	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	502	NAG	O5-C1	-4.26	1.36	1.43
13	В	101	CPL	O2-C31	3.39	1.43	1.34
13	В	101	CPL	O3-C11	3.34	1.43	1.33
13	G	503	CPL	O2-C31	3.28	1.43	1.34
13	А	801	CPL	O3-C11	3.25	1.42	1.33
13	G	503	CPL	O3-C11	3.25	1.42	1.33
13	А	801	CPL	O2-C31	3.20	1.43	1.34
14	F	301	PTY	O7-C6	-2.64	1.40	1.46
14	А	802	PTY	O7-C6	-2.43	1.40	1.46
13	G	503	CPL	P-O4P	2.40	1.69	1.59
13	А	801	CPL	O2-C2	-2.36	1.40	1.46
14	F	301	PTY	O4-C30	2.35	1.40	1.33
13	В	101	CPL	P-O4P	2.33	1.68	1.59
14	А	802	PTY	O4-C30	2.33	1.40	1.33
13	В	101	CPL	C32-C31	2.27	1.57	1.50
13	А	801	CPL	P-O4P	2.25	1.68	1.59
13	G	503	CPL	C32-C31	2.23	1.57	1.50



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	503	CPL	O2-C2	-2.17	1.41	1.46
13	А	801	CPL	C32-C31	2.17	1.57	1.50
14	А	802	PTY	O4-C1	-2.15	1.40	1.45
14	F	301	PTY	O4-C1	-2.11	1.40	1.45
17	G	501	NAG	O5-C1	2.10	1.47	1.43
14	А	802	PTY	O7-C8	2.09	1.40	1.34
13	В	101	CPL	O2-C2	-2.08	1.41	1.46
13	G	503	CPL	P-O3P	2.03	1.67	1.59
13	В	101	CPL	P-O3P	2.03	1.67	1.59
14	F	301	PTY	O7-C8	2.00	1.40	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	G	503	CPL	O2-C31-C32	4.07	120.27	111.50
14	А	802	PTY	O7-C8-C11	3.89	119.89	111.50
13	В	101	CPL	O2-C31-C32	3.88	119.86	111.50
17	G	501	NAG	C1-O5-C5	3.83	117.38	112.19
14	F	301	PTY	O7-C8-C11	3.67	119.41	111.50
17	G	502	NAG	C3-C4-C5	3.40	116.31	110.24
13	А	801	CPL	O2-C31-C32	3.27	118.55	111.50
16	А	804	ELU	C6-C7-C8	-3.19	119.97	127.66
16	А	804	ELU	C10-C8-C9	3.00	120.31	115.27
16	А	804	ELU	PA-O3A-PB	-2.84	123.07	132.83
14	F	301	PTY	O4-C30-C31	2.66	120.27	111.91
13	В	101	CPL	O3-C11-C12	2.65	120.21	111.91
16	А	804	ELU	C14-C13-C15	2.61	119.66	115.27
14	А	802	PTY	O4-C30-C31	2.46	119.63	111.91
17	G	502	NAG	C4-C3-C2	2.45	114.61	111.02
16	А	804	ELU	C16-C17-C18	-2.35	119.71	127.75
13	G	503	CPL	O3-C11-C12	2.35	119.28	111.91
13	G	503	CPL	C4-C5-N	-2.33	108.00	115.78
16	A	804	ELU	C19-C18-C20	2.17	119.39	114.60
16	А	804	ELU	C11-C12-C13	-2.11	122.57	127.66

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	В	101	CPL	O4P-C4-C5-N
13	Е	501	CPL	O4P-C4-C5-N
13	Е	501	CPL	C32-C31-O2-C2



