

Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 08:53 AM EDT

PDB ID	:	6E7K
Title	:	Structure of the lipoprotein lipase GPIHBP1 complex that mediates plasma
		triglyceride hydrolysis
Authors	:	Birrane, G.; Meiyappan, M.
Deposited on	:	2018-07-26
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.80 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain							
1	А	448	.% •	72%		19%	• 6%				
1	В	448	2%	74% 16%							
2	С	131	34%	21%	8%	37%					
2	D	131	2% 	21%	6% ·	38%					
3	Е	3	33%		67%						



Mol	Chain	Length	Quality of chain
4	F	4	100%
5	G	3	100%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8045 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	421	Total 3310	C 2101	N 568	O 625	S 16	0	0	0
1	В	422	Total 3321	C 2107	N 572	O 626	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	324	ALA	ARG	engineered mutation	UNP P06858
В	324	ALA	ARG	engineered mutation	UNP P06858

• Molecule 2 is a protein called Glycosylphosphatidylinositol-anchored high density lipoproteinbinding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	83	Total	С	Ν	0	\mathbf{S}	0	0	0
	00	627	376	112	128	11	0	0	0	
0	П	Q1	Total	С	Ν	0	S	0	0	0
	D	01	615	370	110	124	11	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Е	3	Total 39	C 22	N 2	0 15	0	0	0

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



eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose.

 β 4 β 4 β β

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total 49	C 28	N 2	0 19	0	0	0

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	G	3	Total 38	C N 22 2	0 14	0	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Ca 1 1	0	0
6	В	1	Total Ca 1 1	0	0

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	В	1	Total 14	C 8	N 1	O 5	0	0
7	С	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	5	Total O 5 5	0	0
8	В	9	Total O 9 9	0	0
8	С	1	Total O 1 1	0	0
8	D	1	Total O 1 1	0	0



Chain C:

34%

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.



21%

8%

37%

• Molecule 1: Lipoprotein lipase

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• Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



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

Chain E:	33%	67%
NAG1 NAG2 BMA3		

 $\label{eq:manopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose$

Chain F:	100%	
NAG1 NAG2 FUC4		

 • Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	101.95Å 153.21Å 95.78Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.41 - 2.80	Depositor
Resolution (A)	48.37 - 2.80	EDS
% Data completeness	99.2 (48.41-2.80)	Depositor
(in resolution range)	99.3 (48.37-2.80)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.01	Depositor
$< I/\sigma(I) > 1$	$2.06 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
B B.	0.195 , 0.235	Depositor
Λ, Λ_{free}	0.207 , 0.243	DCC
R_{free} test set	1833 reflections (4.90%)	wwPDB-VP
Wilson B-factor $(Å^2)$	89.6	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.31 , 62.3	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8045	wwPDB-VP
Average B, all atoms $(Å^2)$	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CA, FUC, NAG, BMA

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

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.53	1/3389~(0.0%)	0.69	1/4585~(0.0%)	
1	В	0.54	0/3400	0.71	2/4599~(0.0%)	
2	С	0.50	0/638	0.76	0/871	
2	D	0.44	0/626	0.79	1/855~(0.1%)	
All	All	0.52	1/8053~(0.0%)	0.71	4/10910~(0.0%)	

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	А	0	5
1	В	0	7
2	С	0	1
2	D	1	3
All	All	1	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	447	ARG	NE-CZ	6.06	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	235	ASN	CB-CA-C	6.62	123.63	110.40
1	В	337	PRO	N-CA-CB	-5.14	96.94	102.60
1	А	337	PRO	N-CA-CB	-5.14	96.95	102.60
2	D	117	ILE	CB-CA-C	5.12	121.85	111.60



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	117	ILE	CA

All (16) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	178	ARG	Sidechain
1	А	302	CYS	Peptide
1	А	33	ASP	Peptide
1	А	336	MET	Peptide
1	А	86	GLY	Peptide
1	В	116	ARG	Sidechain
1	В	236	GLY	Peptide
1	В	302	CYS	Peptide
1	В	32	ARG	Sidechain
1	В	321	ARG	Sidechain
1	В	33	ASP	Peptide
1	В	336	MET	Peptide
2	С	64	ARG	Sidechain
2	D	101	GLY	Peptide
2	D	64	ARG	Sidechain
2	D	76	ARG	Sidechain

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	3310	0	3240	54	0
1	В	3321	0	3250	53	0
2	С	627	0	593	30	0
2	D	615	0	583	18	0
3	Е	39	0	34	0	0
4	F	49	0	43	0	0
5	G	38	0	34	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
7	В	14	0	13	0	0
7	C	14	0	13	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	А	5	0	0	0	0
8	В	9	0	0	1	0
8	С	1	0	0	0	0
8	D	1	0	0	0	0
All	All	8045	0	7803	142	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 9.

