

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 3, 2023 - 02:08 am GMT

PDB ID	:	1GZ7
Title	:	Crystal structure of the closed state of lipase 2 from Candida rugosa
Authors	:	Mancheno, J.M.; Hermoso, J.A.
Deposited on	:	2002-05-17
Resolution	:	1.97  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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 1.97 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 $(\#Entries)$	Similar resolution $(\#Entries, resolution range(Å))$
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	534	81%	18%	•
1	В	534	79%	19%	
1	С	534	79%	20%	•
1	D	534	78%	21%	
2	Е	2	50%	50%	
2	F	2	100%		
2	G	2	100%		
2	Н	2	100%		



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	Х	-	-	-
3	GOL	В	1537	-	-	Х	-
3	GOL	С	1537	-	-	Х	-
3	GOL	С	1538	-	-	Х	-



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17843 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	524	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
I A	004	4053	2585	668	781	19	0	0	0	
1	Р	524	Total	С	Ν	0	S	0	0	0
1	ГБ	- 554	4053	2585	668	781	19	0	0	0
1	C	524	Total	С	Ν	0	S	0	0	0
1	U	- 554	4053	2585	668	781	19	0	0	0
1	П	524	Total	С	Ν	0	S	0	0	0
T		554	4053	2585	668	781	19	0	0	0

• Molecule 1 is a protein called LIPASE 2.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	78	LEU	ARG	conflict	UNP P32946
А	79	ASP	HIS	conflict	UNP P32946
В	78	LEU	ARG	conflict	UNP P32946
В	79	ASP	HIS	conflict	UNP P32946
С	78	LEU	ARG	conflict	UNP P32946
С	79	ASP	HIS	conflict	UNP P32946
D	78	LEU	ARG	conflict	UNP P32946
D	79	ASP	HIS	conflict	UNP P32946

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



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
2	Е	2	Total 28	C 16	N 2	O 10	0	0	0



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
2	F	2	Total 28	C 16	N 2	0 10	0	0	0
2	G	2	Total 28	C 16	2 N 2	0 10	0	0	0
2	Н	2	Total 28	C 16		0 10	0	0	0

Continued from previous page...

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	462	Total O 462 462	0	0
4	В	352	Total O   352 352	0	0
4	С	312	Total O 312 312	0	0
4	D	345	Total O 345 345	0	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. 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. 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.

Note EDS was not executed.

• Molecule 1: LIPASE 2





# L508 I377 0182 A1 A521 Y381 Y306 111 A521 Y381 Y306 111 P529 T382 S14 E21 P530 Y315 Y316 Y216 Y21 P530 Y216 Y216 Y23 P630 Y365 W24 Y23 P640 Y36 Y36 Y36 P1403 Y346 Y36 Y36 P141 Y36 Y36 Y36 P141 Y36 Y36 Y36 P142 Y36 Y36 Y36 P143 Y39 Y37 Y37 P143 Y39 Y37 Y37 P1445 Y39 Y39 Y44 P1445</

• Molecule 1: LIPASE 2

Ch	aiı	n I	D:											7	8%	ó													21%						·				
A1	888 69	D10	T11	N16	N20	E21	K22 F23	L24	G25	<b>T35</b>		P41	¥44	1.48	N49		F53	P65		508 F69	E70		N76	L78	V81	L82	483 S84	K85	186 F87	<mark>088</mark>	L91	P92	N93	N101	V116		G124 F125	E126	
8130 8131	L132	D136	K141	M11F	0+TU	N155	F163		L179	H180 D181	Q182	R183	M186	L OCN		Y206	G207 E208		S214	1215 F216	V217 1010	0171	K231	R235	1238	M239	0 <u>47</u> 0	M244	0261			S272	L275		D284	<mark>q288</mark>	тооз	P294	Y299
P300	Y306	1315	T316 D317	D318	H330	V331	F332	13 <mark>35</mark>		0338 N339	D340	E341	R359	T374	# 01	M378	Y381		T386	S389	P390	<b>G</b> 394	1395 	Q402	R405		L409 L410	-	L423 N424		07700	S4 <mark>36</mark>	L439		L442 DAA3		N451 D452	70F.7	W455 Q456
L459	V465	I466	Y467 N468	N469	L478	D479	K482		L485	W486	T493	S494 S405		L508	A521		L525	P529	P530	V534																			

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

Chain E:	50%	50%	r
NAG1 NAG2			
• Molecule 2: opyranose	2-acetamido-2-deoxy-beta-I	D-glucopyranose-(1-4)-2-acetamid	lo-2-deoxy-beta-D-gluc
Chain F:	10	00%	1
NAG1 NAG2			
• Molecule 2: opyranose	2-acetamido-2-deoxy-beta-I	D-glucopyranose-(1-4)-2-acetamid	lo-2-deoxy-beta-D-gluc

Chain G:

100%



#### NAG1 NAG2

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

Chain H:

100%

NAG1 NAG2



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants	61.15Å 91.14Å 108.46Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.78^{\circ}$ $106.31^{\circ}$ $86.91^{\circ}$	Depositor
Resolution (Å)	11.98 - 1.97	Depositor
% Data completeness	94 4 (11 98-1 97)	Depositor
(in resolution range)		Depositor
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
$R, R_{free}$	0.200 , $0.236$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17843	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP



