

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

#### Oct 11, 2023 – 12:37 AM EDT

PDB ID	:	7K66
Title	:	Structure of Blood Coagulation Factor VIII in Complex with an Anti-C1 Do-
		main Pathogenic Antibody Inhibitor
Authors	:	Childers, K.C.; Gish, J.; Jarvis, L.; Peters, S.; Garrels, C.; Smith, I.W.;
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Deposited on	:	2020-09-18
Resolution	:	3.92  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.92 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	Qualit	y of chain		
1	А	1467	2% 49%	33%	•	14%
2	В	223	45%	45%		5%••
3	С	213	59%		35%	5%
4	Н	5	1	100%		
5	D	2	1	100%		



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	1265	Total 10216	C 6562	N 1748	0 1854	S 52	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1627	ALA	-	linker	UNP P00451
А	1628	GLN	-	linker	UNP P00451
А	1629	ASN	-	linker	UNP P00451
А	1630	SER	-	linker	UNP P00451
А	1631	ARG	-	linker	UNP P00451
А	1632	PRO	-	linker	UNP P00451
А	1633	PRO	-	linker	UNP P00451
А	1634	SER	-	linker	UNP P00451
А	1635	ALA	-	linker	UNP P00451
А	1636	SER	-	linker	UNP P00451

• Molecule 2 is a protein called 2A9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	217	Total 1649	C 1048	N 266	O 327	S 8	0	0	0

• Molecule 3 is a protein called 2A9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	213	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
<b>J</b>		210	1634	1019	271	335	9	0	0	0

• Molecule 4 is an oligosaccharide called 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-a



cetamido-2-deoxy-beta-D-glucopyranose.



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

• Molecule 5 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
5	D	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
6	А	1	Total 14	C 8	N 1	O 5	0	0



• Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Cu 1 1	0	0

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total Ca 1 1	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	А	1	Total 1	Zn 1	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total O 1 1	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: Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII







# S176 532 T179 593 T179 593 F186 593 F192 619 S199 597 S199 1103 S196 1103 F199 4106 F199 4106 F199 4106 F199 4110 F201 1113 T201 7113 F203 7113 F204 7113 F205 7116 F206 7113 F207 7113 F208 7113 F209 7113 F143 7143

 $\bullet$  Molecule 4: 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-deo

100%	
cetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido	o-2-deoxy-beta-D-gluc
U	100% acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido

Chain D:

100%

NAG1 NAG2



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	116.72Å 116.72Å 371.06Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.49 - 3.92	Depositor
Resolution (A)	49.49 - 3.92	EDS
% Data completeness	97.7 (49.49-3.92)	Depositor
(in resolution range)	97.7 (49.49 - 3.92)	EDS
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.99 (at 3.88 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
P. P.	0.226 , $0.322$	Depositor
$n, n_{free}$	0.238 , $0.324$	DCC
$R_{free}$ test set	1991 reflections $(8.50\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	147.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 125.2	EDS
L-test for $twinning^2$	$ < L >=0.40, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13606	wwPDB-VP
Average B, all atoms $(Å^2)$	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.26% 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: BMA, NAG, ZN, MAN, CU, CA

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.28	0/10502	0.50	0/14238	
2	В	0.31	0/1693	0.59	3/2312~(0.1%)	
3	С	0.27	0/1672	0.52	0/2269	
All	All	0.29	0/13867	0.52	3/18819~(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
2	В	0	4
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	116	VAL	N-CA-C	-6.30	93.99	111.00
2	В	119	SER	N-CA-C	-5.96	94.91	111.00
2	В	119	SER	CA-C-N	-5.40	105.31	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	316	HIS	Peptide
2	В	117	THR	Peptide



Continued from previous page...

Mol	Chain	Res	Type	Group
2	В	119	SER	Mainchain
2	В	120	SER	Peptide
2	В	153	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	10216	0	9961	347	0
2	В	1649	0	1593	133	0
3	С	1634	0	1560	68	0
4	Н	61	0	51	2	0
5	D	28	0	25	0	0
6	А	14	0	13	0	0
7	А	1	0	0	0	0
8	А	1	0	0	0	0
9	А	1	0	0	0	0
10	B	1	0	0	0	0
All	All	13606	0	13203	540	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 20.

All (540) 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)
2:B:91:THR:CB	2:B:117:THR:HG21	1.03	1.48
2:B:91:THR:CB	2:B:117:THR:CG2	1.98	1.40
2:B:91:THR:OG1	2:B:117:THR:CG2	1.68	1.38
2:B:91:THR:CA	2:B:117:THR:HG21	1.57	1.34
2:B:91:THR:CA	2:B:117:THR:CG2	2.07	1.33
2:B:91:THR:HA	2:B:117:THR:CG2	1.60	1.31
2:B:91:THR:OG1	2:B:117:THR:HG21	1.08	1.26
2:B:88:ASN:O	2:B:118:VAL:HG23	1.36	1.25
2:B:88:ASN:O	2:B:118:VAL:CG2	1.86	1.22
2:B:91:THR:OG1	2:B:117:THR:CB	1.89	1.19