All (142) 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:B:359:ASN:O	1:B:380:LEU:O	1.86	0.94
2:C:65:CYS:SG	2:C:89:CYS:HB3	2.13	0.88
1:B:447:ARG:HH11	1:B:447:ARG:HB3	1.38	0.87
1:A:350:SER:OG	1:A:427:ALA:O	1.96	0.82
2:C:91:THR:HG23	2:C:108:THR:HG22	1.62	0.81
1:A:467:ASP:HB2	2:C:109:TRP:HE1	1.46	0.81
1:A:447:ARG:HH12	2:C:96:GLY:H	1.28	0.80
1:A:447:ARG:HH21	2:C:105:THR:HG22	1.45	0.80
1:B:412:ASP:O	1:B:413:SER:HB2	1.84	0.78
1:B:45:THR:OG1	1:B:47:GLU:O	2.04	0.75
2:C:89:CYS:SG	2:C:131:CYS:O	2.45	0.74
2:D:91:THR:HG23	2:D:129:THR:OG1	1.91	0.71
1:B:72:SER:O	1:B:73:SER:HB3	1.93	0.69
1:A:447:ARG:HH12	2:C:96:GLY:N	1.91	0.68
1:A:303:LEU:O	1:A:304:SER:HB3	1.95	0.67
1:B:303:LEU:O	1:B:304:SER:HB3	1.97	0.65
1:B:336:MET:O	1:B:338:TYR:N	2.29	0.65
1:B:35:ILE:HG22	1:B:35:ILE:O	1.95	0.65
1:A:353:GLU:H	1:A:353:GLU:CD	2.01	0.65
1:B:335:GLN:O	1:B:336:MET:O	2.16	0.63
1:A:336:MET:O	1:A:338:TYR:N	2.30	0.63
2:C:89:CYS:HB2	2:C:137:ASN:HB3	1.80	0.63
1:B:411:SER:HA	1:B:455:LYS:HE3	1.79	0.63
1:A:335:GLN:O	1:A:336:MET:O	2.17	0.63
1:A:178:ARG:NH1	1:A:207:ASP:OD1	2.31	0.62
1:A:35:ILE:O	1:A:35:ILE:HG22	2.00	0.61
2:C:89:CYS:SG	2:C:131:CYS:C	2.78	0.61
1:A:48:ASP:OD2	1:A:53:THR:HG21	2.00	0.61
1:A:447:ARG:NH2	2:C:105:THR:HG22	2.14	0.61