# 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, GOL

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	Chain	Bo	nd lengths	Bond angles	
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.36	0/4159	0.63	1/5668~(0.0%)
1	В	0.35	0/4159	0.62	0/5668
1	С	0.35	1/4159~(0.0%)	0.63	2/5668~(0.0%)
1	D	0.34	0/4159	0.62	1/5668~(0.0%)
All	All	0.35	1/16636~(0.0%)	0.63	4/22672~(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	С	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	39	LYS	N-CA	5.60	1.57	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	39	LYS	N-CA-C	-7.31	91.27	111.00
1	С	39	LYS	N-CA-CB	5.72	120.90	110.60
1	А	315	ILE	N-CA-C	-5.41	96.41	111.00
1	D	315	ILE	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	С	38	PHE	Peptide

## 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	4053	0	3913	74	0
1	В	4053	0	3912	85	1
1	С	4053	0	3913	93	1
1	D	4053	0	3913	97	1
2	Е	28	0	25	0	1
2	F	28	0	25	2	0
2	G	28	0	25	2	0
2	Н	28	0	25	0	0
3	А	12	0	16	1	0
3	В	12	0	16	5	0
3	С	12	0	16	9	0
3	D	12	0	16	2	0
4	А	462	0	0	5	1
4	В	352	0	0	6	1
4	С	312	0	0	6	2
4	D	345	0	0	10	4
All	All	17843	0	15815	347	8

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 11.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLY:HA2	4:C:2099:HOH:O	1.59	1.02
1:A:359:ARG:HH11	1:A:378:MET:HE1	1.26	0.97
1:D:11:THR:H	1:D:49:ASN:HD22	1.11	0.95
1:C:20:ASN:HD21	1:C:22:LYS:HE3	1.31	0.93
1:D:180:HIS:ND1	3:D:1538:GOL:H12	1.82	0.93
1:A:66:MET:CE	1:A:295:GLY:H	1.83	0.92
1:A:66:MET:HE2	1:A:295:GLY:H	1.38	0.88



	lo as pagem	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:180:HIS:ND1	3:C:1538:GOL:H32	1.88	0.87
1:A:20:ASN:HD21	1:A:22:LYS:HE3	1.42	0.84
1:B:182:GLN:HE22	1:B:214:SER:HB3	1.43	0.84
1:C:183:ARG:HG2	3:C:1538:GOL:H11	1.60	0.82
1:B:498:SER:OG	4:B:2318:HOH:O	1.63	0.82
1:C:146:GLY:O	4:C:2098:HOH:O	1.97	0.82
1:B:424:ASN:HD21	1:B:495:SER:H	1.23	0.81
1:A:424:ASN:HD21	1:A:495:SER:H	1.25	0.81
1:D:11:THR:H	1:D:49:ASN:ND2	1.77	0.81
1:D:424:ASN:HD21	1:D:495:SER:H	1.26	0.80
1:D:182:GLN:HE22	1:D:214:SER:HB3	1.47	0.79
1:D:331:VAL:HG12	3:D:1537:GOL:H11	1.64	0.79
1:D:359:ARG:HH11	1:D:378:MET:HE1	1.48	0.78
1:B:13:THR:CG2	1:B:52:GLN:HG2	2.14	0.78
1:A:182:GLN:HE22	1:A:214:SER:HB3	1.47	0.78
1:B:359:ARG:HH11	1:B:378:MET:CE	1.97	0.78
1:D:359:ARG:HH11	1:D:378:MET:CE	1.97	0.77
1:C:182:GLN:HE22	1:C:214:SER:HB3	1.49	0.76
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.33	0.76
1:A:359:ARG:HH11	1:A:378:MET:CE	1.99	0.73
1:A:465:VAL:O	1:A:469:ASN:HB2	1.88	0.73
1:A:66:MET:HE1	1:A:294:PRO:HA	1.72	0.72
1:B:280:GLY:HA2	4:B:2182:HOH:O	1.90	0.72
1:B:180:HIS:ND1	3:B:1538:GOL:H12	2.05	0.72
1:D:130:SER:H	1:D:155:ASN:ND2	1.88	0.72
1:C:359:ARG:HH11	1:C:378:MET:CE	2.03	0.71
1:D:272:SER:HA	4:D:2177:HOH:O	1.89	0.71
1:C:11:THR:H	1:C:49:ASN:HD22	1.38	0.71
1:B:330:HIS:H	3:B:1537:GOL:H32	1.55	0.71
1:D:183:ARG:HH11	1:D:218:HIS:HD1	1.38	0.71
1:C:130:SER:H	1:C:155:ASN:ND2	1.89	0.71
1:B:330:HIS:H	3:B:1537:GOL:C3	2.03	0.71
1:D:70:GLU:CD	1:D:70:GLU:H	1.94	0.70
1:B:141:LYS:O	1:B:145:MET:HG2	1.91	0.70
1:C:424:ASN:HD21	1:C:495:SER:H	1.38	0.69
1:D:402:GLN:OE1	1:D:405:ARG:HD2	1.94	0.68
1:D:83:GLN:HE22	1:D:459:LEU:HD11	1.59	0.67
1:B:338:GLN:HE21	1:B:451:ASN:HD21	1.41	0.67
1:C:359:ARG:HG3	1:C:378:MET:HE1	1.76	0.67
1:C:465:VAL:O	1:C:469:ASN:HB2	1.95	0.67
1:D:130:SER:H	1:D:155:ASN:HD21	1.41	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:20:ASN:HD21	1:A:22:LYS:CE	2.07	0.67
1:C:330:HIS:H	3:C:1537:GOL:C3	2.08	0.67
1:D:493:THR:HG23	4:D:2312:HOH:O	1.95	0.66
2:F:1:NAG:H61	2:F:2:NAG:H82	1.77	0.66
1:A:25:GLY:H	1:A:101:ASN:HD22	1.44	0.66
1:C:261:GLN:HG3	4:C:2170:HOH:O	1.94	0.66
1:B:359:ARG:HH11	1:B:378:MET:HE1	1.60	0.65
1:A:130:SER:H	1:A:155:ASN:ND2	1.94	0.65
1:D:25:GLY:H	1:D:101:ASN:ND2	1.93	0.65
1:B:25:GLY:H	1:B:101:ASN:HD22	1.43	0.65
1:A:7:ALA:O	4:A:2005:HOH:O	2.13	0.65
1:D:91:LEU:HD23	1:D:93:ASN:ND2	2.11	0.65
1:B:179:LEU:HD13	1:B:217:VAL:HG11	1.79	0.65
1:D:25:GLY:H	1:D:101:ASN:HD22	1.43	0.64
1:C:486:TRP:HA	1:C:486:TRP:CE3	2.32	0.64
1:C:24:LEU:O	1:C:53:PHE:HB3	1.98	0.63
1:A:183:ARG:HH11	1:A:218:HIS:HD1	1.47	0.62
1:B:13:THR:HG21	1:B:52:GLN:HG2	1.81	0.62
1:A:395:ILE:O	4:A:2362:HOH:O	2.15	0.62
1:A:179:LEU:HD13	1:A:217:VAL:HG11	1.81	0.62
1:D:84:SER:OG	1:D:86:ILE:HG12	2.00	0.62
1:B:124:GLY:O	1:B:126:GLU:HG3	2.01	0.61
1:B:65:PRO:HG3	1:B:127:LEU:CD2	2.30	0.61
1:C:124:GLY:O	1:C:126:GLU:HG3	1.99	0.61
1:A:338:GLN:NE2	1:A:451:ASN:HD21	1.99	0.61
1:C:299:TYR:HB3	2:G:2:NAG:H81	1.83	0.61
1:C:486:TRP:HA	1:C:486:TRP:HE3	1.66	0.60
1:A:66:MET:HE1	1:A:295:GLY:H	1.65	0.60
1:C:216:PHE:CZ	1:C:244:MET:HG3	2.36	0.60
1:D:65:PRO:HG3	1:D:127:LEU:HD21	1.81	0.60
1:D:465:VAL:O	1:D:469:ASN:HB2	2.00	0.60
1:C:508:LEU:CG	1:D:70:GLU:HG3	2.32	0.60
1:D:83:GLN:NE2	1:D:459:LEU:HD11	2.15	0.60
1:B:20:ASN:C	1:B:20:ASN:HD22	2.05	0.60
1:B:442:LEU:HD12	1:B:443:PRO:HD2	1.84	0.60
1:C:330:HIS:H	3:C:1537:GOL:H32	1.65	0.60
1:D:76:ASN:HD21	1:D:443:PRO:HD2	1.66	0.60
1:C:465:VAL:CG1	1:C:485:LEU:HD22	2.32	0.59
1:C:354:THR:OG1	1:C:357:GLN:HG3	2.03	0.59
1:B:465:VAL:O	1:B:469:ASN:HB2	2.02	0.59
1:D:235:ARG:HD2	4:D:2135:HOH:O	2.02	0.59



