

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

### Jan 19, 2022 - 02:53 am GMT

PDB ID	:	7P7P
Title	:	Crystal structure of ERAP2 aminopeptidase in complex with phosphinic pseu
		$dotripeptide((1R)-1-Amino-3-phenylpropyl) \{(2S)-3-[((2S)-1-amino-1-oxo-3-phenylpropyl)] \} = 0.000000000000000000000000000000000$
		$enylpropan-2-yl)amino]-2-\{[3-(2-hydroxyphenyl)-isoxazol-5-yl]methyl\}-3-oxop$
		ropyl}phosphinic acid
Authors	:	Giastas, P.; Stratikos, E.; Mpakali, A.
Deposited on	:	2021-07-20
Resolution	:	3.00 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 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 as $541$ be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.24
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

# 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 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 chair	1	
1	А	962	% • 65%	28%	• 5%
1	В	962	57%	32%	• 9%
2	С	4	100%		
3	D	4	50%	50%	
4	Е	2	100%		



Mol	Chain	Length	Quality of chain							
4	Н	2	100%							
4	Ι	2	50%	50%						
5	F	3		100%						
6	G	5	20%	80%	_					

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
12	EDO	А	1111	-	_	-	Х



# 2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 14990 atoms, of which 76 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	Atoms					ZeroOcc	AltConf	Trace
1	А	911	Total 7330	C 4719	N 1219	O 1359	S 33	0	1	0
1	В	871	Total 6839	C 4407	N 1134	0 1274	S 24	0	0	0

• Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	392	ASN	LYS	variant	UNP Q6P179
А	961	ARG	-	expression tag	UNP Q6P179
А	962	HIS	-	expression tag	UNP $Q6P179$
В	392	ASN	LYS	variant	UNP Q6P179
В	961	ARG	-	expression tag	UNP Q6P179
В	962	HIS	-	expression tag	UNP $Q6P179$

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	С	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total 50	C 28	N 2	O 20	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	Е	2	Total         C         N         O           28         16         2         10	0	0	0
4	Н	2	Total         C         N         O           28         16         2         10	0	0	0
4	Ι	2	Total         C         N         O           28         16         2         10	0	0	0

• Molecule 5 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
5	F	3	Total 39	C 22	N 2	0 15	0	0	0

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





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
6	G	5	Total 61	С 34	N 2	O 25	0	0	0

• Molecule 7 is [(2 {S})-3-[[(2 {S})-1-azanyl-1-oxidanylidene-3-phenyl-propan-2-yl]amino]-2-[[  $3-(2-hydroxyphenyl)-1,2-oxazol-5-yl]methyl]-3-oxidanylidene-propyl]-[(1 {R})-1-azanyl-3-phenyl-propyl]phosphinic acid (three-letter code: 62S) (formula: <math>C_{31}H_{35}N_4O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
7	Δ	1	Total	С	Η	Ν	0	Р	0	0
	I	77	31	35	4	6	1	0	0	
7	В	1	Total	С	Η	Ν	0	Р	0	0
í D	1	77	31	35	4	6	1	0	0	

• Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

• Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total         C         O           10         6         4	0	0

• Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)



(formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
11	А	1	Total 12	С 6	N 1	0 4	${ m S}$ 1	0	0

• Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
12	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{H} & \text{O} \\ 10 & 2 & 6 & 2 \end{array}$	0	0
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
12	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

Continued from previous page...

• Molecule 13 is 1,3-PROPANDIOL (three-letter code: PDO) (formula:  $C_3H_8O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 5 & 3 & 2 \end{array}$	0	0
13	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 5 & 3 & 2 \end{array}$	0	0

• Molecule 14 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	А	1	Total 5	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	N 2	0	0

• Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	1	Total Zn 1 1	0	0
15	В	1	Total Zn 1 1	0	0

• Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	А	121	Total O 121 121	0	0
16	В	35	Total O 35 35	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 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.



• Molecule 1: Endoplasmic reticulum aminopeptidase 2





 $\bullet \ Molecule \ 2: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ eta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyra$ 

Chain C:

100%

#### NAG1 NAG2 BMA3 MAN4

 $\bullet \ Molecule \ 3: \ alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ eta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyra$ 

Chain D:

50%

50%



#### NAG1 NAG2 BMA3 MAN4

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

Cha	in	E:
-----	----	----

100%

#### NAG1 NAG2

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

Chain H:	100%
NAG1 NAG2	
• Molecule 4:	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-

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

Chain I:	50%	50%
M.G.2 M.G.2		

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

Chain F:	100%	
NAGI BNAG BNAG		

 • Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:	20%	80%	•
NAG1 NAG2 BMA3 MAN4 MAN5			



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.34Å 134.62Å 129.14Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.48^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	50.19 - 3.00	Depositor
Resolution (A)	50.19 - 3.00	EDS
% Data completeness	94.5 (50.19-3.00)	Depositor
(in resolution range)	94.5(50.19-3.00)	EDS
R <sub>merge</sub>	0.06	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
B B.	0.180 , $0.231$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.180 , $0.231$	DCC
$R_{free}$ test set	2265 reflections $(4.64%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	79.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
	0.010 for -h,-l,-k	
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
	0.025 for h,-k,-l	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14990	wwPDB-VP
Average B, all atoms $(Å^2)$	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: PEG, NAG, PDO, ZN, MAN, BMA, MES, 62S, IMD, EDO, PGE

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		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.55	0/7514	0.75	5/10190~(0.0%)	
1	В	0.49	0/7009	0.69	3/9536~(0.0%)	
All	All	0.52	0/14523	0.72	8/19726~(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	1
1	В	0	2
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	511	GLY	N-CA-C	-5.56	99.20	113.10
1	А	215	LEU	CA-CB-CG	5.46	127.86	115.30
1	А	859	LEU	CA-CB-CG	-5.31	103.09	115.30
1	А	341	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	В	67	LEU	CA-CB-CG	5.13	127.09	115.30
1	А	843	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	В	717	ASP	CB-CG-OD1	5.07	122.87	118.30
1	В	620	TRP	CA-CB-CG	5.07	123.33	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	270	ASP	Peptide
1	В	637	GLY	Peptide
1	В	638	HIS	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	7330	0	7172	177	0
1	В	6839	0	6480	270	0
2	С	50	0	43	2	0
3	D	50	0	43	0	0
4	Е	28	0	25	0	0
4	Н	28	0	25	0	0
4	Ι	28	0	25	0	0
5	F	39	0	34	4	0
6	G	61	0	52	4	0
7	А	42	35	0	3	0
7	В	42	35	0	1	0
8	А	56	0	52	4	0
8	В	84	0	78	0	0
9	А	14	0	20	0	0
10	А	10	0	14	1	0
11	А	12	0	12	1	0
12	А	28	6	42	3	0
13	А	5	0	8	0	0
13	В	5	0	8	0	0
14	А	5	0	5	0	0
15	А	1	0	0	0	0
15	В	1	0	0	0	0
16	А	121	0	0	1	0
16	В	35	0	0	1	0
All	All	14914	76	14138	454	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 16.

All (454) 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:945:LEU:HB3	1:B:949:LEU:CD2	1.61	1.29
1:B:945:LEU:HB3	1:B:949:LEU:HD22	1.13	1.09
1:B:945:LEU:HA	1:B:949:LEU:HD13	1.10	1.08
1:B:945:LEU:CB	1:B:949:LEU:HD22	1.94	0.98
1:B:945:LEU:CA	1:B:949:LEU:HD13	1.95	0.95
1:B:182:SER:HB2	1:B:330:ASP:HB2	1.48	0.95
1:B:342:ILE:HG22	1:B:344:TYR:CE1	2.09	0.87
1:B:945:LEU:HB3	1:B:949:LEU:HD21	1.57	0.86
1:B:866:PRO:HA	1:B:869:GLN:HG3	1.60	0.83
1:B:945:LEU:HA	1:B:949:LEU:CD1	2.02	0.83
1:B:703:LEU:HD23	1:B:726:LEU:HD22	1.60	0.81
1:B:762:ASN:HA	1:B:767:ILE:HD11	1.63	0.81
1:B:316:ILE:HD11	1:B:483:LYS:HG2	1.62	0.81
1:B:623:PHE:HB2	1:B:633:VAL:HG21	1.61	0.80
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.62	0.79
1:B:80:LEU:HD23	1:B:222:ILE:CD1	2.12	0.79
1:B:678:ASP:HA	1:B:955:TRP:CH2	2.18	0.77
1:A:67:LEU:HD23	1:A:441:GLU:HB3	1.66	0.77
1:B:465:LEU:HG	1:B:469:LEU:HD13	1.68	0.75
1:B:838:LEU:HD22	1:B:842:GLU:HG3	1.67	0.75
1:B:549:LEU:HD21	1:B:564:GLU:HG3	1.69	0.73
1:B:196:VAL:HG13	1:B:267:ILE:HD11	1.69	0.72
1:B:549:LEU:HB3	1:B:566:PHE:HD2	1.53	0.72
1:B:713:ARG:HH12	1:B:906:SER:HB2	1.55	0.72
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.25	0.71
1:B:678:ASP:HA	1:B:955:TRP:HH2	1.53	0.71
1:A:505:GLU:HB3	1:A:508:PHE:CE2	2.26	0.71
1:B:282:VAL:HG21	1:B:318:TYR:HD2	1.57	0.70
1:B:548:PRO:HB3	1:B:586:TRP:CE3	2.26	0.70
1:A:354:LYS:HE2	12:A:1113:EDO:H21	1.73	0.69
1:B:697:LEU:HD21	1:B:750:LEU:HD13	1.74	0.69
1:A:442:THR:O	1:A:446:ILE:HG13	1.91	0.69
1:B:722:LEU:O	1:B:724:ARG:N	2.19	0.69
1:A:603:HIS:CD2	1:A:612:LEU:HD21	2.27	0.69
1:B:54:PRO:HG2	1:B:65:GLN:CB	2.22	0.69
1:B:285:SER:HB2	1:B:324:ASP:OD1	1.94	0.68
1:B:737:GLN:HG3	1:B:754:LEU:HD12	1.75	0.68
1:A:331:PHE:CE2	1:A:333:PRO:HG2	2.29	0.68
1:B:337:GLU:HA	1:B:342:ILE:HD13	1.75	0.67
1:B:342:ILE:CG2	1:B:344:TYR:CE1	2.76	0.67
1:B:436:ILE:HG22	1:B:542:THR:HA	1.75	0.67
1:B:364:VAL:O	1:B:368:ILE:HG13	1.94	0.67
		Continue	ed on next page