	louo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:D:67:THR:HG21	2:D:81:GLN:HG3	1.84	0.60	
1:B:48:ASP:OD2	1:B:53:THR:HG21	2.02	0.60	
1:A:361:ALA:HA	1:A:379:THR:HG22	1.84	0.59	
2:C:67:THR:HG21	2:C:81:GLN:HG3	1.83	0.59	
2:C:133:SER:O	2:C:136:CYS:SG	2.61	0.59	
1:A:467:ASP:HB2	2:C:109:TRP:NE1	2.16	0.58	
1:B:439:GLN:O	1:B:470:LEU:HD12	2.04	0.58	
2:C:118:THR:HG22	2:C:127:THR:HG23	1.86	0.58	
1:B:326:SER:O	1:B:327:LYS:HB2	2.03	0.58	
1:A:206:VAL:H	1:A:229:HIS:HD2	1.52	0.57	
1:B:206:VAL:H	1:B:229:HIS:HD2	1.52	0.56	
2:D:133:SER:O	2:D:136:CYS:SG	2.63	0.56	
1:B:177:ASN:ND2	8:B:601:HOH:O	2.35	0.56	
1:B:32:ARG:O	1:B:33:ASP:OD1	2.24	0.55	
2:D:98:THR:HG23	2:D:101:GLY:N	2.20	0.55	
1:B:447:ARG:HH12	2:D:103:LEU:HB3	1.73	0.54	
1:B:454:GLN:HG2	1:B:457:LYS:HG3	1.89	0.54	
1:A:219:ARG:CZ	1:B:424:PRO:HB3	2.37	0.54	
1:B:36:ASP:CG	1:B:37:ILE:N	2.62	0.53	
1:B:385:THR:HG22	1:B:426:PHE:HE1	1.74	0.53	
2:D:92:LEU:HD22	2:D:128:MET:HG3	1.90	0.53	
1:A:469:SER:C	1:A:470:LEU:HG	2.28	0.52	
2:D:94:ALA:HB3	2:D:105:THR:CG2	2.40	0.52	
2:C:112:ASP:O	2:C:113:SER:C	2.48	0.52	
2:D:92:LEU:HD22	2:D:128:MET:CG	2.40	0.52	
1:B:153:VAL:HB	1:B:176:VAL:HG22	1.91	0.51	
1:A:80:HIS:CE1	1:A:113:TRP:CD1	2.99	0.51	
1:B:72:SER:O	1:B:73:SER:CB	2.58	0.51	
1:A:384:SER:OG	1:A:389:TYR:OH	2.28	0.50	
1:A:247:GLU:O	1:A:248:ALA:C	2.50	0.50	
1:A:367:TYR:CZ	2:C:122:GLU:HG3	2.47	0.50	
1:A:158:TYR:CG	1:A:272:ILE:HD11	2.46	0.49	
1:B:113:TRP:CE3	1:B:131:VAL:HG21	2.48	0.49	
1:B:247:GLU:O	1:B:248:ALA:C	2.51	0.49	
1:A:447:ARG:NH2	2:C:94:ALA:O	2.46	0.49	
1:B:368:GLY:HA3	1:B:399:ILE:HG22	1.94	0.49	
1:A:368:GLY:HA3	1:A:399:ILE:HG22	1.95	0.49	
1:A:248:ALA:HB1	1:A:262:GLN:OE1	2.13	0.48	
2:C:98:THR:OG1	2:C:99:GLU:N	2.47	0.48	
1:A:447:ARG:HH21	2:C:105:THR:CG2	2.23	0.48	
1:A:405:LEU:HD23	1:A:405:LEU:C	2.35	0.48	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:80:HIS:CE1	1:B:113:TRP:CD1	3.02	0.48
2:C:78:ASN:O	2:C:78:ASN:OD1	2.32	0.48
1:B:158:TYR:CG	1:B:272:ILE:HD11	2.49	0.47
2:D:65:CYS:SG	2:D:83:CYS:SG	3.11	0.47
2:C:94:ALA:HB3	2:C:105:THR:CG2	2.43	0.47
1:B:405:LEU:C	1:B:405:LEU:HD23	2.34	0.47
2:D:112:ASP:O	2:D:113:SER:C	2.52	0.47
1:B:353:GLU:O	1:B:385:THR:HG21	2.15	0.47
1:A:113:TRP:CE3	1:A:131:VAL:HG21	2.49	0.46
1:A:259:ASP:O	1:A:262:GLN:NE2	2.48	0.46
1:B:35:ILE:O	1:B:35:ILE:CG2	2.61	0.46
1:B:36:ASP:OD2	1:B:37:ILE:N	2.48	0.46
1:B:92:VAL:N	1:B:93:PRO:HD2	2.31	0.46
2:D:67:THR:HG22	2:D:109:TRP:HA	1.96	0.46
1:A:163:HIS:O	1:A:167:ILE:HG13	2.15	0.46
2:C:102:LEU:HD12	2:C:102:LEU:C	2.35	0.46
1:B:320:VAL:HG23	1:B:321:ARG:N	2.31	0.46
2:C:65:CYS:SG	2:C:89:CYS:CB	2.97	0.45
2:C:63:LEU:HD21	2:C:133:SER:C	2.36	0.45
1:A:353:GLU:O	1:A:385:THR:HG21	2.17	0.45
1:B:51:GLU:HB2	1:B:53:THR:HG22	1.99	0.45
2:C:92:LEU:HD22	2:C:128:MET:CG	2.46	0.45
2:D:98:THR:OG1	2:D:99:GLU:N	2.49	0.45
1:A:36:ASP:OD1	1:A:37:ILE:N	2.50	0.45
1:B:91:TRP:CD2	1:B:272:ILE:HD13	2.52	0.44
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.98	0.44
1:B:194:ALA:N	1:B:195:PRO:CD	2.81	0.44
1:A:91:TRP:CD2	1:A:272:ILE:HD13	2.53	0.44
1:A:320:VAL:HG23	1:A:321:ARG:N	2.32	0.44
1:B:307:LYS:O	1:B:307:LYS:CD	2.64	0.44
1:A:194:ALA:N	1:A:195:PRO:CD	2.80	0.44
2:C:67:THR:HG22	2:C:109:TRP:HA	1.99	0.44
1:A:411:SER:HA	1:A:455:LYS:HE3	1.99	0.44
1:A:362:PHE:CE2	1:A:380:LEU:HD12	2.53	0.43
1:B:362:PHE:CE2	1:B:380:LEU:HD12	2.53	0.43
2:D:116:PRO:O	2:D:117:ILE:HD13	2.18	0.43
1:B:206:VAL:N	1:B:229:HIS:HD2	2.16	0.43
2:C:64:ARG:O	2:C:134:SER:HA	2.19	0.43
1:B:239:PHE:CE2	1:B:243:CYS:O	2.72	0.43
2:C:92:LEU:HD22	2:C:128:MET:HG3	2.01	0.43
1:A:358:THR:O	1:A:359:ASN:C	2.57	0.42