Mol	Chain	Res	Type	Atoms
13	Е	501	CPL	O31-C31-O2-C2
13	Е	501	CPL	C1-O3P-P-O2P
13	G	503	CPL	C32-C31-O2-C2
14	А	802	PTY	C3-O11-P1-O13
14	А	802	PTY	C3-O11-P1-O14
14	F	301	PTY	O4-C1-C6-O7
14	F	301	PTY	N1-C2-C3-O11
14	F	301	PTY	C3-O11-P1-O12
16	А	804	ELU	C1-O1-PA-O2A
16	А	804	ELU	C1-O1-PA-O1A
16	А	804	ELU	O1-C1-C2-C3
16	А	804	ELU	C1-C2-C3-C4
16	А	804	ELU	C12-C13-C15-C16
16	А	804	ELU	C14-C13-C15-C16
13	G	503	CPL	O31-C31-O2-C2
13	Е	501	CPL	C41-C42-C43-C44
13	G	503	CPL	O11-C11-O3-C3
13	G	503	CPL	C12-C11-O3-C3
16	А	804	ELU	C10-C8-C9-C11
16	А	804	ELU	C7-C8-C9-C11
17	G	501	NAG	O5-C5-C6-O6
13	В	101	CPL	C12-C11-O3-C3
17	G	501	NAG	C4-C5-C6-O6
16	А	804	ELU	C4-C3-C5-C6
13	G	503	CPL	C31-C32-C33-C34
13	Ε	501	CPL	C12-C11-O3-C3
14	F	301	PTY	C31-C32-C33-C34
16	А	804	ELU	C12-C11-C9-C8
13	G	503	CPL	C11-C12-C13-C14
13	В	101	CPL	O11-C11-O3-C3
13	Ε	501	CPL	C1-O3P-P-O4P
14	F	301	PTY	C3-O11-P1-O14
13	Е	501	CPL	C32-C33-C34-C35
13	Ε	501	CPL	O11-C11-O3-C3
13	В	101	CPL	C12-C13-C14-C15
13	G	$50\overline{3}$	CPL	C16-C17-C18-C19
13	G	503	CPL	C15-C16-C17-C18
13	Е	501	CPL	C15-C16-C17-C18
13	E	501	CPL	C11-C12-C13-C14
13	E	501	CPL	C16-C17-C18-C19
13	E	501	CPL	C12-C13-C14-C15
13	G	503	CPL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
14	F	301	PTY	C32-C33-C34-C35
13	В	101	CPL	C13-C14-C15-C16
14	А	802	PTY	C30-C31-C32-C33
13	В	101	CPL	C21-C22-C23-C24
14	А	802	PTY	C32-C33-C34-C35
14	А	802	PTY	C16-C17-C18-C19
14	А	802	PTY	C17-C18-C19-C20
13	А	801	CPL	C4-C5-N-C8
13	А	801	CPL	C34-C35-C36-C37
14	F	301	PTY	C8-C11-C12-C13
14	А	802	PTY	C39-C40-C41-C42
14	F	301	PTY	C36-C37-C38-C39
16	А	804	ELU	C13-C15-C16-C17
14	А	802	PTY	C11-C8-O7-C6
13	А	801	CPL	C16-C17-C18-C19
14	А	802	PTY	O10-C8-O7-C6
14	А	802	PTY	O4-C1-C6-O7
14	F	301	PTY	C35-C36-C37-C38
13	В	101	CPL	C35-C36-C37-C38
14	F	301	PTY	C37-C38-C39-C40
14	F	301	PTY	C30-C31-C32-C33
16	А	804	ELU	C1-C2-C3-C5
13	В	101	CPL	C23-C24-C25-C26
13	Е	501	CPL	C23-C24-C25-C26
13	А	801	CPL	C4-C5-N-C6
14	А	802	PTY	O14-C5-C6-C1
14	А	802	PTY	N1-C2-C3-O11
13	Е	501	CPL	C18-C19-C20-C21
13	Е	501	CPL	C1-C2-C3-O3
13	G	503	CPL	C1-C2-C3-O3
14	А	802	PTY	O4-C1-C6-C5
14	F	301	PTY	O4-C1-C6-C5
13	G	503	CPL	C23-C24-C25-C26
13	А	801	CPL	C4-C5-N-C7
13	G	503	CPL	C13-C14-C15-C16
13	A	801	CPL	C39-C40-C41-C42
13	E	501	CPL	C39-C40-C41-C42
13	G	503	CPL	C40-C41-C42-C43
17	G	502	NAG	C4-C5-C6-O6
13	G	503	CPL	O3P-C1-C2-O2
14	A	802	PTY	O14-C5-C6-O7
13	В	101	CPL	C15-C16-C17-C18