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:838:LEU:CD2	1:B:842:GLU:HG3	2.24	0.67	
1:B:957:MET:HA	1:B:960:THR:HB	1.75	0.67	
1:B:943:LYS:HA	1:B:946:GLU:HG2	1.77	0.67	
1:B:571:PHE:HB2	1:B:574:ASP:HB2	1.77	0.67	
1:A:710:MET:HB2	1:A:719:SER:HB3	1.77	0.66	
1:B:323:LEU:HD12	1:B:340:GLY:HA2	1.78	0.66	
1:B:389:ILE:HG21	1:B:449:MET:HB3	1.76	0.66	
1:A:365:THR:HG21	1:A:411:LEU:CD1	2.27	0.65	
1:A:465:LEU:HD11	1:A:469:LEU:HD11	1.77	0.65	
5:F:1:NAG:O7	5:F:1:NAG:O3	2.13	0.65	
1:A:542:THR:HG22	1:A:543:LEU:CD2	2.27	0.64	
1:B:928:LEU:HG	1:B:930:ILE:HG22	1.78	0.64	
1:A:421:CYS:O	1:A:425:ILE:HG13	1.97	0.64	
1:A:563:GLN:OE1	1:A:585:LEU:HA	1.97	0.64	
1:A:273:SER:H	6:G:5:MAN:H62	1.62	0.64	
1:B:124:SER:N	1:B:130:TYR:O	2.31	0.63	
1:B:196:VAL:HG13	1:B:267:ILE:CD1	2.28	0.63	
1:A:945:LEU:HD22	1:A:949:LEU:HD12	1.81	0.63	
1:B:400:GLU:O	1:B:404:VAL:HG12	1.98	0.63	
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.81	0.63	
1:A:786:ILE:HD13	1:A:794:VAL:HG11	1.79	0.63	
1:A:659:ARG:NH1	1:A:690:GLU:OE2	2.29	0.63	
1:B:323:LEU:HD21	1:B:372:LEU:HD21	1.81	0.63	
1:B:703:LEU:HD23	1:B:726:LEU:CD2	2.28	0.63	
1:B:945:LEU:CD2	1:B:949:LEU:HD11	2.29	0.63	
1:A:724:ARG:O	1:A:728:GLN:HG3	1.99	0.63	
1:B:864:ARG:HD2	1:B:864:ARG:O	1.99	0.63	
1:A:238:LYS:HD2	1:A:241:THR:OG1	1.98	0.62	
1:A:398:TYR:OH	1:A:466:LYS:HD3	1.99	0.62	
1:B:141:SER:CB	1:B:148:ILE:HG22	2.29	0.62	
1:B:948:ASN:O	1:B:952:LEU:HB2	2.00	0.62	
1:A:242:ILE:HG12	1:A:250:GLU:HB3	1.81	0.62	
1:B:497:SER:HA	1:B:535:LYS:HE3	1.82	0.62	
1:B:680:ALA:HB2	1:B:683:MET:CB	2.29	0.62	
1:A:545:LYS:HD2	1:A:565:ARG:NH2	2.14	0.62	
1:B:82:VAL:HG22	1:B:224:ILE:HG12	1.80	0.62	
1:A:105:THR:HG22	1:A:107:PHE:H	1.64	0.61	
1:B:792:LYS:O	1:B:796:SER:HB2	2.00	0.61	
1:B:80:LEU:HD23	1:B:222:ILE:HD12	1.80	0.61	
1:B:378:GLY:O	1:B:382:THR:HB	2.00	0.61	
1:B:549:LEU:CD2	1:B:564:GLU:HG3	2.32	0.60	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:363:TRP:HB2	12:A:1116:EDO:H12	1.83	0.60	
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.36	0.60	
1:A:362:LEU:O	1:A:366:ARG:HG3	2.01	0.60	
1:B:140:LEU:HD12	1:B:149:ALA:HB3	1.82	0.60	
1:B:757:LEU:O	1:B:761:LEU:HG	2.01	0.60	
1:A:67:LEU:CD2	1:A:441:GLU:HB3	2.32	0.60	
1:B:566:PHE:CE2	1:B:632:ILE:HD12	2.36	0.60	
1:A:361:LYS:O	1:A:365:THR:HG22	2.02	0.60	
1:A:845:MET:O	1:A:886:LYS:HE3	2.02	0.59	
1:B:351:PHE:CE1	1:B:356:SER:HB3	2.37	0.59	
1:B:382:THR:O	1:B:489:ASN:HA	2.02	0.59	
1:B:196:VAL:HA	1:B:267:ILE:HG12	1.84	0.59	
1:A:663:ILE:HG21	1:A:698:GLU:HG2	1.84	0.59	
1:B:915:LYS:O	1:B:919:GLU:HG2	2.02	0.59	
1:A:128:SER:O	1:A:131:MET:HB2	2.01	0.59	
1:B:224:ILE:HD11	1:B:266:TYR:HB2	1.85	0.59	
1:A:139:VAL:HG22	1:A:150:LEU:HD22	1.84	0.59	
1:B:242:ILE:HD12	1:B:252:HIS:NE2	2.18	0.59	
1:B:140:LEU:CD1	1:B:149:ALA:HB3	2.32	0.58	
1:B:101:VAL:HG12	1:B:158:PRO:HA	1.84	0.58	
1:B:840:LEU:HB3	1:B:858:LEU:HD21	1.84	0.58	
5:F:2:NAG:O3	5:F:3:BMA:H2	2.03	0.58	
1:B:697:LEU:HD21	1:B:750:LEU:CD1	2.34	0.58	
1:B:64:TRP:CD2	1:B:70:PRO:HG3	2.39	0.58	
1:B:591:THR:HG23	1:B:600:ILE:HG23	1.85	0.58	
1:A:96:LYS:HD2	10:A:1108:PGE:H32	1.86	0.58	
1:A:293:ARG:O	1:A:296:THR:HG22	2.03	0.58	
1:B:852:THR:HG21	1:B:886:LYS:HE3	1.86	0.58	
1:B:918:PHE:O	1:B:922:GLU:HG2	2.03	0.58	
1:B:680:ALA:HA	1:B:683:MET:N	2.19	0.58	
1:A:395:PHE:HE2	1:A:495:LEU:HD21	1.68	0.57	
1:B:111:HIS:HA	1:B:147:GLN:HA	1.86	0.57	
1:B:452:GLU:HG3	7:B:1501:62S:C25	2.34	0.57	
1:B:907:SER:OG	1:B:909:ASP:HB3	2.05	0.57	
1:B:674:ARG:O	1:B:675:LEU:HD23	2.05	0.57	
1:A:367:VAL:HG22	7:A:1101:62S:C27	2.35	0.57	
1:B:63:PRO:HB2	1:B:107:PHE:CE2	2.39	0.57	
1:B:727:LEU:O	1:B:731:LYS:HB2	2.04	0.56	
1:A:95:GLU:OE1	1:A:209:PRO:HD2	2.06	0.56	
1:B:201:PRO:HG2	1:B:202:THR:HG23	1.87	0.56	
1:A:660:VAL:HG12	1:A:695:ALA:HA	1.87	0.56	