A + 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:378:PHE:CZ	1:A:391:PHE:CZ	3.07	0.42
1:B:406:LYS:HG2	1:B:461:VAL:HG22	2.01	0.42
1:B:453:LEU:O	1:B:454:GLN:CB	2.66	0.42
2:D:89:CYS:HB3	2:D:137:ASN:HB3	2.02	0.42
1:A:35:ILE:O	1:A:35:ILE:CG2	2.66	0.42
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.85	0.42
1:A:232:ILE:HG22	1:A:234:PRO:HD3	2.00	0.42
1:B:378:PHE:CZ	1:B:391:PHE:CZ	3.07	0.42
1:A:219:ARG:NH1	1:B:424:PRO:HB3	2.34	0.42
1:A:36:ASP:CG	1:A:37:ILE:N	2.73	0.42
1:B:64:VAL:HG13	1:B:69:PHE:HB3	2.01	0.42
1:A:139:ILE:CG2	1:A:150:LEU:HD22	2.50	0.42
1:A:183:ASP:OD2	1:A:268:HIS:HD2	2.02	0.42
2:D:117:ILE:CG1	2:D:118:THR:H	2.33	0.42
1:B:341:PHE:O	1:B:394:TYR:HA	2.19	0.42
1:A:341:PHE:O	1:A:394:TYR:HA	2.20	0.41
1:A:367:TYR:HB3	2:C:121:VAL:HG23	2.02	0.41
1:B:183:ASP:OD2	1:B:268:HIS:HD2	2.03	0.41
1:B:307:LYS:O	1:B:307:LYS:HD2	2.21	0.41
2:D:76:ARG:HG2	2:D:142:GLN:OE1	2.20	0.41
1:A:386:ASN:O	1:A:387:LYS:HD2	2.21	0.41
1:A:239:PHE:CE2	1:A:243:CYS:O	2.74	0.41
1:A:353:GLU:CD	1:A:353:GLU:N	2.72	0.41
1:B:79:ILE:HD12	1:B:165:ALA:HB2	2.03	0.41
2:D:117:ILE:HG13	2:D:118:THR:H	1.86	0.41
1:A:260:VAL:HG13	1:A:261:ASP:OD1	2.21	0.41
1:B:158:TYR:CD1	1:B:272:ILE:HD11	2.56	0.40
2:C:106:HIS:CG	2:C:139:PRO:HG3	2.56	0.40
2:D:63:LEU:HD21	2:D:133:SER:CA	2.51	0.40
1:B:36:ASP:CG	1:B:37:ILE:H	2.24	0.40
1:B:336:MET:HB3	1:B:337:PRO:CD	2.50	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 X-ray entries followed by that with respect to entries of similar resolution.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	415/448~(93%)	378~(91%)	30~(7%)	7~(2%)	9 29
1	В	416/448~(93%)	371 (89%)	33~(8%)	12 (3%)	4 15
2	С	81/131~(62%)	76~(94%)	3~(4%)	2(2%)	5 19
2	D	79/131~(60%)	73~(92%)	4(5%)	2(2%)	5 19
All	All	991/1158~(86%)	898 (91%)	70 (7%)	23 (2%)	6 21

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

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	37	ILE
1	А	336	MET
1	А	337	PRO
1	А	423	SER
1	В	33	ASP
1	В	37	ILE
1	В	336	MET
1	В	337	PRO
1	В	423	SER
1	В	453	LEU
2	С	121	VAL
2	D	113	SER
1	В	73	SER
2	С	113	SER
2	D	121	VAL
1	А	359	ASN
1	В	454	GLN
1	А	327	LYS
1	В	327	LYS
1	В	360	GLN
1	А	304	SER
1	В	304	SER
1	В	35	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 X-ray entries followed by that with respect to entries of similar resolution.