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:91:THR:HA	2:B:117:THR:HG22	1.22	1.13
2:B:10:GLU:O	2:B:116:VAL:HG21	1.48	1.12
2:B:11:LEU:HA	2:B:116:VAL:CG1	1.80	1.10
2:B:11:LEU:CB	2:B:116:VAL:HG11	1.87	1.03
1:A:31:PHE:H	1:A:32:PRO:CD	1.70	1.03
2:B:10:GLU:O	2:B:116:VAL:CG2	2.08	1.02
2:B:11:LEU:CD1	2:B:116:VAL:CG1	2.37	1.01
2:B:88:ASN:CA	2:B:118:VAL:CG2	2.39	1.01
2:B:91:THR:CG2	2:B:117:THR:HG21	1.91	1.00
2:B:11:LEU:HA	2:B:116:VAL:HG11	1.41	0.99
2:B:91:THR:HG23	2:B:117:THR:HG23	1.44	0.97
2:B:88:ASN:HA	2:B:118:VAL:HG22	1.46	0.97
2:B:13:LYS:NZ	2:B:119:SER:OG	1.99	0.95
2:B:11:LEU:CA	2:B:116:VAL:HG11	1.94	0.95
1:A:369:ILE:HG22	1:A:522:THR:HG23	1.49	0.95
1:A:31:PHE:CD1	1:A:32:PRO:HD3	2.02	0.94
2:B:91:THR:CG2	2:B:117:THR:CG2	2.43	0.94
2:B:11:LEU:HD13	2:B:116:VAL:CG1	1.97	0.94
2:B:88:ASN:O	2:B:118:VAL:HG21	1.69	0.93
2:B:88:ASN:C	2:B:118:VAL:CG2	2.35	0.93
1:A:1999:GLU:HB3	1:A:2006:LEU:HD11	1.50	0.93
2:B:88:ASN:CA	2:B:118:VAL:HG22	1.97	0.92
1:A:31:PHE:H	1:A:32:PRO:HD3	1.36	0.91
1:A:43:PRO:O	1:A:45:VAL:N	2.04	0.90
2:B:88:ASN:HA	2:B:118:VAL:CG2	2.01	0.90
2:B:11:LEU:HD12	2:B:116:VAL:CG1	2.07	0.85
2:B:88:ASN:HD22	2:B:118:VAL:HG13	1.43	0.83
2:B:11:LEU:CD1	2:B:116:VAL:HG11	2.07	0.83
2:B:91:THR:HG23	2:B:117:THR:CG2	2.05	0.82
1:A:1925:VAL:HG22	1:A:1926:MET:HG3	1.61	0.82
1:A:105:SER:HB3	1:A:140:GLN:HB2	1.61	0.82
1:A:31:PHE:HD1	1:A:32:PRO:HD3	1.45	0.81
2:B:35:HIS:HE1	2:B:99:CYS:HB3	1.45	0.81
2:B:91:THR:CA	2:B:117:THR:HG22	1.91	0.81
3:C:61:PHE:CE2	3:C:74:ILE:CD1	2.64	0.81
2:B:11:LEU:HD12	2:B:116:VAL:HG12	1.64	0.79
3:C:74:ILE:HG21	3:C:77:VAL:HG12	1.66	0.78
1:A:31:PHE:N	1:A:32:PRO:CD	2.42	0.78
1:A:2156:TYR:HD2	1:A:2160:SER:HG	1.32	0.78
2:B:11:LEU:HD13	2:B:116:VAL:HG13	1.65	0.78
2:B:11:LEU:HB2	2:B:116:VAL:HG11	1.64	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:631:LEU:HD11	1:A:685:PRO:HG3	1.68	0.76
3:C:109:ASP:N	3:C:109:ASP:OD1	2.18	0.74
2:B:88:ASN:CB	2:B:118:VAL:HG22	2.16	0.74
3:C:200:LYS:HZ2	3:C:204:ILE:CG1	2.00	0.74
1:A:233:HIS:HB3	1:A:321:MET:HG2	1.70	0.74
2:B:88:ASN:C	2:B:118:VAL:HG21	2.05	0.74
2:B:91:THR:OG1	2:B:117:THR:OG1	2.06	0.74
2:B:11:LEU:HA	2:B:116:VAL:CB	2.17	0.74
2:B:12:LYS:NZ	2:B:17:THR:O	2.20	0.74
2:B:11:LEU:HD11	2:B:119:SER:OG	1.89	0.73
3:C:200:LYS:HZ2	3:C:204:ILE:HG13	1.54	0.73
1:A:2102:ILE:HD11	2:B:103:VAL:HG11	1.70	0.72
1:A:419:ILE:O	1:A:421:ARG:N	2.22	0.72
1:A:164:ASP:OD1	1:A:2007:GLN:NE2	2.25	0.70
1:A:73:LEU:HD21	1:A:199:LEU:HB2	1.74	0.70
1:A:1825:PRO:HG3	1:A:1833:LYS:H	1.57	0.70
1:A:189:ARG:HB3	1:A:192:ASN:HB2	1.73	0.70
2:B:13:LYS:HZ3	2:B:119:SER:C	1.96	0.69
2:B:145:LEU:HD21	2:B:217:ILE:HG21	1.75	0.68
1:A:2192:ALA:HB2	1:A:2230:LEU:HD12	1.74	0.68
1:A:1789:LEU:HD12	1:A:1855:LEU:HD13	1.75	0.68
3:C:61:PHE:CE2	3:C:74:ILE:HD11	2.27	0.68
1:A:418:ARG:NH1	1:A:607:GLU:O	2.27	0.67
1:A:435:THR:HG23	1:A:437:LYS:H	1.60	0.67
3:C:4:LEU:HD21	3:C:89:GLN:HG2	1.76	0.67
3:C:74:ILE:CG2	3:C:77:VAL:HG12	2.25	0.67
2:B:88:ASN:C	2:B:118:VAL:HG23	2.10	0.67
2:B:9:PRO:HB3	2:B:114:THR:HA	1.77	0.66
2:B:88:ASN:CB	2:B:118:VAL:CG2	2.72	0.66
3:C:112:PRO:HB2	3:C:135:LEU:HD22	1.75	0.66
3:C:15:LEU:H	3:C:106:LYS:HB2	1.59	0.66
1:A:5:TYR:HB2	1:A:87:VAL:HG22	1.78	0.66
1:A:687:LEU:HD12	1:A:707:LYS:HG3	1.76	0.65
1:A:3:ARG:NH1	1:A:83:ASP:OD2	2.29	0.65
1:A:1933:VAL:HG22	1:A:2015:LEU:HB3	1.78	0.65
1:A:1782:PRO:HB3	1:A:1809:PRO:HD3	1.78	0.65
1:A:31:PHE:H	1:A:32:PRO:HD2	1.60	0.65
1:A:1808:GLN:HG3	1:A:1809:PRO:HD2	1.78	0.65
1:A:391:GLU:HG2	1:A:392:ASP:H	1.62	0.65
1:A:162:HIS:O	1:A:162:HIS:ND1	2.30	0.64
3:C:130:SER:HA	3:C:179:THR:HB	1.80	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:145:LEU:HD22	2:B:146:GLY:H	1.63	0.64
3:C:60:ARG:HH21	3:C:61:PHE:HE1	1.43	0.64
2:B:2:ILE:HA	2:B:25:SER:HB3	1.79	0.64
2:B:33:SER:O	2:B:34:MET:HG2	1.97	0.63
1:A:16:TYR:HE2	1:A:232:MET:HG3	1.63	0.63
1:A:1733:VAL:HG22	1:A:1851:LEU:HD21	1.80	0.63
2:B:13:LYS:NZ	2:B:119:SER:O	2.23	0.63
3:C:150:ASP:H	3:C:190:SER:HB2	1.64	0.63
1:A:1939:ARG:NH2	1:A:1987:GLU:OE1	2.32	0.62
1:A:106:PHE:HB2	1:A:110:SER:HB2	1.81	0.62
1:A:2141:ASN:O	1:A:2143:PRO:HD3	2.00	0.61
3:C:24:ARG:HG2	3:C:69:SER:HB2	1.82	0.61
1:A:705:LEU:H	1:A:705:LEU:HD23	1.65	0.61
1:A:69:TRP:HZ3	1:A:197:VAL:H	1.48	0.60
1:A:300:PHE:HD2	1:A:302:MET:HG3	1.65	0.60
1:A:708:VAL:HG23	1:A:709:SER:H	1.66	0.60
3:C:61:PHE:CE2	3:C:74:ILE:HD13	2.36	0.60
1:A:697:PHE:O	1:A:699:ASN:N	2.33	0.60
2:B:51:ILE:HD12	2:B:58:PRO:HG3	1.82	0.60
2:B:151:GLY:HA2	2:B:181:LEU:HD21	1.83	0.60
1:A:2193:SER:OG	1:A:2228:GLU:OE1	2.20	0.60