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.39	0.56		
1:A:663:ILE:CG2	1:A:698:GLU:HG2	2.36	0.56		
1:B:362:LEU:O	1:B:365:THR:HG22	2.05	0.56		
1:A:778:MET:HG3	1:A:807:TYR:CD2	2.41	0.56		
1:B:272:HIS:ND1	1:B:290:PRO:HB3	2.21	0.56		
1:B:421:CYS:O	1:B:425:ILE:HG13	2.05	0.56		
1:A:293:ARG:NH2	6:G:2:NAG:O3	2.39	0.55		
1:B:238:LYS:O	1:B:238:LYS:HG3	2.06	0.55		
1:B:465:LEU:HD13	1:B:538:MET:CE	2.36	0.55		
1:B:917:PHE:CE1	1:B:921:LEU:HD21	2.41	0.55		
1:B:933:THR:O	1:B:937:THR:HG22	2.07	0.55		
1:A:272:HIS:CD2	1:A:290:PRO:HB3	2.42	0.55		
1:B:199:PHE:CD1	1:B:204:ALA:HA	2.41	0.55		
1:B:623:PHE:CB	1:B:633:VAL:HG21	2.34	0.55		
1:A:192:ARG:HA	1:B:190:GLU:HG2	1.89	0.55		
1:A:492:ASN:OD1	1:A:542:THR:HG21	2.07	0.55		
1:B:197:THR:HG23	1:B:266:TYR:O	2.07	0.55		
1:B:433:SER:O	1:B:545:LYS:HD3	2.06	0.55		
1:A:802:THR:HG22	1:A:836:LYS:HZ1	1.72	0.55		
1:B:479:ILE:O	1:B:483:LYS:HG3	2.06	0.55		
1:A:193:ILE:HG13	1:B:190:GLU:HG3	1.89	0.55		
1:A:579:ALA:O	1:A:582:GLU:HG2	2.07	0.54		
5:F:1:NAG:H62	5:F:2:NAG:C1	2.36	0.54		
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.88	0.54		
1:A:647:LEU:HD13	1:A:686:TYR:CE2	2.42	0.54		
1:B:954:THR:HG22	1:B:958:VAL:HG21	1.89	0.54		
1:B:743:GLY:H	1:B:751:ARG:NH2	2.05	0.54		
1:B:930:ILE:HA	1:B:933:THR:CG2	2.37	0.54		
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.42	0.54		
1:B:442:THR:O	1:B:446:ILE:HG13	2.08	0.54		
1:B:839:LYS:O	1:B:843:LEU:HG	2.08	0.54		
1:A:226:ARG:HG3	1:A:227:GLU:O	2.08	0.54		
1:A:418:LEU:HD21	1:A:627:SER:HB3	1.91	0.53		
1:A:626:ASP:OD2	1:A:655:ARG:NH1	2.41	0.53		
1:A:702:TYR:O	1:A:705:SER:HB3	2.07	0.53		
1:B:397:LYS:O	1:B:400:GLU:HG2	2.07	0.53		
1:B:551:VAL:HG21	1:B:564:GLU:OE2	2.08	0.53		
1:B:762:ASN:HA	1:B:767:ILE:CD1	2.35	0.53		
1:A:351:PHE:HA	16:A:1203:HOH:O	2.09	0.53		
1:A:479:ILE:O	1:A:483:LYS:HG3	2.09	0.53		
1:A:670:VAL:HG11	1:A:677:LEU:CD1	2.38	0.53		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:863:ALA:HB2	1:A:901:THR:HG22	1.90	0.52
1:A:764:ALA:HB3	1:A:765:PRO:HD3	1.91	0.52
1:A:870:GLN:O	1:A:873:TRP:N	2.42	0.52
1:B:362:LEU:O	1:B:362:LEU:HD12	2.09	0.52
1:A:791:LEU:HD11	1:A:795:TYR:CZ	2.44	0.52
1:B:937:THR:O	1:B:941:ASN:HB2	2.09	0.52
1:A:796:SER:HB3	1:A:827:ALA:HA	1.92	0.52
1:B:468:PHE:HD1	1:B:469:LEU:HD12	1.73	0.52
1:A:622:LYS:HE3	1:A:658:ASP:CG	2.29	0.52
1:B:224:ILE:HD11	1:B:266:TYR:CB	2.40	0.52
1:B:372:LEU:O	1:B:375:GLN:HG2	2.10	0.52
1:B:475:GLN:O	1:B:479:ILE:HG13	2.09	0.52
1:B:438:LYS:HG2	1:B:439:PRO:CD	2.40	0.52
1:B:104:ALA:HB2	1:B:158:PRO:CD	2.37	0.51
1:A:127:ASP:HB2	1:A:160:LEU:HD23	1.91	0.51
1:B:945:LEU:HD23	1:B:949:LEU:HD11	1.91	0.51
1:B:122:LEU:HD23	1:B:163:TYR:O	2.10	0.51
1:B:101:VAL:HG21	1:B:156:LEU:CB	2.40	0.51
1:B:870:GLN:OE1	1:B:910:LYS:NZ	2.43	0.51
1:B:930:ILE:HA	1:B:933:THR:HG22	1.93	0.51
1:A:399:MET:HE3	1:A:402:ILE:HD11	1.93	0.51
1:B:127:ASP:OD1	1:B:129:ARG:HG3	2.11	0.51
1:B:365:THR:HG21	1:B:411:LEU:HD12	1.92	0.51
1:B:362:LEU:HA	1:B:365:THR:HG22	1.92	0.51
1:A:448:GLU:OE2	1:A:929:ASP:N	2.39	0.51
1:B:141:SER:HB2	1:B:148:ILE:HG22	1.93	0.50
1:B:395:PHE:HE2	1:B:495:LEU:HD21	1.76	0.50
1:A:710:MET:CB	1:A:719:SER:HB3	2.39	0.50
1:A:905:PHE:HB2	1:A:938:ILE:HD13	1.92	0.50
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.93	0.50
1:B:945:LEU:O	1:B:949:LEU:HB2	2.12	0.50
1:B:157:THR:N	1:B:162:TYR:OH	2.44	0.50
1:B:214:PRO:HA	1:B:260:SER:HB3	1.93	0.50
1:B:95:GLU:OE1	1:B:209:PRO:HD2	2.12	0.50
1:B:103:ASN:O	1:B:105:THR:HG23	2.12	0.50
1:B:126:GLU:OE1	1:B:160:LEU:HA	2.12	0.50
1:B:786:ILE:HD13	1:B:794:VAL:HG11	1.94	0.50
1:A:362:LEU:HD13	1:A:411:LEU:HB3	1.94	0.50
1:A:670:VAL:HG11	1:A:677:LEU:HD13	1.94	0.50
1:A:888:ASP:O	1:A:894:ILE:HG13	2.12	0.50
1:B:63:PRO:HB2	1:B:107:PHE:CD2	2.47	0.50



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:100:LEU:O	1:B:100:LEU:HD12	2.11	0.50	
1:A:122:LEU:HD12	1:A:163:TYR:O	2.12	0.50	
1:B:438:LYS:HG2	1:B:439:PRO:HD2	1.93	0.50	
1:B:497:SER:HB2	1:B:535:LYS:CE	2.42	0.49	
1:B:805:TRP:CE2	1:B:828:LEU:HD22	2.47	0.49	
1:B:934:VAL:HA	1:B:937:THR:CG2	2.42	0.49	
1:A:666:VAL:HG12	1:A:680:ALA:HB2	1.95	0.49	
1:A:780:SER:CB	1:A:784:LEU:HG	2.43	0.49	
1:A:774:PHE:HB2	1:A:794:VAL:HG13	1.94	0.49	
1:B:344:TYR:HE2	1:B:367:VAL:HG12	1.77	0.49	
1:B:76:LEU:HD11	1:B:100:LEU:HG	1.95	0.49	
1:B:591:THR:HG23	1:B:600:ILE:CG2	2.42	0.49	
1:B:641:ASP:OD1	1:B:641:ASP:N	2.41	0.49	
1:B:452:GLU:O	1:B:456:ASN:HB2	2.12	0.49	
1:B:777:TRP:HB2	1:B:784:LEU:HD22	1.95	0.49	
1:A:382:THR:O	1:A:489:ASN:HA	2.13	0.49	
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.48	0.49	
1:B:737:GLN:HA	1:B:737:GLN:OE1	2.12	0.49	
1:B:786:ILE:CD1	1:B:794:VAL:HG11	2.42	0.49	
1:B:366:ARG:HD2	1:B:413:PHE:CE1	2.48	0.48	
1:B:397:LYS:HD2	1:B:455:TYR:HB3	1.94	0.48	
1:B:707:TYR:HE2	1:B:761:LEU:CD2	2.26	0.48	
1:B:676:THR:OG1	1:B:678:ASP:OD1	2.29	0.48	
1:A:337:GLU:OE2	7:A:1101:62S:N10	2.46	0.48	
1:B:342:ILE:HD11	1:B:375:GLN:NE2	2.29	0.48	
1:B:934:VAL:HA	1:B:937:THR:HG22	1.94	0.48	
1:A:286:ILE:HG13	1:A:300:LEU:HB2	1.95	0.48	
1:A:884:LEU:HA	1:A:884:LEU:HD23	1.64	0.48	
1:B:750:LEU:HD12	1:B:750:LEU:O	2.13	0.48	
1:B:751:ARG:O	1:B:755:LEU:HG	2.14	0.48	
1:B:955:TRP:H	1:B:955:TRP:HE3	1.61	0.48	
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.48	0.48	
1:B:395:PHE:CD2	1:B:462:LEU:HD11	2.49	0.48	
1:A:547:ILE:HG13	1:A:548:PRO:HD2	1.96	0.48	
1:A:88:SER:HB3	1:A:90:ASP:OD2	2.13	0.47	
1:A:239:VAL:HG23	1:A:240:LYS:HB2	1.95	0.47	
1:A:875:PHE:O	1:A:879:ASN:ND2	2.46	0.47	
1:B:910:LYS:HD3	1:B:913:GLU:OE2	2.12	0.47	
1:A:244:LEU:HB2	1:A:248:LEU:O	2.13	0.47	
1:B:674:ARG:C	1:B:675:LEU:HD23	2.35	0.47	
1:B:754:LEU:O	1:B:757:LEU:N	2.47	0.47	