Mol	Chain	Analysed	Rotameric	Outliers	P	erce	entiles
1	А	365/388~(94%)	335~(92%)	30 (8%)		11	33
1	В	366/388~(94%)	342~(93%)	24 (7%)		16	44
2	С	78/122~(64%)	64 (82%)	14 (18%)		2	5
2	D	76/122~(62%)	63~(83%)	13~(17%)		2	6
All	All	885/1020 (87%)	804 (91%)	81 (9%)		9	27

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

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	53	THR
1	А	56	LEU
1	А	83	THR
1	А	143	GLU
1	А	152	ASN
1	А	238	THR
1	А	245	ILE
1	А	263	LEU
1	А	278	SER
1	А	303	LEU
1	А	307	LYS
1	А	310	CYS
1	А	323	LYS
1	А	326	SER
1	А	334	SER
1	А	337	PRO
1	А	340	VAL
1	А	353	GLU
1	А	358	THR
1	А	384	SER
1	А	385	THR
1	А	390	SER
1	А	412	ASP
1	А	429	GLN
1	А	430	LYS
1	А	450	VAL
1	А	451	SER
1	А	454	GLN
1	А	467	ASP
1	А	470	LEU



Mol	Chain	Res	Type
1	В	32	ARG
1	В	47	GLU
1	В	53	THR
1	В	152	ASN
1	В	176	VAL
1	В	238	THR
1	В	245	ILE
1	В	278	SER
1	В	303	LEU
1	В	307	LYS
1	В	310	CYS
1	В	323	LYS
1	В	326	SER
1	В	334	SER
1	В	337	PRO
1	В	350	SER
1	В	379	THR
1	В	385	THR
1	В	388	THR
1	В	412	ASP
1	В	413	SER
1	В	448	GLU
1	В	450	VAL
1	В	470	LEU
2	С	63	LEU
2	С	70	SER
2	С	78	ASN
2	С	90	THR
2	С	91	THR
2	С	92	LEU
2	C	97	ASN
2	С	98	THR
2	C	99	GLU
2	С	103	LEU
2	C	119	LYS
2	С	124	THR
2	С	134	SER
2	С	143	SER
2	D	63	LEU
2	D	70	SER
2	D	85	HIS
2	D	91	THR



Continuaca from pretioas page						
Mol	Chain	\mathbf{Res}	Type			
2	D	92	LEU			
2	D	98	THR			
2	D	100	SER			
2	D	102	LEU			
2	D	103	LEU			
2	D	117	ILE			
2	D	124	THR			
2	D	130	CYS			
2	D	134	SER			

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	147	ASN
1	А	224	GLN
1	А	229	HIS
1	А	244	ASN
1	А	268	HIS
1	А	308	ASN
1	А	454	GLN
1	А	466	HIS
1	В	229	HIS
1	В	262	GLN
1	В	268	HIS
1	В	308	ASN
1	В	466	HIS
2	D	95	HIS

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)

10 monosaccharides are modelled in this entry.



6E7K

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	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	les
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3,1	14,14,15	0.44	0	17,19,21	1.81	4 (23%)
3	NAG	Е	2	3	14,14,15	0.58	0	17,19,21	1.61	2 (11%)
3	BMA	Е	3	3	11,11,12	0.44	0	$15,\!15,\!17$	0.92	0
4	NAG	F	1	1,4	14,14,15	0.42	0	17,19,21	1.26	1 (5%)
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	1.77	1 (5%)
4	BMA	F	3	4	11,11,12	0.50	0	$15,\!15,\!17$	1.21	1 (6%)
4	FUC	F	4	4	10,10,11	0.31	0	14,14,16	1.39	3 (21%)
5	NAG	G	1	1,5	14,14,15	0.52	0	17,19,21	1.39	2 (11%)
5	NAG	G	2	5	14,14,15	0.47	0	17,19,21	1.72	2 (11%)
5	FUC	G	3	5	10,10,11	0.27	0	14,14,16	0.88	1 (7%)