2:B:11:LEU:HA	2:B:116:VAL:HB	1.82	0.60
1:A:1807:VAL:HG22	1:A:1813:ARG:HH11	1.65	0.59
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.84	0.59
2:B:106:ALA:O	2:B:107:ILE:HD12	2.03	0.59
1:A:1949:SER:O	1:A:1952:ASN:ND2	2.36	0.59
1:A:453:LEU:HD23	1:A:513:TRP:HZ3	1.67	0.59
1:A:2101:PHE:HA	1:A:2154:THR:HG23	1.84	0.59
2:B:16:GLU:H	2:B:86:LEU:HD12	1.67	0.59
1:A:1797:GLU:O	1:A:1799:GLY:N	2.36	0.59
1:A:193:LEU:O	1:A:195:GLU:N	2.36	0.59
3:C:148:LYS:HA	3:C:153:GLU:HG3	1.84	0.58
1:A:525:ASP:N	1:A:525:ASP:OD1	2.36	0.58
1:A:2110:LYS:HA	1:A:2112:TRP:HD1	1.69	0.58
2:B:131:LEU:HD12	3:C:117:PHE:HB3	1.84	0.58
1:A:2141:ASN:HB3	1:A:2142:PRO:HD3	1.86	0.58
3:C:14:SER:HA	3:C:106:LYS:HB2	1.85	0.58
2:B:3:GLN:O	2:B:25:SER:OG	2.15	0.58
3:C:205:VAL:O	3:C:206:LYS:NZ	2.32	0.58
1:A:16:TYR:CE2	1:A:232:MET:HG3	2.39	0.58
1:A:452:LEU:HA	1:A:550:PRO:HG2	1.85	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:175:ALA:HB2	2:B:184:LEU:HB3	1.86	0.58
3:C:149:ILE:O	3:C:151:GLY:N	2.37	0.58
1:A:2110:LYS:HA	1:A:2112:TRP:CD1	2.38	0.57
2:B:91:THR:OG1	2:B:117:THR:HB	1.97	0.57
1:A:1750:GLY:HA2	1:A:1754:LYS:HG3	1.86	0.57
2:B:15:GLY:HA2	2:B:86:LEU:N	2.19	0.57
1:A:31:PHE:CD1	1:A:32:PRO:CD	2.85	0.57
1:A:2114:THR:HG21	1:A:2123:LEU:HD22	1.87	0.57
1:A:200:PHE:HE2	1:A:270:ILE:HG21	1.69	0.57
1:A:634:VAL:HG13	1:A:679:PHE:HE1	1.70	0.57
1:A:2261:LEU:HD22	1:A:2280:VAL:HG12	1.87	0.57
1:A:320:GLY:O	1:A:322:GLU:N	2.36	0.57
1:A:664:TYR:HB2	1:A:1833:LYS:HE3	1.87	0.57
1:A:1870:GLN:OE1	1:A:1941:ARG:NH2	2.37	0.57
2:B:88:ASN:HD22	2:B:118:VAL:CG1	2.17	0.57
1:A:1825:PRO:HD2	1:A:1859:ARG:HB2	1.86	0.56
2:B:88:ASN:HB3	2:B:118:VAL:HG21	1.87	0.56
1:A:503:ILE:HG23	1:A:507:GLU:HB2	1.87	0.56
3:C:61:PHE:HE2	3:C:74:ILE:HD11	1.71	0.56
3:C:191:TYR:N	3:C:208:PHE:HB2	2.20	0.56
1:A:166:VAL:O	1:A:170:ASN:ND2	2.36	0.56
1:A:412:LEU:HD22	1:A:421:ARG:HH21	1.70	0.56
1:A:571:ARG:HD3	1:A:635:ALA:HA	1.88	0.56
1:A:2092:LYS:HB3	1:A:2093:PHE:CD1	2.41	0.56
1:A:255:TYR:OH	1:A:364:ASP:O	2.24	0.55
1:A:1838:PHE:HB3	1:A:1852:ILE:HD12	1.87	0.55
2:B:36:TRP:O	2:B:48:MET:HB2	2.06	0.55
2:B:117:THR:OG1	2:B:118:VAL:HB	2.07	0.55
1:A:2261:LEU:HD23	1:A:2282:VAL:HA	1.89	0.55
1:A:402:PRO:HA	1:A:413:ASN:HD21	1.70	0.55
1:A:137:TYR:O	1:A:138:VAL:HG12	2.05	0.55
1:A:642:ILE:HD13	1:A:673:PHE:HA	1.89	0.55
1:A:669:THR:HG21	1:A:1979:TYR:HB3	1.89	0.55
1:A:1787:SER:O	1:A:1788:SER:OG	2.17	0.55
3:C:61:PHE:CZ	3:C:74:ILE:HD13	2.41	0.55
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.42	0.55
2:B:205:ALA:HA	2:B:212:LYS:HA	1.89	0.55
1:A:634:VAL:HG13	1:A:679:PHE:CE1	2.42	0.54
3:C:48:PHE:HE1	3:C:54:ALA:HA	1.71	0.54
1:A:497:HIS:CD2	1:A:499:LYS:HG2	2.42	0.54
1:A:516:THR:OG1	1:A:517:VAL:N	2.40	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2116:ARG:HG2	1:A:2122:THR:O	2.08	0.54
2:B:11:LEU:CG	2:B:116:VAL:HG11	2.37	0.54
3:C:104:LYS:HA	3:C:165:GLN:HE22	1.71	0.54
1:A:2072:LYS:HD3	1:A:2150:ARG:HH21	1.73	0.54
2:B:88:ASN:HB3	2:B:118:VAL:CG2	2.37	0.54
3:C:150:ASP:N	3:C:190:SER:HB2	2.23	0.54
1:A:382:TRP:HB2	1:A:461:LEU:HD12	1.90	0.53
1:A:2067:PRO:HG3	3:C:55:PRO:HD2	1.90	0.53
1:A:2263:SER:HB3	1:A:2273:LEU:HD23	1.89	0.53
3:C:120:SER:OG	3:C:121:SER:N	2.41	0.53
1:A:381:THR:HA	1:A:460:THR:HB	1.90	0.53
1:A:644:ALA:O	1:A:646:THR:N	2.39	0.53
2:B:35:HIS:CE1	2:B:99:CYS:HB3	2.35	0.53
2:B:153:PHE:HB3	2:B:154:PRO:HD2	1.90	0.53
1:A:107:TRP:O	1:A:109:SER:N	2.33	0.53
1:A:1878:LEU:HD11	1:A:1998:ILE:HD13	1.89	0.53
2:B:33:SER:O	2:B:34:MET:CG	2.55	0.53
1:A:313:ILE:HG22	1:A:315:SER:H	1.73	0.53
1:A:134:SER:OG	1:A:135:GLN:N	2.38	0.53
2:B:157:VAL:HG21	2:B:204:VAL:HG13	1.91	0.53
3:C:104:LYS:HA	3:C:165:GLN:NE2	2.23	0.53
1:A:1751:GLU:H	1:A:1754:LYS:HE2	1.74	0.53
2:B:11:LEU:CA	2:B:116:VAL:CG1	2.61	0.53
1:A:2242:GLY:HA2	1:A:2297:LEU:HG	1.91	0.53
1:A:301:LEU:HB3	1:A:327:VAL:HG11	1.91	0.52
2:B:135:CYS:O	2:B:138:THR:N	2.42	0.52
1:A:187:ARG:NH1	1:A:189:ARG:HD3	2.24	0.52
1:A:165:LEU:HD23	1:A:2003:GLY:HA2	1.90	0.52
1:A:165:LEU:HD22	1:A:2006:LEU:HD22	1.91	0.52
1:A:582:ASN:OD1	1:A:612:ASN:ND2	2.41	0.52
1:A:104:VAL:HG12	1:A:141:VAL:HG12	1.91	0.52
1:A:111:GLU:OE2	1:A:1959:SER:OG	2.25	0.52
1:A:399:VAL:HG11	1:A:421:ARG:HD3	1.90	0.52
1:A:1878:LEU:HD23	1:A:1922:ASN:HD21	1.73	0.52
3:C:114:VAL:HG21	3:C:206:LYS:HZ1	1.75	0.52
1:A:2063:SER:HA	1:A:2160:SER:O	2.09	0.52
1:A:2106:SER:HB2	1:A:2112:TRP:CE2	2.45	0.52
2:B:53:THR:HG22	2:B:72:LEU:HD21	1.92	0.52
1:A:293:THR:HG22	1:A:295:LEU:HD13	1.91	0.52
1:A:616:SER:HA	1:A:621:VAL:HG12	1.92	0.52
2:B:107:ILE:HB	3:C:35:TYR:OH	2.10	0.52