	• • • • • • •	Interatomic	nic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:298:TYR:OH	1:A:365:THR:HB	2.13	0.47		
1:A:873:TRP:CH2	1:A:877:ARG:HD3	2.49	0.47		
1:B:278:THR:HG22	1:B:308:ASP:OD1	2.14	0.47		
1:B:945:LEU:HD22	1:B:949:LEU:HD11	1.94	0.47		
1:A:232:ALA:HA	1:A:267:ILE:O	2.15	0.47		
1:A:75:PRO:HD2	1:A:216:PHE:HD1	1.78	0.47		
1:B:325:LEU:HD23	1:B:349:LEU:HD11	1.96	0.47		
1:A:587:HIS:CD2	1:A:606:LYS:HD3	2.49	0.47		
1:A:660:VAL:HG12	1:A:695:ALA:CA	2.44	0.47		
1:B:248:LEU:HD22	6:G:1:NAG:H83	1.95	0.47		
1:A:62:PHE:CZ	1:A:149:ALA:HB2	2.50	0.47		
1:A:95:GLU:O	1:A:165:ALA:HA	2.15	0.47		
1:A:106:GLN:O	1:A:152:VAL:HG22	2.14	0.47		
1:A:659:ARG:HH11	1:A:690:GLU:CD	2.18	0.47		
1:B:106:GLN:HA	1:B:152:VAL:CG2	2.44	0.47		
1:B:182:SER:CB	1:B:330:ASP:HB2	2.33	0.47		
1:B:307:LEU:O	1:B:311:GLU:HG3	2.14	0.47		
1:B:465:LEU:HD13	1:B:538:MET:HE3	1.95	0.47		
1:B:549:LEU:HB3	1:B:566:PHE:CD2	2.41	0.47		
1:B:624:ASN:CB	1:B:631:TYR:HE1	2.28	0.47		
1:B:731:LYS:N	1:B:732:PRO:HD2	2.29	0.47		
1:B:733:VAL:HG12	1:B:754:LEU:CD1	2.45	0.47		
1:B:944:TRP:O	1:B:948:ASN:HB2	2.14	0.47		
1:B:952:LEU:C	1:B:953:ARG:HD3	2.34	0.47		
1:A:561:LEU:HD12	1:A:610:ASP:HB3	1.97	0.47		
1:A:731:LYS:N	1:A:732:PRO:HD2	2.29	0.47		
1:B:236:MET:HE3	1:B:256:THR:HA	1.96	0.47		
1:A:756:LYS:HE3	1:A:760:ASP:OD2	2.15	0.47		
1:A:588:ILE:HB	1:A:590:LEU:HD21	1.96	0.46		
1:B:337:GLU:HA	1:B:342:ILE:CD1	2.45	0.46		
1:A:421:CYS:O	1:A:424:VAL:HG12	2.14	0.46		
8:A:1105:NAG:C8	8:A:1105:NAG:C3	2.94	0.46		
1:B:337:GLU:HG3	1:B:374:HIS:HB3	1.98	0.46		
1:B:226:ARG:HG3	1:B:227:GLU:O	2.16	0.46		
1:B:559:LEU:O	1:B:612:LEU:N	2.31	0.46		
1:B:662:LEU:O	1:B:666:VAL:HG22	2.15	0.46		
1:B:194:LEU:HD23	1:B:194:LEU:N	2.31	0.46		
1:A:182:SER:OG	1:A:330:ASP:HB2	2.16	0.46		
1:A:570:VAL:HG12	1:A:577:TRP:HD1	1.81	0.46		
1:B:58:ASN:HB3	1:B:60:GLU:H	1.79	0.46		
1:B:566:PHE:O	1:B:567:LEU:HD22	2.16	0.46		