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	Е	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Е	3	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	FUC	F	4	4	-	-	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	2	NAG	C1-O5-C5	6.66	121.22	112.19
5	G	2	NAG	C1-O5-C5	5.75	119.98	112.19
3	Е	1	NAG	C3-C4-C5	4.44	118.16	110.24
3	Е	2	NAG	C4-C3-C2	3.97	116.83	111.02
5	G	1	NAG	C4-C3-C2	3.48	116.12	111.02
5	G	1	NAG	C1-C2-N2	-3.38	104.71	110.49
4	F	1	NAG	C1-C2-N2	-3.29	104.87	110.49
4	F	3	BMA	O5-C1-C2	-3.17	105.87	110.77
4	F	4	FUC	O5-C1-C2	-3.16	105.89	110.77
5	G	2	NAG	O5-C5-C6	3.12	112.10	107.20
3	Е	1	NAG	C1-O5-C5	3.04	116.31	112.19
3	Е	1	NAG	O5-C1-C2	-2.92	106.68	111.29
3	Е	1	NAG	C1-C2-N2	2.88	115.42	110.49
3	Е	2	NAG	C1-O5-C5	-2.45	108.88	112.19
4	F	4	FUC	C2-C3-C4	-2.21	107.07	110.89
5	G	3	FUC	O5-C5-C6	2.12	111.89	107.33
4	F	4	FUC	C1-C2-C3	-2.03	107.17	109.67

There are no chirality outliers.

All	(11)) torsion	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms
3	Е	2	NAG	O5-C5-C6-O6
3	Е	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	Е	1	NAG	C4-C5-C6-O6
3	Ε	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	Ε	3	BMA	O5-C5-C6-O6
3	Ē	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	В	504	1	14,14,15	0.64	0	17,19,21	2.27	1 (5%)
7	NAG	С	201	2	14,14,15	0.63	0	17,19,21	1.69	2 (11%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	В	504	1	-	2/6/23/26	0/1/1/1
7	NAG	С	201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	В	504	NAG	C1-O5-C5	8.52	123.74	112.19
7	С	201	NAG	C1-O5-C5	5.23	119.28	112.19
7	С	201	NAG	C3-C4-C5	2.56	114.80	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	В	504	NAG	O5-C5-C6-O6
7	В	504	NAG	C4-C5-C6-O6
7	С	201	NAG	C4-C5-C6-O6
7	С	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	421/448~(93%)	0.13	6 (1%) 75 70	69, 91, 132, 149	0
1	В	422/448~(94%)	0.20	10 (2%) 59 49	59, 85, 125, 145	0
2	С	83/131~(63%)	0.06	0 100 100	88, 110, 137, 161	0
2	D	81/131~(61%)	-0.20	2 (2%) 57 47	79, 107, 138, 151	0
All	All	1007/1158~(86%)	0.12	18 (1%) 68 61	59, 91, 133, 161	0

All (18) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	258	GLY	5.0
1	В	258	GLY	3.4
1	А	352	THR	3.2
1	А	422	SER	3.2
1	В	323	LYS	2.8
1	В	173	ASN	2.7
1	А	425	GLY	2.7
1	В	353	GLU	2.6
2	D	95	HIS	2.4
1	А	351	GLY	2.4
1	В	352	THR	2.3
1	В	413	SER	2.2
1	В	389	TYR	2.2
1	А	289	TYR	2.1
1	В	425	GLY	2.1
1	В	386	ASN	2.1
1	В	355	GLU	2.1
2	D	74	ASP	2.0



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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	BMA	Е	3	11/12	0.76	0.31	141,152,157,159	0
4	BMA	F	3	11/12	0.79	0.29	158,167,169,169	0
5	NAG	G	2	14/15	0.83	0.26	119,130,135,138	0
3	NAG	Е	2	14/15	0.86	0.29	139,150,155,156	0
3	NAG	Е	1	14/15	0.86	0.15	105,118,131,142	0
5	NAG	G	1	14/15	0.89	0.23	97,112,121,121	0
4	NAG	F	1	14/15	0.90	0.12	93,102,109,113	0
4	NAG	F	2	14/15	0.94	0.21	120,126,136,148	0
4	FUC	F	4	10/11	0.94	0.27	106,113,116,119	0
5	FUC	G	3	10/11	0.95	0.15	112,113,116,116	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.









6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
7	NAG	С	201	14/15	0.47	0.38	$139,\!153,\!159,\!159$	0
7	NAG	В	504	14/15	0.76	0.35	107, 117, 125, 127	0
6	CA	А	501	1/1	0.96	0.09	98,98,98,98	0
6	CA	В	505	1/1	0.97	0.08	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.