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:C:66:SER:HA	3:C:70:TYR:CZ	2.45	0.52
1:A:371:ILE:HG12	1:A:517:VAL:HG21	1.92	0.52
1:A:1946:SER:HB2	1:A:1978:LEU:HB3	1.91	0.52
1:A:2106:SER:HB2	1:A:2112:TRP:CD2	2.44	0.52
2:B:98:ARG:NH2	2:B:108:ASP:OD2	2.34	0.52
1:A:601:VAL:HG12	1:A:602:GLN:H	1.75	0.51
1:A:107:TRP:C	1:A:109:SER:H	2.13	0.51
1:A:243:LEU:HB3	1:A:323:ALA:HB1	1.93	0.51
3:C:88:GLN:OE1	3:C:97:SER:OG	2.27	0.51
2:B:34:MET:SD	2:B:97:ALA:O	2.68	0.51
3:C:61:PHE:CD2	3:C:74:ILE:HG12	2.46	0.51
1:A:270:ILE:O	1:A:287:LEU:N	2.41	0.51
3:C:6:GLN:HE21	3:C:101:LEU:HD12	1.74	0.51
1:A:279:VAL:HG22	1:A:284:GLN:HG3	1.93	0.51
1:A:650:SER:O	1:A:693:HIS:HB2	2.10	0.51
2:B:195:TRP:HA	2:B:197:SER:H	1.76	0.51
1:A:2062:TRP:O	1:A:2161:THR:HA	2.10	0.51
1:A:2114:THR:HG22	1:A:2115:TYR:H	1.75	0.51
2:B:18:VAL:O	2:B:82:GLN:HA	2.10	0.51
3:C:21:MET:SD	3:C:101:LEU:HD13	2.51	0.51
1:A:7:LEU:HD21	1:A:52:PHE:HB3	1.92	0.51
1:A:106:PHE:HB3	1:A:139:TRP:HD1	1.76	0.51
1:A:268:HIS:HB2	1:A:289:ILE:HG12	1.91	0.51
3:C:191:TYR:H	3:C:208:PHE:HB2	1.76	0.51
1:A:192:ASN:OD1	1:A:252:LYS:HD2	2.10	0.50
1:A:474:ASN:HB2	1:A:537:VAL:HG13	1.94	0.50
1:A:1732:LYS:HB3	1:A:1849:SER:O	2.11	0.50
2:B:16:GLU:O	2:B:84:ASN:HA	2.12	0.50
1:A:208:SER:OG	1:A:209:TRP:N	2.45	0.50
1:A:687:LEU:HD22	1:A:1802:PRO:HG3	1.93	0.50
2:B:173:PHE:CG	3:C:175:SER:HB2	2.47	0.50
2:B:152:TYR:OH	2:B:184:LEU:HD22	2.11	0.50
2:B:157:VAL:HG12	2:B:206:HIS:HA	1.93	0.50
1:A:608:PHE:O	1:A:611:SER:OG	2.29	0.50
1:A:637:TRP:HB2	1:A:678:VAL:HG23	1.94	0.50
1:A:116:GLU:HB3	1:A:2013:THR:HG21	1.94	0.50
1:A:642:ILE:HD13	1:A:673:PHE:HD1	1.76	0.50
1:A:2058:SER:OG	1:A:2059:ILE:N	2.43	0.50
1:A:1958:PHE:HB2	1:A:1961:HIS:HB2	1.94	0.49
2:B:88:ASN:ND2	2:B:118:VAL:HG22	2.27	0.49
1:A:11:GLU:HB3	1:A:48:LYS:HE2	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:80:GLU:O	1:A:83:ASP:HB2	2.12	0.49
1:A:517:VAL:O	1:A:519:ASP:N	2.41	0.49
1:A:422:LYS:HD2	1:A:594:PHE:HZ	1.77	0.49
1:A:423:TYR:OH	1:A:612:ASN:HB3	2.11	0.49
3:C:154:ARG:HE	3:C:156:ASN:HB2	1.77	0.49
3:C:9:ALA:O	3:C:101:LEU:HA	2.13	0.49
1:A:188:GLU:HB2	1:A:193:LEU:HD22	1.93	0.49
1:A:311:CYS:SG	1:A:313:ILE:HG12	2.53	0.49
1:A:504:LEU:HB2	1:A:507:GLU:HG2	1.93	0.49
1:A:2106:SER:HB3	1:A:2148:TYR:HB2	1.94	0.49
1:A:1935:ALA:HA	1:A:2017:TYR:CE1	2.48	0.49
1:A:2218:ALA:HB2	1:A:2248:VAL:HG11	1.94	0.49
1:A:2098:ILE:HD11	1:A:2162:LEU:HB2	1.95	0.49
2:B:37:VAL:HG21	2:B:110:TRP:CZ3	2.48	0.49
1:A:2261:LEU:HD21	1:A:2282:VAL:HG22	1.94	0.48
2:B:39:GLN:NE2	2:B:44:GLY:O	2.46	0.48
1:A:637:TRP:CD1	1:A:680:MET:HG2	2.48	0.48
1:A:664:TYR:CZ	1:A:1822:HIS:HB2	2.48	0.48
2:B:10:GLU:O	2:B:116:VAL:CB	2.59	0.48
2:B:177:LEU:HB2	2:B:182:TYR:HE1	1.77	0.48
3:C:63:GLY:HA3	3:C:72:LEU:HA	1.95	0.48
1:A:128:LYS:HG2	1:A:163:VAL:HG12	1.95	0.48
1:A:1870:GLN:O	1:A:1872:THR:N	2.43	0.48
1:A:418:ARG:NH1	1:A:611:SER:HB3	2.28	0.48
1:A:425:LYS:HB3	1:A:545:SER:O	2.13	0.48
3:C:6:GLN:NE2	3:C:85:TYR:O	2.45	0.48
2:B:191:THR:O	2:B:193:SER:N	2.44	0.48
3:C:2:ASN:OD1	3:C:27:SER:OG	2.30	0.48
1:A:2228:GLU:O	1:A:2310:PRO:HD2	2.13	0.48
2:B:218:GLU:HG3	2:B:219:PRO:HD2	1.95	0.48
1:A:652:PHE:HE1	1:A:691:GLY:HA3	1.78	0.48
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.49	0.48
2:B:148:LEU:HD23	2:B:185:SER:HB3	1.95	0.48
1:A:1789:LEU:HD22	1:A:1823:MET:HG2	1.95	0.48
1:A:2021:CYS:HB2	1:A:2176:MET:SD	2.54	0.48
1:A:50:THR:HG21	1:A:95:HIS:CE1	2.49	0.47
1:A:660:HIS:NE2	1:A:676:GLU:OE1	2.43	0.47
1:A:690:LEU:HB2	1:A:704:ALA:O	2.14	0.47
1:A:2186:SER:OG	1:A:2189:GLN:OE1	2.26	0.47
2:B:88:ASN:ND2	2:B:118:VAL:HG13	2.19	0.47
1:A:417:GLN:HA	1:A:595:LEU:HD11	1.97	0.47