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:200:GLU:HG2	1:A:201:PRO:HA	1.98	0.46	
1:A:802:THR:HG22	1:A:836:LYS:CE	2.45	0.46	
1:B:112:SER:HB2	1:B:209:PRO:HB3	1.98	0.46	
1:B:80:LEU:HB3	1:B:222:ILE:HD13	1.97	0.46	
1:B:273:SER:HB3	1:B:287:TYR:CD1	2.51	0.46	
1:B:72:VAL:HG23	1:B:73:VAL:HG13	1.98	0.46	
1:B:687:LEU:CB	1:B:696:LEU:HD13	2.46	0.46	
1:A:548:PRO:HG2	1:A:631:TYR:HB3	1.99	0.45	
1:A:830:THR:HA	1:A:865:ARG:NE	2.30	0.45	
1:B:795:TYR:O	1:B:827:ALA:HB1	2.17	0.45	
1:B:889:LEU:CD1	1:B:928:LEU:HD22	2.45	0.45	
1:B:817:SER:O	1:B:821:GLN:HG3	2.16	0.45	
1:B:918:PHE:CE2	1:B:931:PHE:HA	2.52	0.45	
1:A:434:ARG:NH2	1:A:454:SER:OG	2.47	0.45	
1:A:889:LEU:HG	1:A:928:LEU:HD21	1.98	0.45	
1:A:739:TRP:HE3	1:A:790:VAL:HG21	1.80	0.45	
1:B:737:GLN:CG	1:B:754:LEU:HD12	2.43	0.45	
1:A:220:PHE:O	1:A:256:THR:HG23	2.16	0.45	
1:A:550:LEU:O	1:A:633:VAL:HA	2.16	0.45	
1:B:96:LYS:HA	1:B:164:VAL:O	2.17	0.45	
1:B:678:ASP:HA	1:B:955:TRP:CZ2	2.49	0.45	
1:A:542:THR:HG22	1:A:543:LEU:HG	1.99	0.45	
11:A:1109:MES:H81	11:A:1109:MES:H51	1.74	0.45	
1:B:707:TYR:CE1	1:B:711:ASP:HB2	2.52	0.45	
1:A:148:ILE:HD12	1:A:148:ILE:HA	1.67	0.45	
1:A:718:ILE:HG23	1:A:956:LEU:HD12	1.99	0.45	
1:B:271:PHE:CD2	1:B:326:ILE:HD11	2.51	0.45	
6:G:3:BMA:H62	6:G:5:MAN:H2	1.48	0.45	
1:A:638:HIS:O	1:A:642:GLN:HG2	2.16	0.45	
1:A:647:LEU:HD21	1:A:659:ARG:HG2	1.98	0.45	
1:A:140:LEU:HD11	1:A:151:LEU:HD11	1.98	0.45	
1:A:457:LYS:HE3	1:A:630:TYR:CE2	2.52	0.45	
1:A:510:SER:HA	1:A:511:GLY:HA2	1.64	0.45	
1:B:482:LEU:O	1:B:486:SER:HB3	2.17	0.45	
1:B:954:THR:CG2	1:B:958:VAL:HG21	2.45	0.45	
1:A:54:PRO:HG2	1:A:62:PHE:HB3	1.99	0.44	
1:A:474:PHE:O	1:A:478:ILE:HG12	2.17	0.44	
8:A:1105:NAG:C8	8:A:1105:NAG:H3	2.46	0.44	
1:B:604:ILE:HG22	1:B:605:LEU:H	1.81	0.44	
1:B:952:LEU:O	1:B:953:ARG:HD3	2.16	0.44	
1:B:221:SER:OG	1:B:255:THR:HG22	2.17	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:877:ARG:HG2	1:B:917:PHE:CZ	2.52	0.44	
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.98	0.44	
1:A:544:GLN:HG2	12:A:1110:EDO:H11	1.99	0.44	
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.82	0.44	
1:A:770:ALA:CB	1:A:797:VAL:HG21	2.46	0.44	
1:A:915:LYS:O	1:A:919:GLU:HG3	2.16	0.44	
1:A:432:SER:N	1:A:936:GLU:OE2	2.49	0.44	
1:B:152:VAL:HG11	16:B:1627:HOH:O	2.16	0.44	
1:B:248:LEU:C	1:B:249:LEU:HD12	2.38	0.44	
1:A:723:LYS:HG3	1:A:761:LEU:HB3	2.00	0.44	
1:B:352:ASP:O	1:B:356:SER:HB2	2.17	0.44	
1:B:552:VAL:HG12	1:B:561:LEU:HD22	2.00	0.44	
1:B:588:ILE:HG23	1:B:631:TYR:CE2	2.53	0.44	
1:B:282:VAL:HA	1:B:321:SER:O	2.18	0.44	
1:B:497:SER:HB2	1:B:535:LYS:HE2	2.00	0.44	
1:A:238:LYS:HD2	1:A:241:THR:HG1	1.82	0.44	
1:B:86:LEU:N	1:B:86:LEU:HD23	2.33	0.44	
1:B:272:HIS:HE1	2:C:2:NAG:H81	1.82	0.44	
1:B:277:PHE:CE1	3:277:PHE:CE1 1:B:283:LYS:HG3		0.44	
1:B:318:TYR:CE2	1:B:323:LEU:HB2	2.53	0.44	
1:B:453:VAL:O	1:B:457:LYS:HB3	2.17	0.44	
1:A:123:GLN:HG2	1:A:134:GLY:HA3	1.99	0.44	
1:A:715:ILE:HG22	1:A:715:ILE:O	2.18	0.44	
1:A:841:ILE:HD13	1:A:859:LEU:HD21	2.00	0.44	
1:B:666:VAL:O	1:B:670:VAL:HG23	2.18	0.44	
1:A:200:GLU:CG	1:A:201:PRO:HA	2.48	0.43	
1:A:484:LYS:HD3	1:A:485:PHE:CE2	2.53	0.43	
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.18	0.43	
1:A:732:PRO:O	1:A:736:ARG:HG3	2.19	0.43	
1:A:922:GLU:HA	1:A:926:SER:O	2.16	0.43	
1:B:104:ALA:H	1:B:158:PRO:HG3	1.83	0.43	
1:B:379:ASN:OD1	1:B:379:ASN:N	2.52	0.43	
1:A:285:SER:HB2	1:A:324:ASP:OD1	2.18	0.43	
1:B:436:ILE:HG22	1:B:542:THR:CA	2.47	0.43	
1:B:603:HIS:ND1	1:B:604:ILE:HD12	2.32	0.43	
1:A:330:ASP:OD1	1:A:851:LYS:HD2	2.18	0.43	
1:A:802:THR:HG22	1:A:836:LYS:NZ	2.33	0.43	
1:B:404:VAL:HG11	1:B:413:PHE:CD2	2.53	0.43	
1:B:141:SER:HB3	1:B:148:ILE:HG22	1.99	0.43	
1:B:928:LEU:HG	1:B:930:ILE:CG2	2.47	0.43	
5:F:2:NAG:H4	5:F:3:BMA:O2	2.18	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:666:VAL:HG11	1:A:680:ALA:HA	2.01	0.43	
1:A:770:ALA:HB3	1:A:797:VAL:HG21	2.01	0.43	
1:B:548:PRO:CG	1:B:588:ILE:HD11	2.49	0.43	
1:A:745:VAL:O	1:A:749:MET:HG3	2.18	0.43	
1:B:857:ALA:HA	1:B:896:MET:CE	2.49	0.43	
1:B:928:LEU:HB3	1:B:931:PHE:CE2	2.54	0.43	
1:B:444:THR:O	1:B:448:GLU:HG3	2.19	0.43	
1:B:677:LEU:HD13	1:B:952:LEU:HD13	1.99	0.43	
1:A:139:VAL:HG22	1:A:150:LEU:CD2	2.47	0.43	
1:B:465:LEU:HD13	1:B:538:MET:HE2	2.00	0.43	
1:A:236:MET:SD	1:A:320:LEU:HD13	2.59	0.42	
1:A:624:ASN:HB2	1:A:631:TYR:CE1	2.54	0.42	
1:A:833:HIS:HB2	1:A:836:LYS:HD2	2.00	0.42	
1:B:64:TRP:CE2	1:B:70:PRO:HG3	2.54	0.42	
1:B:217:LYS:HE3	1:B:382:THR:HG22	2.00	0.42	
1:B:337:GLU:HB3	1:B:371:GLU:OE2	2.20	0.42	
1:B:791:LEU:HD12	1:B:791:LEU:HA	1.70	0.42	
1:B:479:ILE:CG2	1:B:483:LYS:HE3	2.49	0.42	
1:B:830:THR:O	1:B:830:THR:HG22	2.19	0.42	
1:A:610:ASP:OD1	1:A:611:THR:N	2.48	0.42	
1:A:641:ASP:O	1:A:645:THR:OG1	2.35	0.42	
1:A:654:LEU:N	1:A:654:LEU:HD12	2.34	0.42	
1:B:318:TYR:CZ	1:B:320:LEU:HB2	2.54	0.42	
1:B:377:PHE:HE2	1:B:399:MET:HG3	1.84	0.42	
1:A:279:SER:HB2	1:A:308:ASP:OD1	2.18	0.42	
1:A:300:LEU:O	1:A:300:LEU:HD12	2.20	0.42	
1:B:955:TRP:HA	1:B:958:VAL:HB	2.02	0.42	
1:A:792:LYS:HD2	1:A:826:TYR:CD1	2.55	0.42	
1:A:68:ARG:HH11	1:A:68:ARG:HD2	1.67	0.42	
1:B:591:THR:CG2	1:B:625:VAL:HG12	2.50	0.42	
1:B:738:SER:O	1:B:751:ARG:HD3	2.19	0.42	
1:B:743:GLY:H	1:B:751:ARG:HH22	1.66	0.42	
1:A:323:LEU:HD12	1:A:324:ASP:H	1.84	0.42	
1:A:334:GLY:N	7:A:1101:62S:O30	2.41	0.42	
1:A:683:MET:O	1:A:686:TYR:HD2	2.03	0.42	
1:A:838:LEU:O	1:A:842:GLU:HG3	2.19	0.42	
1:B:78:TYR:HB2	1:B:220:PHE:CD2	2.55	0.42	
1:B:894:ILE:HA	1:B:894:ILE:HD13	1.80	0.42	
1:B:414:ASP:OD2	1:B:657:LYS:NZ	2.32	0.42	
1:B:190:GLU:OE1	1:B:192:ARG:NH1	2.39	0.42	
1:B:677:LEU:O	1:B:677:LEU:HD23	2.20	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:112:SER:HB3	1:B:148:ILE:HD13	2.02	0.41	
1:B:187:LEU:O	1:B:187:LEU:HD23	2.20	0.41	
1:B:338:ASN:HB2	1:B:341:LEU:O	2.19	0.41	
1:B:576:GLU:H	1:B:576:GLU:HG3	1.59	0.41	
1:A:96:LYS:HA	1:A:164:VAL:O	2.20	0.41	
1:A:620:TRP:NE1	1:A:646:GLN:HG3	2.34	0.41	
1:B:571:PHE:CE2	1:B:943:LYS:HD2	2.56	0.41	
1:A:866:PRO:HA	1:A:869:GLN:HG2	2.02	0.41	
1:B:75:PRO:HA	1:B:99:VAL:HG12	2.03	0.41	
1:B:772:GLU:O	1:B:776:GLN:HG2	2.20	0.41	
1:A:677:LEU:HD12	1:A:677:LEU:HA	1.81	0.41	
1:B:954:THR:HB	1:B:955:TRP:CE3	2.55	0.41	
1:A:713:ARG:HD2	1:A:713:ARG:HA	1.90	0.41	
1:B:271:PHE:CE2	1:B:326:ILE:HD11	2.56	0.41	
1:B:318:TYR:CE2	1:B:320:LEU:HB2	2.56	0.41	
1:A:219:ASN:OD1	1:A:258:LYS:HD3	2.20	0.41	
1:A:263:LEU:O	1:A:338:ASN:HB3	2.21	0.41	
1:A:537:MET:HG3	1:A:587:HIS:O	2.21	0.41	
1:A:739:TRP:CE3	739:TRP:CE3 1:A:790:VAL:HG21		0.41	
1:B:693:SER:N	1:B:694:PRO:HD2	2.36	0.41	
1:A:193:ILE:HG13	1:B:190:GLU:CG	2.51	0.41	
8:A:1105:NAG:H3	8:A:1105:NAG:H82	2.02	0.41	
1:B:249:LEU:HD12	1:B:249:LEU:N	2.35	0.41	
1:A:106:GLN:HB3	1:A:107:PHE:HD1	1.86	0.41	
1:A:227:GLU:HG3	2:C:1:NAG:H83	2.02	0.41	
1:B:74:ILE:O	1:B:74:ILE:HG22	2.20	0.41	
1:B:330:ASP:OD2	1:B:851:LYS:HE3	2.21	0.41	
1:B:496:TRP:HA	1:B:499:LEU:HD12	2.03	0.41	
1:A:324:ASP:C	1:A:325:LEU:HD12	2.41	0.41	
1:A:626:ASP:HA	1:A:657:LYS:HB2	2.03	0.41	
1:B:224:ILE:CD1	1:B:266:TYR:HB2	2.50	0.41	
1:B:777:TRP:HB2	1:B:784:LEU:CD2	2.51	0.41	
1:B:184:TYR:CE2	1:B:192:ARG:HB2	2.55	0.40	
1:B:547:ILE:HB	1:B:630:TYR:CE2	2.56	0.40	
1:B:106:GLN:C	1:B:152:VAL:HG22	2.41	0.40	
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.76	0.40	
1:A:342:ILE:CG2	1:A:371:GLU:HG3	2.51	0.40	
1:B:386:TRP:CB	1:B:446:ILE:HG23	2.52	0.40	
8:A:1105:NAG:H83	8:A:1105:NAG:O3	2.22	0.40	
1:B:295:GLN:HB3	1:B:350:LEU:HB3	2.04	0.40	
1:A:91:PHE:CE2	1:A:170:ALA:HB3	2.56	0.40	



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Atom 1	n-1 Atom-2 In dis	Interatomic	$\operatorname{Clash}$	
Atom-1		distance $(\text{\AA})$	overlap (Å)	
1:A:352:ASP:OD2	1:A:355:THR:OG1	2.39	0.40	
1:B:282:VAL:HG22	1:B:320:LEU:O	2.22	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.