Mol	Chain	Res	Type	Atoms
13	Е	501	CPL	C42-C43-C44-C45
13	Е	501	CPL	C33-C34-C35-C36
13	Е	501	CPL	C34-C35-C36-C37
16	А	804	ELU	PB-O3A-PA-O1
13	Е	501	CPL	O3P-C1-C2-C3
16	А	804	ELU	C2-C3-C5-C6
13	Е	501	CPL	C38-C39-C40-C41
14	А	802	PTY	C11-C12-C13-C14
13	А	801	CPL	C14-C15-C16-C17
13	А	801	CPL	C1-C2-C3-O3
13	G	503	CPL	C35-C36-C37-C38
13	Е	501	CPL	O3P-C1-C2-O2
13	G	503	CPL	O2-C2-C3-O3
13	А	801	CPL	C43-C44-C45-C46
13	G	503	CPL	C19-C20-C21-C22
13	G	503	CPL	C34-C35-C36-C37
13	В	101	CPL	C18-C19-C20-C21
14	F	301	PTY	C3-O11-P1-O13
14	F	301	PTY	O14-C5-C6-C1
14	F	301	PTY	C11-C12-C13-C14
14	F	301	PTY	O14-C5-C6-O7
13	В	101	CPL	C16-C17-C18-C19
13	G	503	CPL	O4P-C4-C5-N
13	Е	501	CPL	O2-C2-C3-O3
14	А	802	PTY	O4-C30-C31-C32
13	А	801	CPL	C15-C16-C17-C18
14	А	802	PTY	C5-C6-O7-C8
13	Ε	501	CPL	C13-C14-C15-C16
14	F	301	PTY	O4-C30-C31-C32
13	В	101	CPL	C1-O3P-P-O4P
14	F	301	PTY	C5-O14-P1-O11
13	A	801	CPL	O2-C2-C3-O3
13	G	503	CPL	C42-C43-C44-C45
13	А	801	CPL	O11-C11-O3-C3
13	А	801	CPL	C12-C11-O3-C3
13	В	101	CPL	C36-C37-C38-C39
14	F	301	PTY	C12-C11-C8-O7
14	A	802	PTY	C6-C5-O14-P1
13	A	801	CPL	C32-C33-C34-C35
14	A	802	PTY	C15-C16-C17-C18
14	A	802	PTY	C12-C11-C8-O7
13	G	503	CPL	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
14	А	802	PTY	C37-C38-C39-C40
13	А	801	CPL	C1-O3P-P-O4P
13	Е	501	CPL	C43-C44-C45-C46
14	F	301	PTY	C16-C17-C18-C19
14	А	802	PTY	C31-C32-C33-C34
13	В	101	CPL	C37-C38-C39-C40
13	G	503	CPL	C37-C38-C39-C40
16	А	804	ELU	C1-O1-PA-O3A
14	F	301	PTY	C34-C35-C36-C37
14	F	301	PTY	C40-C41-C42-C43
13	Е	501	CPL	C37-C38-C39-C40
13	А	801	CPL	C1-O3P-P-O1P
13	В	101	CPL	C4-O4P-P-O1P
13	В	101	CPL	C32-C33-C34-C35
14	F	301	PTY	C15-C16-C17-C18
14	А	802	PTY	C38-C39-C40-C41

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There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	А	802	PTY	1	0
13	В	101	CPL	1	0
13	А	801	CPL	3	0
13	G	503	CPL	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.





















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-15419. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

6.2.2 Raw map



X Index: 192

Y Index: 192

Z Index: 192

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: 206



Y Index: 193



Z Index: 147

6.3.2 Raw map



X Index: 205

Y Index: 194



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





6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.417. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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 90 $\rm nm^3;$ this corresponds to an approximate mass of 81 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 0.333 ${\rm \AA^{-1}}$



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 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	3.00	-	-		
Author-provided FSC curve	-	-	-		
Unmasked-calculated*	3.90	7.08	4.00		

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15419 and PDB model 8AGB. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.417 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 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 (0.417).



9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.417) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.7860	0.5530	_ 10
А	0.8460	0.5810	1.0
В	0.7990	0.5680	
С	0.7370	0.5350	
D	0.7610	0.5340	
Е	0.7860	0.5530	
F	0.6160	0.4740	
G	0.8240	0.5590	
Н	0.7830	0.5570	
Ι	0.8310	0.5620	0.0
J	0.6670	0.5690	<0.0
K	0.1790	0.3840	
L	0.5350	0.5350	