A + 1	<b>A t</b> and <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:2055:TYR:H	1:A:2163:ARG:HH11	1.60	0.47
3:C:92:SER:OG	3:C:93:SER:N	2.47	0.47
1:A:2234:PHE:C	1:A:2236:LYS:H	2.17	0.47
1:A:504:LEU:O	1:A:506:GLY:N	2.48	0.47
1:A:2026:GLY:HA3	1:A:2031:HIS:HB3	1.95	0.47
1:A:1786:TYR:OH	1:A:1788:SER:HB3	2.14	0.47
1:A:2059:ILE:HD12	1:A:2059:ILE:O	2.15	0.47
1:A:1789:LEU:HD11	1:A:1835:TRP:CG	2.50	0.47
1:A:2116:ARG:HA	1:A:2123:LEU:HA	1.96	0.47
1:A:99:LEU:HB3	1:A:137:TYR:CE2	2.50	0.47
1:A:666:ASP:OD2	1:A:1788:SER:OG	2.32	0.47
1:A:2141:ASN:HB3	1:A:2142:PRO:CD	2.44	0.47
3:C:184:GLU:O	3:C:188:HIS:HB2	2.15	0.47
1:A:1785:PHE:HB3	1:A:1815:TYR:CE2	2.50	0.47
2:B:23:LYS:HG3	2:B:24:ALA:N	2.30	0.47
1:A:1764:ARG:HD3	1:A:1863:LEU:HD11	1.97	0.47
1:A:310:PHE:HB2	1:A:322:GLU:HG2	1.96	0.47
1:A:1777:ASN:ND2	1:A:1809:PRO:HA	2.30	0.46
2:B:92:ALA:O	2:B:115:SER:HB3	2.16	0.46
3:C:38:LYS:HA	3:C:83:ALA:HB1	1.98	0.46
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.96	0.46
1:A:2236:LYS:O	1:A:2304:ARG:HG3	2.13	0.46
1:A:272:LEU:HD23	1:A:275:HIS:HB2	1.97	0.46
1:A:396:ALA:O	1:A:399:VAL:HG13	2.14	0.46
1:A:1790:ILE:HD12	1:A:1790:ILE:O	2.15	0.46
1:A:80:GLU:HA	1:A:180:CYS:O	2.16	0.46
1:A:178:LEU:HD11	1:A:257:HIS:CD2	2.50	0.46
1:A:391:GLU:HG2	1:A:392:ASP:N	2.27	0.46
1:A:1831:ASP:OD1	1:A:1859:ARG:NH2	2.48	0.46
2:B:115:SER:O	2:B:116:VAL:HG23	2.16	0.46
1:A:1997:ARG:NE	1:A:2011:SER:OG	2.49	0.46
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.98	0.46
2:B:155:GLU:HG2	2:B:156:PRO:HA	1.97	0.46
1:A:417:GLN:NE2	1:A:418:ARG:HH21	2.14	0.46
1:A:433:ASP:N	1:A:433:ASP:OD1	2.49	0.46
1:A:655:GLY:H	1:A:1786:TYR:HE1	1.64	0.46
3:C:39:SER:O	3:C:39:SER:OG	2.32	0.46
1:A:278:LEU:HB2	1:A:298:GLN:HG2	1.97	0.45
1:A:1704:GLU:OE1	1:A:1779:ALA:HA	2.15	0.45
1:A:1750:GLY:HA3	1:A:2116:ARG:HD2	1.97	0.45
1:A:2174:CYS:HB3	1:A:2241:THR:HG21	1.98	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:19:SER:OG	1:A:20:GLU:N	2.49	0.45
1:A:121:GLN:HA	1:A:124:LYS:HB2	1.98	0.45
2:B:20:ILE:HG22	2:B:21:SER:H	1.80	0.45
1:A:271:PHE:HE2	1:A:478:HIS:HE2	1.64	0.45
1:A:412:LEU:HD23	1:A:421:ARG:HA	1.99	0.45
1:A:50:THR:HG21	1:A:95:HIS:NE2	2.32	0.45
1:A:115:TYR:O	1:A:117:ASP:N	2.48	0.45
2:B:122:LYS:HD3	2:B:124:THR:OG1	2.16	0.45
1:A:543:LEU:HD21	1:A:643:GLY:HA2	1.99	0.45
1:A:2101:PHE:HE2	1:A:2103:ILE:HD11	1.82	0.45
2:B:158:THR:O	2:B:158:THR:OG1	2.35	0.45
3:C:32:MET:HE3	3:C:87:CYS:HB2	1.99	0.45
1:A:16:TYR:O	1:A:239:VAL:HG22	2.17	0.45
1:A:649:LEU:HG	1:A:692:CYS:SG	2.56	0.45
1:A:1935:ALA:HB3	1:A:1938:GLN:HB2	1.99	0.45
1:A:2241:THR:O	1:A:2297:LEU:N	2.49	0.45
2:B:126:PRO:HG3	2:B:204:VAL:HG12	1.99	0.45
1:A:1843:LEU:HD12	1:A:1843:LEU:H	1.81	0.45
1:A:2258:LYS:H	1:A:2313:TRP:HA	1.82	0.45
1:A:280:ARG:HD2	1:A:1971:TYR:HE2	1.82	0.44
1:A:2077:ALA:O	1:A:2147:ARG:HB3	2.17	0.44
1:A:28:ASP:OD2	1:A:30:ARG:HB2	2.17	0.44
1:A:578:VAL:HG23	1:A:645:GLN:HG2	1.99	0.44
1:A:1998:ILE:HG13	1:A:2014:PHE:CD1	2.52	0.44
1:A:2110:LYS:HB2	1:A:2110:LYS:HE3	1.71	0.44
1:A:2119:SER:O	1:A:2121:GLY:N	2.51	0.44
2:B:159:LEU:HD13	2:B:184:LEU:HD11	1.98	0.44
2:B:173:PHE:CD2	3:C:175:SER:HB2	2.52	0.44
2:B:178:GLN:HA	2:B:179:SER:HA	1.66	0.44
1:A:456:GLU:HB2	1:A:459:ASP:OD1	2.17	0.44
3:C:14:SER:O	3:C:16:GLY:N	2.51	0.44
2:B:11:LEU:HD11	2:B:119:SER:CB	2.46	0.44
1:A:318:HIS:CD2	1:A:318:HIS:N	2.85	0.44
1:A:1778:GLN:HB3	1:A:1779:ALA:H	1.48	0.44
1:A:54:GLU:HB2	1:A:75:PRO:HG2	1.99	0.44
1:A:85:VAL:O	1:A:138:VAL:HA	2.18	0.44
1:A:2087:GLN:HG2	1:A:2088:GLY:H	1.83	0.44
1:A:280:ARG:HD2	1:A:1971:TYR:CE2	2.53	0.44
2:B:64:PHE:HB3	2:B:68:PHE:CE1	2.53	0.44
3:C:110:ALA:HB3	3:C:139:TYR:N	2.33	0.44
1:A:2115:TYR:OH	1:A:2140:PHE:HB2	2.18	0.44