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	ntiles
1	А	906/962~(94%)	858~(95%)	48 (5%)	0	100	100
1	В	859/962~(89%)	801 (93%)	56~(6%)	2~(0%)	47	82
All	All	1765/1924~(92%)	1659 (94%)	104 (6%)	2(0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	638	HIS
1	В	723	LYS

#### 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	Percentiles
1	А	796/865~(92%)	771 (97%)	25~(3%)	40 75
1	В	707/865~(82%)	674~(95%)	33~(5%)	26 63



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0 0 1 0 0 1 0 0 0 0 0 0	J	<i>P</i> · · · · · · · · · · · · · · · · · · ·	r ~g ~···

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1503/1730~(87%)	1445~(96%)	58~(4%)	32 69

All (58) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	79	ASP
1	А	95	GLU
1	А	132	LYS
1	А	185	ARG
1	А	192	ARG
1	А	194	LEU
1	А	312	LYS
1	А	339	TRP
1	А	371	GLU
1	А	383	MET
1	А	476	LYS
1	А	504	LEU
1	A	505	GLU
1	A	508	PHE
1	А	545	LYS
1	А	563	GLN
1	А	571	PHE
1	А	582	GLU
1	А	627	SER
1	А	650	ASN
1	А	678	ASP
1	А	746	TRP
1	А	829	SER
1	А	864	ARG
1	А	893	ASP
1	В	53	PHE
1	В	64	TRP
1	В	68	ARG
1	В	107	PHE
1	В	122	LEU
1	В	140	LEU
1	В	179	PHE
1	В	185	ARG
1	В	194	LEU
1	В	203	GLN
1	В	331	PHE
1	В	383	MET



Mol	Chain	Res	Type
1	В	395	PHE
1	В	497	SER
1	В	502	SER
1	В	549	LEU
1	В	553	LYS
1	В	560	ARG
1	В	568	GLN
1	В	581	GLN
1	В	587	HIS
1	В	620	TRP
1	В	707	TYR
1	В	729	TYR
1	В	746	TRP
1	В	751	ARG
1	В	796	SER
1	В	865	ARG
1	В	929	ASP
1	В	943	LYS
1	В	946	GLU
1	В	953	ARG
1	В	959	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	806	ASN
1	В	272	HIS
1	В	581	GLN
1	В	879	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)

22 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	Type	Chain	Bos	Link	Bo	ond leng	ths	Bond angles		
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	NAG	С	1	1,2	$14,\!14,\!15$	0.63	0	$17,\!19,\!21$	0.60	0
2	NAG	С	2	2	$14,\!14,\!15$	0.55	0	$17,\!19,\!21$	0.69	0
2	BMA	С	3	2	11,11,12	1.22	2 (18%)	$15,\!15,\!17$	1.29	2 (13%)
2	MAN	С	4	2	11,11,12	2.78	3 (27%)	$15,\!15,\!17$	1.91	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.14	0	$17,\!19,\!21$	0.72	0
3	NAG	D	2	3	$14,\!14,\!15$	0.37	0	$17,\!19,\!21$	0.60	0
3	BMA	D	3	3	11,11,12	0.87	1 (9%)	$15,\!15,\!17$	1.70	3 (20%)
3	MAN	D	4	3	$11,\!11,\!12$	1.23	2 (18%)	$15,\!15,\!17$	1.19	2 (13%)
4	NAG	Е	1	4,1	14,14,15	0.43	0	$17,\!19,\!21$	1.11	1 (5%)
4	NAG	Е	2	4	14,14,15	0.88	1 (7%)	$17,\!19,\!21$	0.71	0
5	NAG	F	1	1,5	14,14,15	0.75	1 (7%)	17,19,21	1.16	1 (5%)
5	NAG	F	2	5	14,14,15	1.18	1 (7%)	17,19,21	1.20	1 (5%)
5	BMA	F	3	5	11,11,12	2.07	3 (27%)	$15,\!15,\!17$	1.20	1 (6%)
6	NAG	G	1	6,1	14,14,15	0.65	1 (7%)	17,19,21	0.59	0
6	NAG	G	2	6	14,14,15	1.19	1 (7%)	17,19,21	1.00	1 (5%)
6	BMA	G	3	6	11,11,12	1.00	1 (9%)	$15,\!15,\!17$	1.75	5 (33%)
6	MAN	G	4	6	11,11,12	2.05	5 (45%)	$15,\!15,\!17$	1.19	2 (13%)
6	MAN	G	5	6	11,11,12	3.05	6 (54%)	$15,\!15,\!17$	2.82	5 (33%)
4	NAG	Н	1	4,1	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.53	0
4	NAG	Ι	1	4,1	14,14,15	0.59	0	$17,\!19,\!21$	0.55	0
4	NAG	I	2	4	14,14,15	1.08	1 (7%)	$17,\!19,\!21$	1.67	3 (17%)

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	С	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
2	MAN	С	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
4	NAG	Е	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
6	NAG	G	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1
4	NAG	Н	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Н	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Ι	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Ι	2	4	-	1/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
2	С	4	MAN	O5-C1	6.76	1.54	1.43
6	G	5	MAN	C4-C3	5.54	1.66	1.52
5	F	3	BMA	O5-C1	4.67	1.51	1.43
6	G	5	MAN	C2-C3	4.30	1.58	1.52
2	С	4	MAN	O5-C5	4.17	1.51	1.43
5	F	2	NAG	O5-C1	4.09	1.50	1.43
6	G	5	MAN	C4-C5	3.95	1.61	1.53
2	С	4	MAN	C1-C2	3.86	1.61	1.52
6	G	4	MAN	C2-C3	3.75	1.58	1.52
6	G	2	NAG	O5-C1	-3.70	1.37	1.43
6	G	5	MAN	C1-C2	3.62	1.60	1.52
4	Ι	2	NAG	O5-C1	3.38	1.49	1.43
6	G	4	MAN	C4-C3	3.15	1.60	1.52
4	Е	2	NAG	C1-C2	3.04	1.56	1.52
3	D	4	MAN	O5-C5	2.83	1.49	1.43
6	G	5	MAN	O4-C4	2.83	1.49	1.43
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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
6	G	4	MAN	C1-C2	2.54	1.58	1.52
2	С	3	BMA	C2-C3	-2.49	1.48	1.52
6	G	5	MAN	O5-C1	2.48	1.47	1.43
5	F	3	BMA	C1-C2	2.46	1.57	1.52
6	G	3	BMA	O5-C5	2.39	1.48	1.43
2	С	3	BMA	O3-C3	-2.34	1.37	1.43
5	F	1	NAG	O5-C1	2.29	1.47	1.43
6	G	4	MAN	O5-C1	-2.23	1.40	1.43
6	G	1	NAG	O5-C1	-2.23	1.40	1.43
3	D	4	MAN	C4-C5	2.14	1.57	1.53
6	G	4	MAN	O3-C3	2.13	1.48	1.43
5	F	3	BMA	O4-C4	2.08	1.47	1.43
3	D	3	BMA	C1-C2	2.08	1.56	1.52

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All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	G	5	MAN	C1-O5-C5	6.98	121.65	112.19
2	С	4	MAN	C1-O5-C5	4.77	118.66	112.19
4	Ι	2	NAG	C1-O5-C5	4.53	118.33	112.19
3	D	3	BMA	C1-O5-C5	4.46	118.23	112.19
6	G	5	MAN	C1-C2-C3	4.33	114.99	109.67
6	G	5	MAN	C2-C3-C4	4.30	118.33	110.89
6	G	5	MAN	C3-C4-C5	4.03	117.42	110.24
4	Е	1	NAG	C1-O5-C5	3.74	117.26	112.19
2	С	4	MAN	O5-C1-C2	3.69	116.46	110.77
5	F	2	NAG	C1-O5-C5	3.64	117.13	112.19
5	F	1	NAG	C1-O5-C5	3.48	116.91	112.19
5	F	3	BMA	C1-O5-C5	3.45	116.86	112.19
6	G	3	BMA	C3-C4-C5	3.31	116.14	110.24
2	С	3	BMA	C1-C2-C3	-3.07	105.89	109.67
4	Ι	2	NAG	C4-C3-C2	-2.89	106.78	111.02
3	D	3	BMA	O5-C1-C2	2.86	115.19	110.77
6	G	3	BMA	C6-C5-C4	-2.84	106.36	113.00
3	D	3	BMA	O2-C2-C3	-2.79	104.54	110.14
2	С	3	BMA	O2-C2-C3	-2.59	104.94	110.14
4	Ι	2	NAG	C1-C2-N2	2.51	114.77	110.49
6	G	3	BMA	O5-C1-C2	-2.48	106.95	110.77
3	D	4	MAN	C1-O5-C5	2.43	115.49	112.19
6	G	5	MAN	O5-C1-C2	2.36	114.41	110.77
2	С	4	MAN	O2-C2-C1	2.35	113.96	109.15
6	G	3	BMA	C2-C3-C4	2.32	114.90	110.89



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	4	MAN	O2-C2-C3	-2.19	105.74	110.14
6	G	2	NAG	C3-C4-C5	2.19	114.15	110.24
6	G	4	MAN	O2-C2-C1	2.08	113.42	109.15
6	G	3	BMA	C1-C2-C3	-2.06	107.14	109.67
6	G	4	MAN	O5-C5-C6	2.04	110.40	107.20

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
5	F	3	BMA	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C1-C2-N2-C7
3	D	4	MAN	C4-C5-C6-O6
2	С	2	NAG	C8-C7-N2-C2
2	С	2	NAG	O7-C7-N2-C2
6	G	2	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
4	Ε	1	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
4	Ι	1	NAG	O5-C5-C6-O6
4	Ι	2	NAG	C4-C5-C6-O6
4	Е	2	NAG	C4-C5-C6-O6
6	G	5	MAN	C4-C5-C6-O6
4	Е	2	NAG	O5-C5-C6-O6

All (20) torsion outliers are listed below:

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1	NAG	1	0
5	F	2	NAG	3	0
6	G	2	NAG	1	0
5	F	1	NAG	2	0
6	G	5	MAN	2	0
6	G	3	BMA	1	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	2	NAG	1	0
6	G	1	NAG	1	0
5	F	3	BMA	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)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	Bos	Link	B	ond leng	gths	E	Bond ang	gles
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
14	IMD	А	1114	-	$3,\!5,\!5$	0.37	0	$4,\!5,\!5$	0.64	0
8	NAG	В	1503	1	14,14,15	0.80	1 (7%)	17,19,21	0.49	0
8	NAG	В	1505	1	14,14,15	0.34	0	17,19,21	0.63	0
12	EDO	А	1115	-	3,3,3	0.68	0	2,2,2	0.12	0
13	PDO	А	1112	-	4,4,4	0.43	0	3,3,3	0.29	0
8	NAG	А	1104	1	14,14,15	0.27	0	17,19,21	0.59	0
8	NAG	В	1504	1	14,14,15	1.10	1 (7%)	17,19,21	0.89	1 (5%)
8	NAG	В	1506	1	14,14,15	1.16	2 (14%)	17,19,21	0.51	0
11	MES	А	1109	-	12,12,12	2.27	1 (8%)	14,16,16	1.83	4 (28%)
10	PGE	А	1108	-	9,9,9	0.53	0	8,8,8	0.38	0
12	EDO	А	1118	-	3,3,3	0.64	0	2,2,2	0.09	0
8	NAG	А	1105	1	14,14,15	0.54	0	17,19,21	2.32	3 (17%)
12	EDO	А	1110	-	3,3,3	0.56	0	2,2,2	0.28	0
13	PDO	В	1508	-	4,4,4	0.36	0	3,3,3	0.40	0
9	PEG	А	1107	-	6,6,6	0.51	0	$5,\!5,\!5$	0.31	0
7	62S	В	1501	15	38,45,45	3.17	13 (34%)	46,62,62	1.81	14 (30%)
7	62S	А	1101	15	38,45,45	<mark>3.28</mark>	6 (15%)	46,62,62	1.91	11 (23%)
12	EDO	А	1116	-	3,3,3	0.52	0	2,2,2	0.28	0
9	PEG	А	1106	-	6,6,6	0.51	0	$5,\!5,\!5$	0.38	0
12	EDO	А	1117	-	3,3,3	0.73	0	2,2,2	0.09	0
8	NAG	А	1102	1	14,14,15	0.58	0	17,19,21	0.65	0
8	NAG	В	1507	1	14,14,15	1.05	1 (7%)	17,19,21	1.20	2 (11%)
12	EDO	А	1113	-	3,3,3	0.84	0	2,2,2	0.29	0
8	NAG	А	1103	1	14,14,15	2.17	4 (28%)	17,19,21	1.82	4 (23%)
8	NAG	В	1502	1	14,14,15	0.99	1 (7%)	17,19,21	1.14	1 (5%)
12	EDO	A	1111	-	3,3,3	0.55	0	2,2,2	0.15	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.



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	IMD	А	1114	-	-	-	0/1/1/1
8	NAG	В	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	В	1505	1	-	2/6/23/26	0/1/1/1
12	EDO	А	1115	-	-	1/1/1/1	-
13	PDO	А	1112	-	-	1/2/2/2	-
8	NAG	А	1104	1	-	3/6/23/26	0/1/1/1
8	NAG	В	1504	1	-	2/6/23/26	0/1/1/1
8	NAG	В	1506	1	-	1/6/23/26	0/1/1/1
11	MES	А	1109	-	-	4/6/14/14	0/1/1/1
10	PGE	А	1108	-	-	3/7/7/7	-
12	EDO	А	1118	-	-	0/1/1/1	-
8	NAG	А	1105	1	-	3/6/23/26	0/1/1/1
12	EDO	А	1110	-	-	0/1/1/1	-
13	PDO	В	1508	-	-	1/2/2/2	-
9	PEG	А	1107	-	-	3/4/4/4	-
7	62S	В	1501	15	-	14/32/40/40	0/4/4/4
7	62S	А	1101	15	-	9/32/40/40	0/4/4/4
12	EDO	А	1116	-	-	1/1/1/1	-
9	PEG	A	1106	-	-	1/4/4/4	-
12	EDO	A	1117	-	-	0/1/1/1	-
8	NAG	A	1102	1	-	0/6/23/26	0/1/1/1
8	NAG	В	1507	1	-	1/6/23/26	0/1/1/1
12	EDO	А	1113	-	-	0/1/1/1	-
8	NAG	A	1103	1	-	1/6/23/26	0/1/1/1
8	NAG	В	1502	1	-	2/6/23/26	0/1/1/1
12	EDO	A	1111	-	-	0/1/1/1	-

'-' means no outliers of that kind were identified.

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
7	А	1101	62S	P11-C14	16.41	1.95	1.79
7	В	1501	62S	P11-C14	13.92	1.93	1.79
7	В	1501	62S	C29-N31	7.60	1.50	1.34
11	А	1109	MES	C8-S	-7.29	1.67	1.77
7	А	1101	62S	C29-N31	7.23	1.50	1.34
7	В	1501	62S	C33-N35	6.51	1.49	1.32
7	А	1101	62S	C33-N35	5.51	1.46	1.32
8	А	1103	NAG	O5-C1	5.18	1.52	1.43
8	В	1504	NAG	O5-C1	3.78	1.49	1.43



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	Ideal(Å)
8	А	1103	NAG	C1-C2	3.52	1.57	1.52
8	В	1506	NAG	C1-C2	3.32	1.57	1.52
8	В	1502	NAG	O5-C1	3.31	1.49	1.43
8	В	1507	NAG	O5-C1	3.25	1.48	1.43
8	А	1103	NAG	C8-C7	-3.24	1.43	1.50
8	А	1103	NAG	O7-C7	3.12	1.30	1.23
7	В	1501	62S	C19-N20	2.86	1.38	1.33
7	В	1501	62S	C18-C17	2.77	1.43	1.39
7	В	1501	62S	C32-C33	2.70	1.58	1.52
8	В	1503	NAG	C1-C2	2.57	1.56	1.52
7	В	1501	62S	C15-C29	2.56	1.56	1.51
8	В	1506	NAG	O5-C1	2.54	1.47	1.43
7	В	1501	62S	C06-C01	2.54	1.44	1.38
7	А	1101	62S	O28-C23	2.43	1.41	1.36
7	В	1501	62S	C27-C22	2.40	1.43	1.40
7	В	1501	62S	C22-C19	2.33	1.55	1.48
7	В	1501	62S	O28-C23	2.31	1.41	1.36
7	В	1501	62S	C04-C03	2.25	1.44	1.38
7	A	1101	62S	C04-C03	2.24	1.43	1.38
7	В	1501	62S	C36-C37	2.03	1.56	1.51
7	А	1101	62S	C06-C01	2.00	1.43	1.38

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All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	А	1105	NAG	C2-N2-C7	8.65	135.23	122.90
7	А	1101	62S	C17-C16-C15	-6.26	105.93	114.21
7	В	1501	62S	P11-C09-C08	4.96	121.06	111.10
8	А	1103	NAG	C1-O5-C5	4.58	118.40	112.19
7	А	1101	62S	P11-C09-C08	-4.48	102.11	111.10
11	А	1109	MES	C5-N4-C3	4.01	117.85	108.83
8	В	1502	NAG	C1-O5-C5	3.86	117.42	112.19
7	В	1501	62S	C15-C29-N31	3.73	122.66	116.21
7	В	1501	62S	C22-C19-N20	3.63	126.75	120.96
8	А	1103	NAG	C2-N2-C7	-3.50	117.92	122.90
7	А	1101	62S	C08-C07-C01	3.41	125.03	113.18
7	В	1501	62S	C32-C33-N35	3.39	122.49	116.69
7	А	1101	62S	C27-C22-C23	3.34	123.68	117.45
7	А	1101	62S	C27-C22-C19	-3.17	111.95	119.68
7	A	1101	62S	O30-C29-C15	-3.14	118.03	122.12
8	В	1507	NAG	C1-O5-C5	3.12	116.41	112.19
7	В	1501	62S	O30-C29-C15	-3.07	118.13	122.12



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	В	1501	62S	C36-C32-N31	3.05	117.21	110.79
8	В	1504	NAG	C1-O5-C5	3.00	116.25	112.19
7	В	1501	62S	C19-C18-C17	2.97	110.02	106.02
7	А	1101	62S	O13-P11-C09	-2.85	100.47	106.87
8	А	1103	NAG	O5-C5-C4	2.80	117.63	110.83
7	В	1501	62S	C18-C19-N20	-2.79	104.90	109.97
7	А	1101	62S	C19-C18-C17	-2.69	102.41	106.02
7	А	1101	62S	C22-C19-N20	-2.68	116.67	120.96
7	В	1501	62S	C08-C07-C01	2.66	122.44	113.18
8	А	1105	NAG	C1-O5-C5	2.58	115.69	112.19
7	А	1101	62S	C06-C01-C02	2.52	122.13	118.17
7	В	1501	62S	C17-C16-C15	2.46	117.46	114.21
7	А	1101	62S	C36-C32-N31	-2.42	105.68	110.79
7	В	1501	62S	O34-C33-N35	-2.38	118.85	123.00
11	А	1109	MES	C7-N4-C5	2.30	117.11	111.23
7	В	1501	62S	C32-N31-C29	2.30	126.59	121.67
11	А	1109	MES	O3S-S-C8	2.17	109.27	105.77
8	В	1507	NAG	C2-N2-C7	2.12	125.92	122.90
7	В	1501	62S	C36-C32-C33	-2.12	104.89	110.94
8	А	1103	NAG	O4-C4-C3	2.09	115.17	110.35
11	А	1109	MES	O2S-S-C8	2.09	109.43	106.92
8	A	1105	NAG	C8-C7-N2	2.06	119.59	116.10
7	В	1501	62S	O30-C29-N31	-2.04	119.16	122.93