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:338:GLN:HE21	1:D:451:ASN:HD21	1.49	0.59
1:B:63:MET:HE2	1:B:126:GLU:HB3	1.83	0.59
1:C:359:ARG:HH11	1:C:378:MET:HE1	1.67	0.59
1:A:11:THR:H	1:A:49:ASN:ND2	2.01	0.58
1:D:235:ARG:HD3	1:D:478:LEU:HD21	1.84	0.58
1:D:124:GLY:O	1:D:126:GLU:HG3	2.03	0.58
1:C:399:ILE:HD11	1:C:444:VAL:HG13	1.87	0.57
1:B:13:THR:HG23	1:B:52:GLN:HG2	1.86	0.57
1:C:141:LYS:O	1:C:145:MET:HG2	2.05	0.57
1:B:130:SER:H	1:B:155:ASN:ND2	2.03	0.57
1:A:124:GLY:O	1:A:126:GLU:HG3	2.05	0.57
1:B:338:GLN:NE2	1:B:451:ASN:HD21	2.02	0.57
1:C:326:GLY:HA2	1:C:328:TYR:CE2	2.41	0.56
1:D:76:ASN:HD21	1:D:443:PRO:CD	2.17	0.56
1:A:20:ASN:HA	1:A:106:PRO:HD3	1.87	0.56
1:A:65:PRO:HG3	1:A:127:LEU:CD2	2.36	0.56
1:C:508:LEU:HG	1:D:70:GLU:HG3	1.87	0.56
1:A:83:GLN:HE22	1:A:459:LEU:HD11	1.69	0.56
1:C:20:ASN:C	1:C:20:ASN:HD22	2.09	0.56
1:D:20:ASN:C	1:D:20:ASN:HD22	2.09	0.56
1:B:359:ARG:HH11	1:B:378:MET:HE2	1.70	0.56
1:A:235:ARG:HD2	4:A:2400:HOH:O	2.05	0.56
1:A:465:VAL:CG1	1:A:485:LEU:HD22	2.36	0.56
1:B:183:ARG:HH11	1:B:218:HIS:HD1	1.52	0.56
1:B:330:HIS:N	3:B:1537:GOL:H32	2.20	0.56
1:B:25:GLY:H	1:B:101:ASN:ND2	2.05	0.55
1:D:389:SER:HA	1:D:390:PRO:C	2.26	0.55
1:C:179:LEU:HD13	1:C:217:VAL:HG11	1.88	0.55
1:B:261:GLN:OE1	1:B:293:THR:HG22	2.06	0.55
1:D:270:SER:HA	4:D:2176:HOH:O	2.06	0.55
1:A:248:ASP:HB3	1:A:249:PRO:HD2	1.88	0.55
1:B:38:PHE:CE1	1:B:164:LEU:HD22	2.42	0.55
1:D:442:LEU:HD12	1:D:443:PRO:HD2	1.89	0.54
1:D:24:LEU:O	1:D:53:PHE:HB3	2.08	0.54
1:D:272:SER:CA	4:D:2177:HOH:O	2.52	0.54
1:A:266:ALA:HB1	1:A:281:LEU:HD11	1.90	0.54
1:C:338:GLN:HE21	1:C:451:ASN:HD21	1.55	0.54
1:D:65:PRO:HG3	1:D:127:LEU:CD2	2.37	0.54
1:B:20:ASN:HA	1:B:106:PRO:HD3	1.90	0.54
1:C:38:PHE:CE1	1:C:164:LEU:HD22	2.42	0.53
1:D:68:SER:HB2	1:D:71:ASP:OD2	2.09	0.53



			Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:D:486:TRP:CE3	1:D:486:TRP:HA	2.43	0.53	
1:A:354:THR:OG1	1:A:357:GLN:HG3	2.09	0.53	
1:B:70:GLU:CD	1:B:70:GLU:H	2.12	0.53	
1:C:183:ARG:CG	3:C:1538:GOL:H11	2.36	0.53	
1:D:20:ASN:HD21	1:D:22:LYS:HE3	1.72	0.53	
1:B:20:ASN:HD21	1:B:22:LYS:HE3	1.73	0.53	
1:A:25:GLY:H	1:A:101:ASN:ND2	2.05	0.53	
1:A:141:LYS:O	1:A:145:MET:HG2	2.09	0.53	
1:C:78:LEU:O	1:C:82:LEU:HG	2.08	0.53	
1:C:330:HIS:H	3:C:1537:GOL:H31	1.74	0.52	
1:A:127:LEU:C	1:A:127:LEU:HD12	2.30	0.52	
1:B:24:LEU:HD23	1:B:101:ASN:HB3	1.91	0.52	
1:C:235:ARG:HD2	4:C:2135:HOH:O	2.10	0.52	
1:A:11:THR:H	1:A:49:ASN:HD22	1.56	0.52	
1:A:130:SER:H	1:A:155:ASN:HD21	1.57	0.52	
1:D:386:THR:HA	1:D:394:GLY:O	2.10	0.52	
1:D:395:ILE:C	1:D:395:ILE:HD12	2.29	0.52	
1:A:180:HIS:ND1	3:A:1538:GOL:H32	2.25	0.52	
1:D:338:GLN:NE2	1:D:451:ASN:HD21	2.06	0.52	
1:B:508:LEU:N	1:B:508:LEU:HD22	2.25	0.51	
1:D:11:THR:N	1:D:49:ASN:HD22	1.95	0.51	
1:B:465:VAL:CG1	1:B:485:LEU:HD22	2.39	0.51	
1:B:41:PRO:HD2	1:B:180:HIS:HB3	1.92	0.51	
1:A:445:LEU:HB3	1:A:448:PHE:HB3	1.92	0.51	
1:A:66:MET:CE	1:A:298:ALA:HB2	2.41	0.51	
1:B:78:LEU:O	1:B:81:VAL:HG22	2.10	0.51	
1:B:359:ARG:NH1	1:B:378:MET:HE2	2.26	0.51	
1:C:130:SER:H	1:C:155:ASN:HD21	1.58	0.51	
1:D:335:ILE:O	1:D:433:SER:HA	2.10	0.51	
1:B:395:ILE:C	1:B:395:ILE:HD12	2.31	0.51	
1:A:66:MET:HE2	1:A:295:GLY:N	2.18	0.50	
1:B:63:MET:CE	1:B:295:GLY:HA2	2.41	0.50	
1:D:76:ASN:ND2	1:D:443:PRO:HD2	2.26	0.50	
1:D:338:GLN:NE2	1:D:436:SER:HB3	2.27	0.50	
1:C:409:LEU:HD23	1:C:409:LEU:C	2.31	0.50	
1:A:439:LEU:HB2	1:A:447:THR:HA	1.92	0.50	
1:A:66:MET:HE3	1:A:298:ALA:HB2	1.92	0.50	
1:C:508:LEU:HD22	1:C:508:LEU:N	2.26	0.50	
1:D:85:LYS:HA	1:D:88:GLN:NE2	2.26	0.50	
1:C:389:SER:HA	1:C:390:PRO:C	2.31	0.50	
1:D:409:LEU:C	1:D:409:LEU:HD23	2.32	0.50	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:389:SER:HA	1:B:390:PRO:C	2.32	0.49	
1:C:338:GLN:NE2	1:C:436:SER:HB3	2.26	0.49	
1:D:141:LYS:O	1:D:145:MET:HG2	2.12	0.49	
2:G:1:NAG:H61	2:G:2:NAG:H82	1.94	0.49	
1:B:232:PRO:HB3	3:B:1537:GOL:H11	1.95	0.49	
1:D:455:TRP:HA	1:D:459:LEU:O	2.12	0.49	
1:B:73:LEU:HD21	1:B:347:LEU:HD11	1.95	0.49	
1:C:37:ARG:HB2	1:C:279:ARG:HG2	1.95	0.49	
1:A:317:ASP:O	1:A:318:ASP:C	2.50	0.49	
1:C:319:MET:O	1:C:323:VAL:HG23	2.13	0.49	
1:A:216:PHE:CZ	1:A:244:MET:HG3	2.47	0.49	
1:C:299:TYR:N	1:C:300:PRO:HD2	2.28	0.49	
1:D:132:LEU:HD12	4:D:2081:HOH:O	2.13	0.48	
1:B:465:VAL:HG13	1:B:485:LEU:HD22	1.95	0.48	
1:C:63:MET:CE	1:C:295:GLY:HA2	2.44	0.48	
1:D:76:ASN:HD21	1:D:443:PRO:CG	2.26	0.48	
1:B:395:ILE:HG13	4:B:2272:HOH:O	2.12	0.48	
1:B:354:THR:OG1	1:B:357:GLN:HG3	2.14	0.48	
1:B:10:ASP:HA	1:B:49:ASN:HD22	1.79	0.48	
1:B:8:ASN:ND2	1:B:10:ASP:OD2	2.44	0.48	
1:C:183:ARG:HH11	1:C:218:HIS:HD1	1.62	0.48	
1:B:359:ARG:NH1	1:B:378:MET:CE	2.73	0.47	
1:D:299:TYR:N	1:D:300:PRO:HD2	2.29	0.47	
1:A:374:ILE:O	1:A:378:MET:HG3	2.14	0.47	
1:A:24:LEU:O	1:A:53:PHE:HB3	2.14	0.47	
1:A:326:GLY:HA2	1:A:328:TYR:CE2	2.49	0.47	
1:B:63:MET:HE3	1:B:295:GLY:HA2	1.95	0.47	
1:C:127:LEU:C	1:C:127:LEU:HD12	2.35	0.47	
1:D:395:ILE:HG13	4:D:2271:HOH:O	2.14	0.47	
1:A:508:LEU:N	1:A:508:LEU:HD22	2.30	0.47	
1:C:87:PHE:CD1	1:C:297:LEU:HD21	2.49	0.47	
1:D:208:GLU:HA	1:D:240:GLN:O	2.14	0.47	
1:C:359:ARG:NH1	1:C:378:MET:CE	2.77	0.47	
1:D:317:ASP:CG	1:D:318:ASP:N	2.68	0.47	
1:A:465:VAL:HG13	1:A:485:LEU:HD22	1.97	0.47	
1:B:176:ASN:OD1	1:B:308:PRO:HA	2.15	0.47	
1:C:25:GLY:H	1:C:101:ASN:HD22	1.63	0.46	
1:C:221:TRP:HZ2	3:C:1538:GOL:H12	1.79	0.46	
1:D:529:PRO:HB2	1:D:530:PRO:HD3	1.96	0.46	
1:B:104:ARG:HD2	1:B:108:THR:HB	1.98	0.46	