A + a 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:11:LEU:HD13	2:B:116:VAL:HG11	1.80	0.44
3:C:9:ALA:O	3:C:101:LEU:HD23	2.18	0.44
1:A:529:LEU:HD23	1:A:529:LEU:H	1.82	0.44
1:A:1773:VAL:HG11	1:A:1785:PHE:CZ	2.53	0.44
3:C:141:LYS:HB3	3:C:172:TYR:CG	2.52	0.44
1:A:2120:THR:HG1	1:A:2121:GLY:H	1.66	0.43
2:B:33:SER:O	2:B:34:MET:SD	2.76	0.43
1:A:121:GLN:HA	1:A:124:LYS:HD2	2.00	0.43
1:A:435:THR:O	1:A:437:LYS:HG2	2.18	0.43
1:A:447:GLY:O	1:A:448:ILE:HG22	2.17	0.43
1:A:605:ASP:HA	1:A:606:PRO:HD3	1.81	0.43
1:A:605:ASP:HB3	1:A:608:PHE:CD2	2.53	0.43
1:A:610:ALA:HA	1:A:613:ILE:HG12	2.00	0.43
1:A:2027:MET:N	1:A:2032:ILE:HD12	2.32	0.43
2:B:33:SER:C	2:B:34:MET:HG2	2.38	0.43
1:A:5:TYR:CZ	1:A:77:ILE:HG23	2.53	0.43
3:C:16:GLY:HA2	3:C:76:SER:HA	1.99	0.43
1:A:290:SER:O	1:A:293:THR:OG1	2.37	0.43
1:A:1856:LEU:HD11	1:A:1943:TYR:CE2	2.53	0.43
1:A:2141:ASN:HD22	1:A:2141:ASN:C	2.21	0.43
1:A:528:CYS:HA	1:A:553:ILE:O	2.18	0.43
1:A:2141:ASN:C	1:A:2141:ASN:ND2	2.72	0.43
1:A:2260:PHE:HE2	1:A:2262:ILE:HD11	1.83	0.43
1:A:174:ILE:HD12	1:A:261:MET:SD	2.58	0.43
1:A:2019:LYS:NZ	4:H:2:NAG:O7	2.52	0.43
1:A:2210:LEU:HB3	1:A:2322:GLU:HB2	2.00	0.43
2:B:3:GLN:H	2:B:25:SER:HB3	1.82	0.43
2:B:37:VAL:O	2:B:94:TYR:HA	2.19	0.43
2:B:67:ARG:HB3	2:B:84:ASN:O	2.18	0.43
1:A:1704:GLU:HG2	1:A:1733:VAL:HB	2.01	0.43
1:A:1763:ILE:HG23	1:A:1855:LEU:HA	2.01	0.43
3:C:38:LYS:HD2	3:C:83:ALA:HB2	2.01	0.43
3:C:114:VAL:O	3:C:115:SER:OG	2.33	0.43
1:A:300:PHE:CD2	1:A:302:MET:HG3	2.50	0.43
1:A:418:ARG:HH11	1:A:611:SER:HB3	1.84	0.43
1:A:617:ILE:HG22	1:A:625:LEU:HD23	2.00	0.43
1:A:2307:ARG:HD3	1:A:2309:HIS:HE1	1.84	0.43
1:A:2209:ARG:O	1:A:2320:ARG:HB3	2.19	0.43
1:A:379:PRO:HB2	1:A:459:ASP:HA	2.00	0.42
1:A:1996:TRP:HB2	1:A:2014:PHE:CE1	2.54	0.42
1:A:2055:TYR:O	1:A:2060:ASN:HB2	2.18	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:2310:PRO:HG3	1:A:2317:ILE:HD13	2.00	0.42
1:A:2087:GLN:HA	1:A:2129:ASN:ND2	2.33	0.42
1:A:115:TYR:CE2	1:A:1997:ARG:HB2	2.54	0.42
1:A:136:THR:HG22	1:A:137:TYR:H	1.85	0.42
1:A:620:TYR:HB3	1:A:624:SER:OG	2.19	0.42
1:A:2059:ILE:H	1:A:2059:ILE:HG13	1.67	0.42
1:A:2072:LYS:HD3	1:A:2150:ARG:NH2	2.34	0.42
1:A:2201:ALA:HB1	1:A:2216:SER:HB3	2.01	0.42
1:A:1781:ARG:HD3	1:A:1889:TRP:HB3	2.00	0.42
1:A:1808:GLN:HG3	1:A:1809:PRO:CD	2.46	0.42
1:A:2209:ARG:HB2	1:A:2212:LEU:HB2	2.01	0.42
1:A:170:ASN:HB3	1:A:204:ASP:O	2.20	0.42
1:A:406:SER:OG	1:A:408:LYS:HG2	2.19	0.42
2:B:147:CYS:HB2	2:B:161:TRP:CH2	2.55	0.42
1:A:115:TYR:HB3	1:A:1997:ARG:NH2	2.35	0.42
1:A:147:PRO:HB2	1:A:181:ARG:HH21	1.83	0.42
1:A:395:TYR:CD2	1:A:614:MET:HG3	2.54	0.42
1:A:598:PRO:O	1:A:600:GLY:N	2.40	0.42
1:A:2115:TYR:OH	1:A:2142:PRO:O	2.28	0.42
2:B:11:LEU:CD1	2:B:119:SER:CB	2.97	0.42
2:B:38:LYS:HD3	2:B:64:PHE:CZ	2.54	0.42
1:A:631:LEU:C	1:A:633:GLU:H	2.22	0.42
1:A:2126:PHE:HD2	1:A:2138:ASN:HB3	1.84	0.42
2:B:89:GLU:C	2:B:91:THR:H	2.22	0.42
1:A:134:SER:O	1:A:135:GLN:HB3	2.20	0.42
1:A:288:GLU:HB3	1:A:671:PHE:CE2	2.55	0.42
1:A:605:ASP:HB3	1:A:608:PHE:CE2	2.54	0.42
1:A:1928:THR:O	1:A:1930:PRO:HD3	2.20	0.42
2:B:18:VAL:HG12	2:B:86:LEU:HD11	2.01	0.42
2:B:37:VAL:HB	2:B:95:PHE:HB2	2.01	0.42
2:B:165:SER:OG	2:B:166:LEU:N	2.53	0.42
1:A:199:LEU:HD12	1:A:259:ILE:O	2.20	0.42
1:A:252:LYS:HE3	1:A:252:LYS:HB2	1.72	0.42
1:A:1693:LYS:HB2	1:A:1694:ARG:HG3	2.02	0.42
1:A:1945:LEU:HB2	1:A:1983:PHE:CE1	2.54	0.42
2:B:70:PHE:CE1	2:B:81:LEU:HD13	2.54	0.42
3:C:6:GLN:HG2	3:C:101:LEU:HD12	2.01	0.42
1:A:56:THR:HG22	1:A:64:ARG:HE	1.85	0.42
1:A:630:CYS:HB2	1:A:633:GLU:CD	2.41	0.41
1:A:1897:ARG:HB3	1:A:1898:ASN:H	1.62	0.41
1:A:1949:SER:OG	1:A:1950:ASN:N	2.53	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:2081:ILE:HG22	1:A:2140:PHE:HZ	1.84	0.41
1:A:2273:LEU:HB2	1:A:2275:PHE:CE1	2.54	0.41
1:A:66:ARG:NH2	1:A:73:LEU:O	2.46	0.41
1:A:2025:LEU:HD13	1:A:2075:LEU:HD11	2.02	0.41
2:B:13:LYS:HA	2:B:13:LYS:HD3	1.79	0.41
3:C:60:ARG:HH12	3:C:78:GLU:HB2	1.85	0.41
1:A:1769:ASP:O	1:A:1819:VAL:HG12	2.20	0.41
1:A:1828:ASP:O	1:A:1966:ARG:HD3	2.21	0.41
1:A:1972:LYS:HE2	1:A:1972:LYS:HB2	1.80	0.41
2:B:156:PRO:HB2	2:B:157:VAL:H	1.55	0.41
2:B:201:THR:HA	2:B:216:LYS:HA	2.02	0.41
3:C:141:LYS:HB3	3:C:172:TYR:CD2	2.54	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.70	0.41
1:A:428:PHE:O	1:A:450:GLY:HA2	2.20	0.41
1:A:1846:ASP:HA	1:A:1849:SER:HB2	2.02	0.41
1:A:1881:THR:HA	1:A:1954:HIS:HE2	1.85	0.41
1:A:2141:ASN:HB2	4:H:1:NAG:H3	2.01	0.41
3:C:154:ARG:NE	3:C:156:ASN:O	2.53	0.41
1:A:3:ARG:NH1	1:A:79:ALA:HA	2.36	0.41
1:A:96:PRO:HB3	1:A:130:LEU:HG	2.01	0.41
1:A:629:VAL:HG22	1:A:706:LEU:HD11	2.03	0.41
1:A:105:SER:O	1:A:140:GLN:N	2.47	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.86	0.41
1:A:428:PHE:HE2	1:A:534:SER:HA	1.85	0.41
1:A:1952:ASN:HB3	1:A:1954:HIS:HE2	1.85	0.41
1:A:2183:LYS:HA	1:A:2209:ARG:NH1	2.36	0.41
1:A:11:GLU:HG2	1:A:50:THR:HB	2.03	0.41
1:A:684:ASN:O	1:A:708:VAL:HG21	2.20	0.41
1:A:1870:GLN:C	1:A:1872:THR:H	2.23	0.41
1:A:2154:THR:HA	3:C:49:PHE:HD2	1.84	0.41
3:C:208:PHE:O	3:C:209:ASN:HB2	2.20	0.41
1:A:98:SER:OG	1:A:162:HIS:N	2.45	0.41
1:A:472:PRO:HB2	1:A:502:PRO:HB2	2.02	0.41
1:A:603:LEU:C	1:A:605:ASP:H	2.24	0.41
1:A:2196:PHE:CD1	1:A:2222:GLN:HA	2.56	0.41
2:B:40:ALA:C	2:B:42:GLY:H	2.24	0.41
3:C:197:HIS:ND1	3:C:199:THR:HG23	2.36	0.41
1:A:89:LEU:HD23	1:A:129:VAL:HG21	2.02	0.41
1:A:382:TRP:HE3	1:A:383:VAL:H	1.69	0.41
1:A:658:PHE:CE2	1:A:668:LEU:HB2	2.56	0.41
1:A:1933:VAL:HA	1:A:2015:LEU:O	2.21	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:2225:ASN:OD1	1:A:2227:LYS:HB2	2.21	0.41
2:B:128:VAL:HA	2:B:149:VAL:HG23	2.03	0.41
2:B:176:VAL:HG23	3:C:161:SER:HB2	2.01	0.41
3:C:121:SER:OG	3:C:122:GLU:N	2.53	0.41
3:C:200:LYS:HZ3	3:C:204:ILE:HD12	0.95	0.41
1:A:31:PHE:N	1:A:32:PRO:HD3	2.15	0.41
1:A:196:PHE:HB2	1:A:256:TRP:HZ3	1.85	0.41
1:A:207:LYS:HE2	1:A:207:LYS:HB3	1.91	0.41
1:A:447:GLY:C	1:A:449:LEU:H	2.23	0.41
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.20	0.41
1:A:2156:TYR:HD2	1:A:2160:SER:OG	1.98	0.41
1:A:428:PHE:CZ	1:A:547:LEU:HD22	2.57	0.40
1:A:1921:ILE:HD12	1:A:2012:THR:HG22	2.03	0.40
1:A:70:MET:O	1:A:236:ASN:HB3	2.21	0.40
1:A:186:THR:O	1:A:188:GLU:N	2.54	0.40
1:A:194:HIS:HB3	1:A:196:PHE:CE1	2.55	0.40
1:A:655:GLY:HA2	1:A:1788:SER:HA	2.02	0.40
1:A:703:THR:HB	1:A:704:ALA:H	1.65	0.40
1:A:1925:VAL:O	1:A:1928:THR:OG1	2.17	0.40
1:A:2087:GLN:HA	1:A:2129:ASN:HD21	1.87	0.40
1:A:2106:SER:OG	1:A:2107:LEU:N	2.54	0.40
3:C:6:GLN:HE22	3:C:86:TYR:HA	1.86	0.40
1:A:2111:LYS:HB2	1:A:2111:LYS:HE3	1.86	0.40
1:A:2180:MET:HG2	1:A:2185:ILE:HD12	2.03	0.40
2:B:4:LEU:HB2	2:B:110:TRP:O	2.22	0.40
1:A:200:PHE:CE2	1:A:270:ILE:HG13	2.56	0.40
2:B:88:ASN:HA	2:B:118:VAL:HG23	1.96	0.40
3:C:6:GLN:NE2	3:C:101:LEU:HB2	2.37	0.40
1:A:104:VAL:HB	1:A:105:SER:H	1.67	0.40
1:A:301:LEU:HD13	1:A:327:VAL:HG12	2.03	0.40
1:A:310:PHE:CB	1:A:322:GLU:HG2	2.50	0.40
1:A:453:LEU:HD23	1:A:513:TRP:CZ3	2.53	0.40
1:A:1993:VAL:HA	1:A:2016:VAL:CG2	2.52	0.40
1:A:2092:LYS:HB3	1:A:2093:PHE:HD1	1.84	0.40
1:A:2229:TRP:HB3	1:A:2309:HIS:ND1	2.37	0.40
1:A:2245:THR:HB	1:A:2319:LEU:HD11	2.03	0.40
2:B:67:ARG:HG2	2:B:85:ASN:HB3	2.04	0.40
2:B:131:LEU:CD2	2:B:148:LEU:H	2.33	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	Ρ	$\mathbf{erc}$	entiles
1	А	1249/1467~(85%)	962 (77%)	222 (18%)	65~(5%)		2	22
2	В	213/223~(96%)	139~(65%)	58 (27%)	16 (8%)		1	16
3	С	211/213~(99%)	149 (71%)	48 (23%)	14 (7%)		1	18
All	All	1673/1903~(88%)	1250 (75%)	328 (20%)	95~(6%)		1	21