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms
7	А	1101	62S	C16-C15-C29-N31
7	А	1101	62S	C16-C15-C29-O30
7	А	1101	62S	C08-C09-P11-O12
7	А	1101	62S	C15-C14-P11-O12
7	А	1101	62S	C15-C14-P11-O13
7	В	1501	62S	P11-C14-C15-C16
7	В	1501	62S	C29-C15-C16-C17
7	В	1501	62S	C16-C15-C29-N31
7	В	1501	62S	C16-C15-C29-O30
7	В	1501	62S	C18-C19-C22-C23
7	В	1501	62S	C15-C14-P11-O12
7	В	1501	62S	C15-C14-P11-O13
8	А	1105	NAG	C3-C2-N2-C7
8	В	1507	NAG	C3-C2-N2-C7



Mol	Chain	Res	Type	Atoms
11	А	1109	MES	N4-C7-C8-S
11	А	1109	MES	C7-C8-S-O2S
13	В	1508	PDO	C1-C2-C3-O3
8	В	1504	NAG	C4-C5-C6-O6
8	В	1502	NAG	O5-C5-C6-O6
8	В	1505	NAG	O5-C5-C6-O6
8	В	1504	NAG	O5-C5-C6-O6
8	В	1502	NAG	C4-C5-C6-O6
8	В	1505	NAG	C4-C5-C6-O6
8	А	1105	NAG	C8-C7-N2-C2
8	А	1105	NAG	O7-C7-N2-C2
9	А	1107	PEG	O1-C1-C2-O2
7	В	1501	62S	C36-C32-N31-C29
11	А	1109	MES	C7-C8-S-O3S
12	А	1115	EDO	O1-C1-C2-O2
8	А	1104	NAG	O5-C5-C6-O6
8	А	1103	NAG	O5-C5-C6-O6
9	А	1107	PEG	O2-C3-C4-O4
8	В	1506	NAG	O5-C5-C6-O6
7	В	1501	62S	N31-C32-C36-C37
7	А	1101	62S	C14-C15-C16-C17
7	В	1501	62S	C33-C32-C36-C37
10	А	1108	PGE	O2-C3-C4-O3
9	А	1106	PEG	C1-C2-O2-C3
8	В	1503	NAG	C4-C5-C6-O6
7	В	1501	62S	C33-C32-N31-C29
10	А	1108	PGE	C4-C3-O2-C2
8	А	1104	NAG	C1-C2-N2-C7
9	А	1107	PEG	C4-C3-O2-C2
10	А	1108	PGE	O3-C5-C6-O4
11	А	1109	MES	C7-C8-S-O1S
7	В	1501	62S	C01-C07-C08-C09
7	В	1501	62S	C15-C16-C17-C18
7	А	1101	62S	C14-C15-C29-N31
8	В	1503	NAG	O5-C5-C6-O6
12	А	1116	EDO	O1-C1-C2-O2
8	А	1104	NAG	C3-C2-N2-C7
13	А	1112	PDO	O1-C1-C2-C3
7	А	1101	62S	C18-C19-C22-C23
7	А	1101	62S	C07-C08-C09-N10
7	В	1501	62S	C07-C08-C09-N10

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There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	А	1109	MES	1	0
10	А	1108	PGE	1	0
8	А	1105	NAG	4	0
12	А	1110	EDO	1	0
7	В	1501	62S	1	0
7	А	1101	62S	3	0
12	А	1116	EDO	1	0
12	А	1113	EDO	1	0

8 monomers are involved in 13 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 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 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>2	$OWAB(Å^2)$	Q<0.9
1	А	911/962~(94%)	-0.35	6 (0%) 87 69	39, 70, 124, 190	0
1	В	871/962~(90%)	-0.13	20 (2%) 60 31	38, 108, 163, 240	0
All	All	1782/1924~(92%)	-0.25	26 (1%) 73 46	38, 85, 153, 240	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	554	GLN	4.2
1	В	502	SER	3.3
1	В	616	GLU	3.1
1	В	623	PHE	3.0
1	В	621	VAL	2.9
1	В	654	LEU	2.8
1	В	637	GLY	2.8
1	В	592	TYR	2.7
1	В	773	LEU	2.6
1	А	514	CYS	2.5
1	А	573	GLU	2.4
1	В	831	SER	2.4
1	В	550	LEU	2.3
1	В	615	PRO	2.3
1	В	837	LEU	2.2
1	В	503	CYS	2.2
1	В	536	GLU	2.2
1	В	164	VAL	2.1
1	А	559	LEU	2.1
1	А	511	GLY	2.1
1	В	551	VAL	2.1
1	В	552	VAL	2.1
1	В	105	THR	2.1
1	В	52	ALA	2.0



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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	515	HIS	2.0
1	А	516	SER	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
2	MAN	С	4	11/12	0.76	0.31	143,171,177,180	0
5	BMA	F	3	11/12	0.77	0.34	115,153,157,163	0
4	NAG	Ι	2	14/15	0.79	0.31	145,161,169,171	0
3	MAN	D	4	11/12	0.82	0.24	175,183,188,195	0
6	MAN	G	4	11/12	0.82	0.24	107,123,148,155	0
6	MAN	G	5	11/12	0.82	0.19	57,104,116,121	0
3	BMA	D	3	11/12	0.84	0.16	141,161,172,181	0
4	NAG	Е	2	14/15	0.84	0.24	156,170,176,177	0
4	NAG	Н	2	14/15	0.85	0.20	97,132,151,156	0
2	BMA	С	3	11/12	0.86	0.17	151,159,169,175	0
4	NAG	Ι	1	14/15	0.86	0.16	99,138,150,160	0
5	NAG	F	2	14/15	0.89	0.30	112,147,152,159	0
6	NAG	G	2	14/15	0.91	0.16	94,114,123,125	0
5	NAG	F	1	14/15	0.93	0.30	161,169,180,186	0
6	BMA	G	3	11/12	0.93	0.09	94,119,126,131	0
4	NAG	Н	1	14/15	0.93	0.21	102,115,139,139	0
2	NAG	С	2	14/15	0.93	0.14	101,116,134,142	0
4	NAG	Е	1	14/15	0.94	0.16	96,114,132,157	0
3	NAG	D	2	14/15	0.96	0.13	90,102,124,151	0
2	NAG	С	1	14/15	0.96	0.14	70,93,109,114	0
3	NAG	D	1	14/15	0.97	0.16	67,83,89,89	0
6	NAG	G	1	14/15	0.97	0.13	54,73,77,94	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
8	NAG	В	1504	14/15	0.75	0.26	144,165,175,182	0
12	EDO	А	1110	4/4	0.75	0.36	121,123,125,127	0
8	NAG	В	1506	14/15	0.79	0.39	172,179,187,187	0
12	EDO	А	1111	4/4	0.80	0.46	116,116,117,117	0
8	NAG	А	1104	14/15	0.81	0.28	153,167,181,184	0
8	NAG	В	1507	14/15	0.81	0.25	149,171,180,180	0
8	NAG	В	1503	14/15	0.82	0.26	175,193,205,212	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	А	1102	14/15	0.82	0.17	124,131,136,139	0
11	MES	А	1109	12/12	0.83	0.23	106,146,352,353	0
8	NAG	А	1103	14/15	0.83	0.19	93,134,148,154	0
10	PGE	А	1108	10/10	0.83	0.41	72,121,132,137	0
12	EDO	А	1115	4/4	0.83	0.82	87,98,100,105	0
8	NAG	В	1502	14/15	0.84	0.26	$136,\!153,\!159,\!160$	0
9	PEG	А	1106	7/7	0.85	0.26	85,100,114,114	0
13	PDO	В	1508	5/5	0.85	0.18	117,122,130,133	0
8	NAG	В	1505	14/15	0.86	0.20	115,142,159,163	0
12	EDO	А	1113	4/4	0.87	0.34	64,83,100,100	0
13	PDO	А	1112	5/5	0.88	0.25	87,91,97,98	0
12	EDO	А	1117	4/4	0.90	0.82	77,77,82,83	0
8	NAG	А	1105	14/15	0.93	0.10	136,151,166,170	0
12	EDO	А	1116	4/4	0.94	0.22	81,98,115,115	0
9	PEG	А	1107	7/7	0.94	0.09	104,113,121,124	0
14	IMD	А	1114	5/5	0.94	0.23	116,117,120,122	0
12	EDO	А	1118	4/4	0.95	0.67	49,72,86,87	0
7	62S	В	1501	42/42	0.95	0.33	70,104,156,175	0
7	62S	A	1101	42/42	0.97	0.31	40,89,181,207	0
15	ZN	А	1119	1/1	0.99	0.21	45,45,45,45	0
15	ZN	В	1509	1/1	1.00	0.21	66,66,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









### 6.5 Other polymers (i)

There are no such residues in this entry.