1:A:389:SER:HA	1:A:390:PRO:C	2.36	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:275:LEU:HB2	4:B:2181:HOH:O	2.15	0.46	
1:C:85:LYS:HA	1:C:88:GLN:NE2	2.31	0.46	
1:D:359:ARG:NH1	1:D:378:MET:HE2	2.30	0.46	
1:D:479:ASP:HB3	1:D:482:LYS:HG2	1.97	0.46	
1:A:235:ARG:HD3	1:A:478:LEU:HD21	1.97	0.46	
1:C:338:GLN:NE2	1:C:451:ASN:HD21	2.13	0.46	
1:C:35:THR:HG23	1:C:36:LEU:HG	1.96	0.46	
1:C:335:ILE:O	1:C:433:SER:HA	2.15	0.46	
1:D:216:PHE:CZ	1:D:244:MET:HG3	2.51	0.46	
1:D:275:LEU:HD12	1:D:275:LEU:HA	1.85	0.46	
1:D:465:VAL:CG1	1:D:485:LEU:HD22	2.45	0.46	
1:A:20:ASN:C	1:A:20:ASN:HD22	2.19	0.46	
1:B:477:ASP:HB2	1:B:482:LYS:HG3	1.98	0.46	
1:A:294:PRO:HG2	4:A:2239:HOH:O	2.14	0.46	
1:C:317:ASP:CG	1:C:318:ASP:H	2.19	0.46	
1:D:317:ASP:CG	1:D:318:ASP:H	2.19	0.46	
1:B:248:ASP:HB3	1:B:249:PRO:HD2	1.97	0.45	
1:C:317:ASP:CG	1:C:318:ASP:N	2.69	0.45	
1:A:95:GLU:OE2	1:A:283:GLN:HG3	2.16	0.45	
1:B:486:TRP:HA	1:B:486:TRP:CE3	2.50	0.45	
1:B:18:ILE:HD12	1:B:18:ILE:N	2.32	0.45	
1:C:266:ALA:HB1	1:C:281:LEU:HD11	1.97	0.45	
1:C:423:LEU:HB3	1:C:492:TYR:CE1	2.51	0.45	
1:B:326:GLY:HA2	1:B:328:TYR:CE2	2.51	0.45	
1:B:261:GLN:HG3	4:B:2178:HOH:O	2.16	0.45	
1:B:395:ILE:HD12	1:B:396:PHE:N	2.32	0.45	
1:B:69:PHE:CZ	1:B:344:LEU:HG	2.51	0.45	
1:C:329:ALA:HB1	3:C:1537:GOL:H11	1.99	0.45	
1:C:338:GLN:O	1:C:341:GLU:HG2	2.16	0.45	
1:C:339:ASN:HB2	1:C:436:SER:O	2.17	0.45	
1:C:435:LEU:HB3	1:C:504:GLN:HG2	1.99	0.45	
1:C:395:ILE:C	1:C:395:ILE:HD12	2.38	0.44	
1:D:41:PRO:HD2	1:D:180:HIS:HB3	1.99	0.44	
1:A:359:ARG:NH1	1:A:378:MET:CE	2.74	0.44	
1:B:24:LEU:O	1:B:53:PHE:HB3	2.18	0.44	
1:C:442:LEU:HD12	1:C:443:PRO:HD2	2.00	0.44	
1:D:78:LEU:O	1:D:82:LEU:HG	2.18	0.44	
1:D:374:ILE:O	1:D:378:MET:HG3	2.18	0.44	
1:C:246:PRO:HD3	4:C:2202:HOH:O	2.16	0.44	
1:A:164:LEU:HD23	1:A:169:ILE:HD11	2.00	0.44	
1:A:334:ILE:HG12	1:A:432:TYR:HB2	1.99	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:294:PRO:HG2	4:D:2194:HOH:O	2.18	0.44	
1:B:334:ILE:HG12	1:B:432:TYR:HB2	1.99	0.44	
1:C:402:GLN:O	1:C:406:ILE:HG13	2.18	0.44	
1:B:39:LYS:HE3	1:B:279:ARG:CZ	2.48	0.43	
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.84	0.43	
1:A:339:ASN:HB2	1:A:436:SER:O	2.18	0.43	
1:C:508:LEU:HD21	1:D:70:GLU:HG3	2.00	0.43	
1:B:319:MET:O	1:B:323:VAL:HG23	2.18	0.43	
1:A:245:VAL:HB	1:A:319:MET:CE	2.49	0.43	
1:B:127:LEU:C	1:B:127:LEU:HD12	2.38	0.43	
1:D:179:LEU:HD13	1:D:217:VAL:HG11	1.99	0.43	
1:A:35:THR:HG21	1:D:35:THR:HB	2.01	0.43	
1:A:442:LEU:HD12	1:A:443:PRO:HD2	1.99	0.43	
1:C:83:GLN:HE22	1:C:459:LEU:HD11	1.82	0.43	
1:B:206:TYR:CB	1:B:238:ILE:HB	2.49	0.43	
1:D:261:GLN:OE1	1:D:293:THR:HG22	2.18	0.43	
1:A:381:TYR:CZ	1:A:521:ALA:HB1	2.54	0.43	
1:C:377:LEU:HD21	1:C:409:LEU:HD11	2.00	0.43	
1:C:382:THR:C	1:C:405:ARG:HH21	2.22	0.43	
1:D:91:LEU:HD23	1:D:93:ASN:HD22	1.84	0.43	
1:B:13:THR:HG23	1:B:52:GLN:HA	2.01	0.43	
1:B:456:GLN:NE2	4:B:2297:HOH:O	2.52	0.43	
1:C:41:PRO:HD2	1:C:180:HIS:HB3	2.00	0.43	
1:C:76:ASN:HD21	1:C:443:PRO:HD2	1.84	0.43	
1:A:266:ALA:HB1	1:A:281:LEU:CD1	2.48	0.43	
1:D:163:PHE:HB2	1:D:306:TYR:HB3	2.01	0.42	
1:B:235:ARG:HD3	1:B:478:LEU:HD21	2.02	0.42	
1:C:84:SER:OG	1:C:86:ILE:HG12	2.19	0.42	
1:C:445:LEU:HB3	1:C:448:PHE:HB3	2.01	0.42	
1:D:508:LEU:N	1:D:508:LEU:HD22	2.33	0.42	
1:A:320:TYR:O	1:A:323:VAL:HG12	2.20	0.42	
1:B:342:GLY:HA3	1:B:407:SER:O	2.18	0.42	
1:C:439:LEU:HB2	1:C:447:THR:HA	2.00	0.42	
1:C:63:MET:HE3	1:C:295:GLY:HA2	2.02	0.42	
1:C:330:HIS:HB2	3:C:1537:GOL:H32	2.01	0.42	
1:D:330:HIS:HE1	4:D:2215:HOH:O	2.00	0.42	
1:A:78:LEU:O	1:A:82:LEU:HG	2.19	0.42	
1:D:69:PHE:C	1:D:71:ASP:H	2.23	0.42	
1:A:409:LEU:HD23	1:A:409:LEU:C	2.40	0.42	
1:C:11:THR:H	1:C:49:ASN:ND2	2.12	0.42	
1:C:409:LEU:HD23	1:C:409:LEU:O	2.18	0.42	