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	44	SER
1	А	187	ARG
1	А	250	HIS
1	А	265	PRO
1	А	291	PRO
1	А	420	GLY
1	А	448	ILE
1	А	492	PRO
1	А	598	PRO
1	А	601	VAL
1	А	708	VAL
1	А	1797	GLU
1	А	1871	VAL
2	В	104	ASP
2	В	118	VAL
2	В	154	PRO
2	В	156	PRO
1	А	33	ALA
1	А	45	VAL
1	A	116	GLU
1	A	138	VAL
1	А	321	MET
1	A	331	ALA
1	A	372	ARG



1         A         446         SER           1         A         519         ASP           1         A         1751         GLU           1         A         1806         PHE           1         A         2058         SER           1         A         2067         PRO           1         A         2067         PRO           1         A         2067         PRO           1         A         2120         THR           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         111         GLU           1         A         111         GLU           1         A         111         GLU           1         A         129         SER           1         A         695         SER           1         A         697         PHE           1         A         2028         ALA           1         A         <	Mol	Chain	Res	Type
1         A         519         ASP           1         A         1751         GLU           1         A         1806         PHE           1         A         2058         SER           1         A         2067         PRO           1         A         2120         THR           2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         112         LEU           1         A         113         GLY           1         A         695         SER           1         A         697         PHE           1         A         2028         ALA           1         A         2028         GLN           1         A         2028         GLN           1         A <td< td=""><td>1</td><td>A</td><td>446</td><td>SER</td></td<>	1	A	446	SER
1         A         1751         GLU           1         A         1806         PHE           1         A         2058         SER           1         A         2067         PRO           1         A         2120         THR           2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         112         LEU           1         A         142         LEU           1         A         142         LEU           1         A         165         SER           1         A         697         PHE           1         A         1798         GLN           1         A         2028         ALA           1         A         2028         GLN           1         A <td< td=""><td>1</td><td>A</td><td>519</td><td>ASP</td></td<>	1	A	519	ASP
1         A         1806         PHE           1         A         2058         SER           1         A         2058         SER           1         A         2067         PRO           1         A         2120         THR           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         112         ARG           3         C         191         TYR           1         A         31         PHE           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         201         SER           1         A         201         SER           1         A         20	1	A	1751	GLU
1         A         2058         SER           1         A         2058         SER           1         A         2067         PRO           1         A         2120         THR           2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         111         GLU           1         A         121         SER           1         A         142         LEU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLN           1         A	1	A	1806	PHE
1         A         2067         PRO           1         A         2120         THR           2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         111         GLU           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         697         PHE           1         A         2028         ALA           1         A         2028         ALA           1         A         208         GLN           1         A         207	1	A	2058	SER
1         A         2120         THR           2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         697         PHE           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLN           1         A         2028         GLY           2         B         117         THR           2         B         20	1	A	2067	PRO
2         B         86         LEU           2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         150         ASP           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLN           1         A         2028         GLY           2         B         117         THR           2         B         207         PRO           3         C         62	1	A	2120	THR
2         B         193         SER           3         C         107         ARG           3         C         129         ALA           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         111         GLU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         1798         GLN           1         A         2028         ALA           1         A         2028         ALA           1         A         208         GLY           2         B         14         PRO           2         B         117         THR           2         B         207<	2	В	86	LEU
3         C         107         ARG           3         C         129         ALA           3         C         150         ASP           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         695         SER           1         A         697         PHE           1         A         704         ALA           1         A         2028         ALA           1         A         2028         ALA           1         A         208         GLN           1         A         208         GLY           2         B         14         PRO           2         B         17         THR           2         B         207         PRO           3         C         62 <td>2</td> <td>В</td> <td>193</td> <td>SER</td>	2	В	193	SER
3       C $129$ ALA $3$ C $150$ ASP $3$ C $191$ TYR $1$ A $31$ PHE $1$ A $111$ GLU $1$ A $142$ LEU $1$ A $142$ LEU $1$ A $211$ SER $1$ A $695$ SER $1$ A $697$ PHE $1$ A $697$ PHE $1$ A $2119$ SER $1$ A $2028$ ALA $1$ A $2028$ ALA $1$ A $2028$ GLN $1$ A $2028$ GLY $2$ B $117$ THR $2$ B $117$ THR $2$ B $207$ PRO $3$ C $62$ SER $3$ C $99$ THR $1$ <t< td=""><td>3</td><td>С</td><td>107</td><td>ARG</td></t<>	3	С	107	ARG
3         C         150         ASP           3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         183         GLY           1         A         695         SER           1         A         697         PHE           1         A         704         ALA           1         A         2028         ALA           1         A         2028         ALA           1         A         208         GLN           1         A         2268         GLY           2         B         14         PRO           2         B         17         THR           2         B         207         PRO           3         C         62         SER           3         C         99         THR           1         A         599 <td>3</td> <td>С</td> <td>129</td> <td>ALA</td>	3	С	129	ALA
3         C         191         TYR           1         A         31         PHE           1         A         111         GLU           1         A         142         LEU           1         A         211         SER           1         A         695         SER           1         A         697         PHE           1         A         704         ALA           1         A         2028         ALA           1         A         2028         ALA           1         A         2068         GLY           2         B         14         PRO           2         B         117         THR           2         B         207         PRO           3         C         62         SER           3         C         99         THR           1         A         599 <td>3</td> <td>C</td> <td>150</td> <td>ASP</td>	3	C	150	ASP
1         A         31         PHE           1         A         111         GLU           1         A         142         LEU           1         A         142         LEU           1         A         142         LEU           1         A         211         SER           1         A         695         SER           1         A         697         PHE           1         A         697         PHE           1         A         704         ALA           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLY           2         B         14         PRO           2         B         14         PRO           2         B         17         THR           2         B         207         PRO           3         C         62         SER           3         C         99         THR           1         A         599         ALA           1         A         1936 <td>3</td> <td>C</td> <td>191</td> <td>TYR</td>	3	C	191	TYR
1         A         111         GLU           1         A         142         LEU           1         A         183         GLY           1         A         211         SER           1         A         695         SER           1         A         697         PHE           1         A         697         PHE           1         A         704         ALA           1         A         1798         GLN           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLY           2         B         14         PRO           2         B         14         PRO           2         B         17         THR           2         B         207         PRO           3         C         15         LEU           3         C         99         THR           1         A         599         ALA           1         A         1796         GLN           1         A         1936<	1	A	31	PHE
1         A         142         LEU           1         A         183         GLY           1         A         211         SER           1         A         695         SER           1         A         697         PHE           1         A         697         PHE           1         A         697         PHE           1         A         704         ALA           1         A         2028         ALA           1         A         2028         ALA           1         A         2028         GLY           2         B         14         PRO           2         B         14         PRO           2         B         14         PRO           2         B         17         THR           2         B         207         PRO           3         C         62         SER           3         C         99         THR           1         A         599         ALA           1         A         1796         GLN           1         A         1936 <td>1</td> <td>А</td> <td>111</td> <td>GLU</td>	1	А	111	GLU
1       A       183       GLY         1       A       211       SER         1       A       695       SER         1       A       697       PHE         1       A       697       PHE         1       A       704       ALA         1       A       2028       ALA         1       A       2028       ALA         1       A       2028       GLY         2       B       14       PRO         2       B       14       PRO         2       B       14       PRO         2       B       14       PRO         2       B       17       THR         2       B       207       PRO         3       C       15       LEU         3       C       99       THR         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1	1	A	142	LEU
1       A       211       SER         1       A       695       SER         1       A       697       PHE         1       A       704       ALA         1       A       1798       GLN         1       A       2028       ALA         1       A       2028       ALA         1       A       2028       GLY         2       B       14       PRO         2       B       14       PRO         2       B       14       PRO         2       B       17       THR         2       B       207       PRO         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2097       TYR         1	1	A	183	GLY
1       A       695       SER         1       A       697       PHE         1       A       704       ALA         1       A       1798       GLN         1       A       2028       ALA         1       A       2028       ALA         1       A       2028       GLY         1       A       2119       SER         1       A       2268       GLY         2       B       14       PRO         2       B       117       THR         2       B       207       PRO         3       C       15       LEU         3       C       99       THR         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2179       GLY         1<	1	A	211	SER
1A $697$ PHE1A $704$ ALA1A $1798$ GLN1A $2028$ ALA1A $2119$ SER1A $2268$ GLY2B $14$ PRO2B $117$ THR2B $207$ PRO3C $62$ SER3C $62$ SER3C $99$ THR1A $599$ ALA1A $614$ MET1A $1796$ GLN1A $1936$ GLN1A $2175$ SER1A $2175$ SER1A $2179$ GLY1A $2186$ PHE1A $2328$ ALA2B $166$ LEU	1	А	695	SER
1       A       704       ALA         1       A       1798       GLN         1       A       2028       ALA         1       A       2119       SER         1       A       2268       GLY         2       B       14       PRO         2       B       14       PRO         2       B       17       THR         2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2179       PHE         1	1	A	697	PHE
1       A       1798       GLN         1       A       2028       ALA         1       A       2119       SER         1       A       2268       GLY         2       B       14       PRO         2       B       14       PRO         2       B       117       THR         2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2196       PHE         1 <td>1</td> <td>А</td> <td>704</td> <td>ALA</td>	1	А	704	ALA
1       A       2028       ALA         1       A       2119       SER         1       A       2268       GLY         2       B       14       PRO         2       B       14       PRO         2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       599       ALA         1       A       1796       GLN         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       2328       ALA         2       B       166       LEU	1	А	1798	GLN
1       A       2119       SER         1       A       2268       GLY         2       B       14       PRO         2       B       117       THR         2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2186       PHE         1       A       2328       ALA         2       B       166       LEU <td>1</td> <td>А</td> <td>2028</td> <td>ALA</td>	1	А	2028	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	2119	SER
2       B       14       PRO         2       B       117       THR         2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2186       PHE         1       A       2328       ALA         2       B       166       LEU	1	А	2268	GLY
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	В	14	PRO
2       B       207       PRO         3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1936       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA	2	В	117	THR
3       C       15       LEU         3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1936       GLN         1       A       1936       GLN         1       A       2097       TYR         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA	2	В	207	PRO
3       C       62       SER         3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA	3	С	15	LEU
3       C       99       THR         1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA	3	С	62	SER
1       A       599       ALA         1       A       614       MET         1       A       1796       GLN         1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA	3	С	99	THR
1       A       614       MET         1       A       1796       GLN         1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       218       ALA         2       B       166       LEU	1	А	599	ALA
1       A       1796       GLN         1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       218       PHE         1       A       2196       PHE         1       A       2328       ALA         2       B       166       LEU	1	А	614	MET
1       A       1830       PHE         1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2179       GLY         1       A       2138       ALA         2       B       166       LEU	1	А	1796	GLN
1       A       1936       GLN         1       A       2097       TYR         1       A       2175       SER         1       A       2179       GLY         1       A       2179       GLY         1       A       218       PHE         1       A       2328       ALA         2       B       166       LEU	1	А	1830	PHE
1         A         2097         TYR           1         A         2175         SER           1         A         2179         GLY           1         A         2196         PHE           1         A         2328         ALA           2         B         166         LEU	1	А	1936	GLN
1         A         2175         SER           1         A         2179         GLY           1         A         2196         PHE           1         A         2328         ALA           2         B         166         LEU	1	А	2097	TYR
1         A         2179         GLY           1         A         2196         PHE           1         A         2328         ALA           2         B         166         LEU	1	А	2175	SER
1         A         2196         PHE           1         A         2328         ALA           2         B         166         LEU	1	А	2179	GLY
1         A         2328         ALA           2         B         166         LEU	1	А	2196	PHE
2 B 166 LEU	1	А	2328	ALA
	2	В	166	LEU



Mol	Chain	Res	Type
3	С	92	SER
3	С	121	SER
1	А	104	VAL
1	А	108	LYS
1	А	134	SER
1	А	401	ALA
1	А	441	ALA
1	А	1897	ARG
1	А	2315	HIS
2	В	192	SER
3	С	209	ASN
1	А	194	HIS
1	А	702	MET
1	А	1850	GLY
3	С	75	SER
3	С	118	PRO
1	А	2041	GLY
1	А	2078	PRO
1	А	2109	GLY
2	В	20	ILE
2	В	116	VAL
2	В	126	PRO
1	А	1854	PRO
1	А	369	ILE
2	В	41	PRO
2	В	42	GLY
3	С	151	GLY
1	А	402	PRO
3	С	93	SER

#### 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	1118/1301 (86%)	1048 (94%)	70 (6%)	18 47
2	В	186/189~(98%)	179 (96%)	7 (4%)	33 59



Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\mathbf{ntiles}$
3	С	186/186~(100%)	178 (96%)	8 (4%)	29	56
All	All	1490/1676~(89%)	1405 (94%)	85 (6%)	20	50

All (85) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	20	GLU
1	А	23	ARG
1	А	24	GLU
1	А	27	VAL
1	А	28	ASP
1	А	29	THR
1	А	30	ARG
1	А	34	THR
1	А	59	LEU
1	А	66	ARG
1	А	115	TYR
1	A	120	SER
1	А	121	GLN
1	А	154	CYS
1	А	162	HIS
1	А	182	GLU
1	А	187	ARG
1	А	189	ARG
1	А	273	GLU
1	А	298	GLN
1	А	304	LEU
1	А	368	PHE
1	А	377	LYS
1	А	407	TYR
1	А	417	GLN
1	А	421	ARG
1	А	459	ASP
1	А	496	LYS
1	А	497	HIS
1	А	499	LYS
1	А	536	PHE
1	А	555	TYR
1	А	592	GLN
1	А	594	PHE
1	А	597	ASN
1	А	605	ASP