	loue page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:44:TYR:CE2	1:D:48:LEU:HD21	2.55	0.42	
1:B:377:LEU:HD21	1:B:409:LEU:HD11	2.00	0.42	
1:C:25:GLY:H	1:C:101:ASN:ND2	2.18	0.42	
1:D:206:TYR:HB2	1:D:238:ILE:HB	2.01	0.42	
1:D:284:ASP:O	1:D:288:GLN:HG2	2.20	0.42	
1:D:409:LEU:HD23	1:D:409:LEU:O	2.19	0.42	
2:F:1:NAG:H61	2:F:2:NAG:C8	2.49	0.42	
1:B:445:LEU:HB3	1:B:448:PHE:HB3	2.01	0.42	
1:A:504:GLN:NE2	1:A:513:GLY:HA3	2.34	0.42	
1:B:336:GLY:HA3	1:B:434:PHE:CZ	2.55	0.42	
1:D:81:VAL:HG23	1:D:82:LEU:N	2.35	0.42	
1:D:335:ILE:CG2	1:D:423:LEU:HD21	2.50	0.42	
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.78	0.41	
1:D:231:LYS:HB2	1:D:231:LYS:HE3	1.80	0.41	
1:A:69:PHE:C	1:A:71:ASP:H	2.22	0.41	
1:A:464:SER:O	1:A:468:ASN:HB2	2.19	0.41	
1:B:91:LEU:HD23	1:B:93:ASN:ND2	2.35	0.41	
1:B:465:VAL:HG13	1:B:485:LEU:CD2	2.50	0.41	
1:C:317:ASP:O	1:C:318:ASP:C	2.59	0.41	
1:C:402:GLN:OE1	1:C:405:ARG:HD2	2.19	0.41	
1:D:456:GLN:HB2	1:D:467:TYR:HB3	2.02	0.41	
1:D:116:VAL:HB	1:D:203:VAL:HG22	2.02	0.41	
1:C:330:HIS:HE1	4:C:2208:HOH:O	2.02	0.41	
1:D:206:TYR:CB	1:D:238:ILE:HB	2.50	0.41	
1:D:381:TYR:CZ	1:D:521:ALA:HB1	2.55	0.41	
1:C:456:GLN:HG2	1:C:457:ASP:OD1	2.20	0.41	
1:D:452:ASP:OD1	1:D:452:ASP:N	2.53	0.41	
1:C:381:TYR:CZ	1:C:521:ALA:HB1	2.56	0.41	
1:C:433:SER:HB3	1:C:502:LEU:HD23	2.02	0.41	
1:A:159:ALA:HB3	1:A:161:TRP:CE3	2.56	0.41	
1:C:508:LEU:CD2	1:D:70:GLU:HG3	2.51	0.41	
1:D:16:ASN:ND2	4:D:2009:HOH:O	2.51	0.41	
1:C:529:PRO:HB2	1:C:530:PRO:HD3	2.03	0.41	
1:D:235:ARG:O	1:D:332:PRO:HD2	2.21	0.41	
1:D:318:ASP:OD2	1:D:530:PRO:HG3	2.20	0.41	
1:B:317:ASP:O	1:B:318:ASP:C	2.59	0.40	
1:B:452:ASP:OD1	1:B:452:ASP:N	2.51	0.40	
1:A:17:ALA:O	1:A:18:ILE:HB	2.21	0.40	
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.79	0.40	
1:B:278:LEU:HA	1:B:281:LEU:CD1	2.51	0.40	
1:B:81:VAL:HG23	$1:B:\overline{82:LEU:N}$	2.37	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:O	1:B:433:SER:HA	2.22	0.40
1:B:431:LYS:HE3	1:B:492:TYR:O	2.22	0.40
1:D:182:GLN:O	1:D:186:MET:HG3	2.20	0.40
1:A:389:SER:HA	1:A:391:PHE:N	2.36	0.40
1:A:395:ILE:HD12	1:A:395:ILE:C	2.41	0.40
1:C:182:GLN:NE2	1:C:218:HIS:NE2	2.65	0.40
1:C:339:ASN:HD22	1:C:339:ASN:HA	1.71	0.40
1:D:338:GLN:O	1:D:341:GLU:HG2	2.22	0.40
1:A:284:ASP:HB3	4:A:2268:HOH:O	2.22	0.40
1:B:374:ILE:HG22	1:B:378:MET:HE2	2.03	0.40
1:C:41:PRO:HG3	1:C:181:ASP:HA	2.03	0.40
1:D:8:ASN:ND2	1:D:10:ASP:OD2	2.53	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:272:SER:OG	2:E:1:NAG:O7[1_655]	1.51	0.69
4:B:2179:HOH:O	4:C:2033:HOH:O[1_645]	1.59	0.61
4:A:2041:HOH:O	4:A:2151:HOH:O[1_655]	1.95	0.25
4:C:2080:HOH:O	4:D:2230:HOH:O[1_455]	2.01	0.19
4:D:2008:HOH:O	4:D:2251:HOH:O[1_455]	2.03	0.17
1:B:280:GLY:O	$1:C:31:PRO:CD[1_645]$	2.07	0.13
4:D:2013:HOH:O	4:D:2338:HOH:O[1_455]	2.09	0.11
4:D:2016:HOH:O	4:D:2095:HOH:O[1_455]	2.12	0.08

# 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.

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	А	532/534~(100%)	507~(95%)	23~(4%)	2~(0%)	34 22

1GZ7



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	532/534~(100%)	509~(96%)	22~(4%)	1 (0%)	47	38
1	С	532/534~(100%)	500 (94%)	32~(6%)	0	100	100
1	D	532/534~(100%)	506~(95%)	25~(5%)	1 (0%)	47	38
All	All	2128/2136~(100%)	2022 (95%)	102 (5%)	4 (0%)	47	38

Continued from previous page...

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	70	GLU
1	В	390	PRO
1	D	390	PRO
1	А	390	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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	ntiles
1	А	435/435~(100%)	425~(98%)	10 (2%)	50	44
1	В	435/435~(100%)	428~(98%)	7 (2%)	62	56
1	С	435/435~(100%)	427~(98%)	8 (2%)	59	51
1	D	435/435~(100%)	423~(97%)	12 (3%)	43	32
All	All	1740/1740~(100%)	1703 (98%)	37 (2%)	53	47

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	20	ASN
1	А	101	ASN
1	А	136	ASP
1	А	206	TYR
1	А	235	ARG
1	А	275	LEU
1	А	339	ASN



Mol	Chain	Res	Type
1	А	364	GLN
1	А	410	LEU
1	А	439	LEU
1	В	13	THR
1	В	20	ASN
1	В	70	GLU
1	В	101	ASN
1	В	235	ARG
1	В	410	LEU
1	В	494	SER
1	С	20	ASN
1	С	206	TYR
1	С	235	ARG
1	С	261	GLN
1	С	275	LEU
1	С	339	ASN
1	С	405	ARG
1	С	486	TRP
1	D	20	ASN
1	D	70	GLU
1	D	127	LEU
1	D	136	ASP
1	D	206	TYR
1	D	235	ARG
1	D	275	LEU
1	D	339	ASN
1	D	405	ARG
1	D	410	LEU
1	D	439	LEU
1	D	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	20	ASN
1	А	49	ASN
1	А	51	GLN
1	А	83	GLN
1	А	101	ASN
1	А	137	GLN
1	А	155	ASN
1	А	182	GLN



Mol	Chain	Res	Type
1	А	240	GLN
1	А	283	GLN
1	А	330	HIS
1	А	338	GLN
1	А	339	ASN
1	А	424	ASN
1	А	456	GLN
1	А	500	ASN
1	А	528	ASN
1	В	20	ASN
1	В	49	ASN
1	В	51	GLN
1	В	93	ASN
1	В	101	ASN
1	В	137	GLN
1	В	155	ASN
1	В	182	GLN
1	В	187	GLN
1	В	240	GLN
1	В	283	GLN
1	В	330	HIS
1	В	338	GLN
1	В	339	ASN
1	В	424	ASN
1	В	456	GLN
1	В	500	ASN
1	В	528	ASN
1	С	20	ASN
1	С	49	ASN
1	С	51	GLN
1	С	83	GLN
1	C	101	ASN
1	С	137	GLN
1	C	155	ASN
1	С	182	GLN
1	С	187	GLN
1	С	222	ASN
1	С	240	GLN
1	С	330	HIS
1	С	338	GLN
1	C	339	ASN
1	С	424	ASN



Mol	Chain	Res	Type
1	С	456	GLN
1	С	488	ASN
1	С	500	ASN
1	С	504	GLN
1	С	528	ASN
1	D	20	ASN
1	D	49	ASN
1	D	51	GLN
1	D	76	ASN
1	D	83	GLN
1	D	93	ASN
1	D	101	ASN
1	D	137	GLN
1	D	155	ASN
1	D	182	GLN
1	D	240	GLN
1	D	283	GLN
1	D	330	HIS
1	D	338	GLN
1	D	339	ASN
1	D	424	ASN
1	D	456	GLN
1	D	500	ASN
1	D	528	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)

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles						
	туре	Unam	nes	nes	nes	nes	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	Е	1	2,1	14,14,15	0.58	0	17,19,21	0.61	0				
2	NAG	Е	2	2	$14,\!14,\!15$	0.54	0	17,19,21	0.72	0				
2	NAG	F	1	2,1	14,14,15	0.75	1 (7%)	17,19,21	0.76	1 (5%)				
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	0.98	1 (5%)				
2	NAG	G	1	2,1	14,14,15	0.56	0	17,19,21	0.71	0				
2	NAG	G	2	2	$14,\!14,\!15$	0.51	0	17,19,21	0.61	0				
2	NAG	Н	1	2,1	14,14,15	0.53	0	17,19,21	0.67	1 (5%)				
2	NAG	Н	2	2	14,14,15	0.48	0	17,19,21	0.66	1 (5%)				

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).

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
2	NAG	Е	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Н	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Н	2	2	_	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	2.10	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	2	NAG	C2-N2-C7	-2.31	119.61	122.90
2	F	1	NAG	C2-N2-C7	-2.11	119.90	122.90
2	Н	1	NAG	C2-N2-C7	-2.09	119.93	122.90
2	Н	2	NAG	C2-N2-C7	-2.00	120.05	122.90



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	Е	2	NAG	C8-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	Е	2	NAG	O7-C7-N2-C2
2	Е	2	NAG	O5-C5-C6-O6
2	Е	2	NAG	C4-C5-C6-O6
2	Н	2	NAG	C8-C7-N2-C2
2	Н	2	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	F	2	NAG	2	0
2	G	2	NAG	2	0
2	Е	1	NAG	0	1
2	F	1	NAG	2	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)

8 ligands are modelled in this entry.

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

Mal	l Type Chain Bes		Tiple	Bond lengths			Bond angles			
MOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	GOL	В	1538	-	$5,\!5,\!5$	0.30	0	$5,\!5,\!5$	0.36	0
3	GOL	В	1537	-	$5,\!5,\!5$	0.25	0	$5,\!5,\!5$	0.44	0
3	GOL	D	1538	-	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.56	0
3	GOL	С	1537	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.56	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	GOL	А	1537	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.40	0
3	GOL	С	1538	-	$5,\!5,\!5$	0.30	0	$5,\!5,\!5$	0.58	0
3	GOL	А	1538	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.51	0
3	GOL	D	1537	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.28	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
3	GOL	В	1538	-	-	2/4/4/4	-
3	GOL	В	1537	-	-	2/4/4/4	-
3	GOL	D	1538	-	-	0/4/4/4	-
3	GOL	С	1537	-	-	0/4/4/4	-
3	GOL	А	1537	-	-	2/4/4/4	-
3	GOL	С	1538	-	-	0/4/4/4	-
3	GOL	A	1538	-	-	0/4/4/4	-
3	GOL	D	1537	-	-	2/4/4/4	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1537	GOL	O1-C1-C2-C3
3	В	1537	GOL	O1-C1-C2-O2
3	В	1537	GOL	O1-C1-C2-C3
3	D	1537	GOL	O1-C1-C2-C3
3	А	1537	GOL	O1-C1-C2-O2
3	D	1537	GOL	O1-C1-C2-O2
3	В	1538	GOL	O1-C1-C2-O2
3	В	1538	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 17 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	1538	GOL	1	0
3	В	1537	GOL	4	0
3	D	1538	GOL	1	0
3	С	1537	GOL	5	0
3	С	1538	GOL	4	0
3	А	1538	GOL	1	0
3	D	1537	GOL	1	0

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

# 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