1       A $652$ PHE         1       A $679$ PHE         1       A $1708$ ASP         1       A $1736$ ARG         1       A $1736$ ARG         1       A $1808$ GLN         1       A $1810$ ASN         1       A $1832$ CYS         1       A $1840$ ASP         1       A $1840$ ASP         1       A $1846$ ASP         1       A $1846$ ASP         1       A $1863$ LEU         1       A $1863$ LEU         1       A $1897$ ARG         1       A $1976$ TYR         1       A $1978$ LEU         1       A $2000$ CYS         1       A $2027$ MET         1       A $2049$ LYS         1       A $2049$ LYS         1       A $2140$ </th
1A $679$ PHE1A $1708$ ASP1A $1736$ ARG1A $1808$ GLN1A $1810$ ASN1A $1832$ CYS1A $1832$ CYS1A $1840$ ASP1A $1846$ ASP1A $1846$ ASP1A $1863$ LEU1A $1885$ GLU1A $1887$ ARG1A $1976$ TYR1A $1976$ TYR1A $1978$ LEU1A $2000$ CYS1A $2000$ CYS1A $2049$ LYS1A $2053$ LEU1A $2053$ LEU1A $2140$ PHE1A $2140$ PHE1A $2156$ TYR1A $2175$ SER1A $2196$ PHE1A $2198$ ASN1A $2198$ ASN1A $2250$ SER
1A1708ASP1A1736ARG1A1808GLN1A1810ASN1A1832CYS1A1840ASP1A1840ASP1A1846ASP1A1863LEU1A1885GLU1A1885GLU1A1887ARG1A1976TYR1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2049LYS1A2140PHE1A2140PHE1A2175SER1A2187ASP1A2196PHE1A2200PHE1A2200PHE1A2200PHE
1A $1736$ ARG1A1808GLN1A1810ASN1A1832CYS1A1840ASP1A1846ASP1A1863LEU1A1885GLU1A1885GLU1A1887ARG1A1897ARG1A1976TYR1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2053LEU1A2140PHE1A2141ASN1A2175SER1A2187ASP1A2198ASN1A2200PHE1A2200PHE
1A1808GLN1A1810ASN1A1832CYS1A1840ASP1A1846ASP1A1863LEU1A1885GLU1A1885GLU1A1887ARG1A1976TYR1A1978LEU1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2049LYS1A2141ASN1A2141ASN1A2175SER1A2187ASP1A2198ASN1A2200PHE1A2200PHE
1A1810ASN1A1832CYS1A1840ASP1A1846ASP1A1863LEU1A1863GLU1A1885GLU1A1885GLU1A1887ARG1A1976TYR1A1978LEU1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2053LEU1A2140PHE1A2141ASN1A2175SER1A2187ASP1A2198ASN1A2200PHE1A2200PHE1A2200PHE
1A $1832$ CYS1A $1840$ ASP1A $1846$ ASP1A $1863$ LEU1A $1863$ GLU1A $1885$ GLU1A $1888$ SER1A $1897$ ARG1A $1976$ TYR1A $1976$ TYR1A $1978$ LEU1A $1978$ LEU1A $2000$ CYS1A $2027$ MET1A $2049$ LYS1A $2053$ LEU1A $2140$ PHE1A $2141$ ASN1A $2156$ TYR1A $2187$ ASP1A $2196$ PHE1A $2198$ ASN1A $2200$ PHE1A $2200$ PHE
1A1840ASP1A1846ASP1A1863LEU1A1863GLU1A1885GLU1A1885GLU1A1897ARG1A1976TYR1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2053LEU1A2140PHE1A2156TYR1A2175SER1A2187ASP1A2198ASN1A2200PHE1A2200PHE1A2200PHE
1A1846ASP1A1863LEU1A1885GLU1A1885GLU1A1888SER1A1897ARG1A1976TYR1A1978LEU1A1978LEU1A1978LEU1A2000CYS1A2027MET1A2049LYS1A2053LEU1A2140PHE1A2141ASN1A2156TYR1A2187ASP1A2198ASN1A2198ASN1A2200PHE1A2200PHE1A2200SER
1       A       1863       LEU         1       A       1885       GLU         1       A       1885       GLU         1       A       1888       SER         1       A       1897       ARG         1       A       1976       TYR         1       A       1978       LEU         1       A       1978       LEU         1       A       1978       LEU         1       A       1978       LEU         1       A       2000       CYS         1       A       2027       MET         1       A       2049       LYS         1       A       2049       LYS         1       A       2049       LYS         1       A       2140       PHE         1       A       2140       PHE         1       A       2141       ASN         1       A       2175       SER         1       A       2187       ASP         1       A       2198       ASN         1       A       2198       ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
1       A       2027       MET         1       A       2049       LYS         1       A       2053       LEU         1       A       2140       PHE         1       A       2141       ASN         1       A       2156       TYR         1       A       2175       SER         1       A       2187       ASP         1       A       2196       PHE         1       A       2198       ASN         1       A       2200       PHE         1       A       2200       SER
1       A       2049       LYS         1       A       2053       LEU         1       A       2140       PHE         1       A       2141       ASN         1       A       2156       TYR         1       A       2175       SER         1       A       2187       ASP         1       A       2196       PHE         1       A       2198       ASN         1       A       2200       PHE         1       A       2250       SER
1       A       2053       LEU         1       A       2140       PHE         1       A       2141       ASN         1       A       2156       TYR         1       A       2175       SER         1       A       2187       ASP         1       A       2196       PHE         1       A       2198       ASN         1       A       2200       PHE         1       A       2250       SER
1       A       2140       PHE         1       A       2141       ASN         1       A       2156       TYR         1       A       2175       SER         1       A       2187       ASP         1       A       2196       PHE         1       A       2198       ASN         1       A       2200       PHE         1       A       2250       SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
1       A       2156       TYR         1       A       2175       SER         1       A       2187       ASP         1       A       2196       PHE         1       A       2198       ASN         1       A       2200       PHE         1       A       2250       SER
1         A         2175         SER           1         A         2187         ASP           1         A         2196         PHE           1         A         2198         ASN           1         A         2200         PHE           1         A         2250         SER
1         A         2187         ASP           1         A         2196         PHE           1         A         2198         ASN           1         A         2200         PHE           1         A         2250         SEB
1         A         2196         PHE           1         A         2198         ASN           1         A         2200         PHE           1         A         2250         SEB
1         A         2198         ASN           1         A         2200         PHE           1         A         2250         SEB
1 A 2200 PHE 1 A 2250 SFR
1 A 2250 SER
1 A 2265 SER
1 A 2267 ASP
1 A 2288 ASP
1 A 2296 SER
1 A 2312 SER
2 B 31 ASP
2 B 39 GLN
2 B 71 SER
2 B 98 ARG
2 B 119 SER
2 B 152 TYR
2 B 153 PHE
3 C 39 SER



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Mol	Chain	Res	Type
3	С	52	SER
3	С	69	SER
3	С	87	CYS
3	С	109	ASP
3	С	133	CYS
3	С	162	TRP
3	С	191	TYR

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

Mol	Chain	Res	Type
1	А	317	HIS
1	А	2007	GLN
2	В	35	HIS
2	В	88	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)

7 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	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	1	1,5	14,14,15	1.33	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	D	2	5	14,14,15	1.25	1 (7%)	17,19,21	1.24	1 (5%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$\mathbf{ths}$	Bond angles		
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	NAG	Н	1	1,4	$14,\!14,\!15$	0.39	0	17,19,21	0.59	0
4	NAG	Н	2	4	$14,\!14,\!15$	0.35	0	17,19,21	0.48	0
4	BMA	Н	3	4	11,11,12	0.94	0	15,15,17	1.58	3 (20%)
4	MAN	Н	4	4	11,11,12	1.14	2 (18%)	15,15,17	1.17	2 (13%)
4	MAN	Н	5	4	11,11,12	0.93	1 (9%)	15,15,17	1.53	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
4	NAG	Н	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Н	2	4	-	3/6/23/26	0/1/1/1
4	BMA	Н	3	4	-	1/2/19/22	0/1/1/1
4	MAN	Н	4	4	-	2/2/19/22	1/1/1/1
4	MAN	Н	5	4	-	1/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	D	1	NAG	O5-C1	4.72	1.51	1.43
5	D	2	NAG	O5-C1	3.95	1.50	1.43
4	Н	4	MAN	C1-C2	2.60	1.58	1.52
4	Н	5	MAN	O5-C5	2.52	1.48	1.43
4	Н	4	MAN	O5-C5	2.15	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	5	MAN	C1-O5-C5	4.66	118.51	112.19
5	D	1	NAG	C1-O5-C5	4.54	118.34	112.19
4	Н	3	BMA	C3-C4-C5	3.46	116.41	110.24
5	D	2	NAG	C1-O5-C5	3.01	116.27	112.19
4	Н	4	MAN	C1-O5-C5	2.99	116.25	112.19
4	Н	3	BMA	C1-O5-C5	2.49	115.57	112.19
4	Н	5	MAN	O2-C2-C3	-2.44	105.26	110.14
4	Н	3	BMA	O2-C2-C3	-2.08	105.98	110.14



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	4	MAN	O2-C2-C3	-2.07	105.99	110.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2	NAG	C4-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	Н	4	MAN	C4-C5-C6-O6
4	Н	1	NAG	O5-C5-C6-O6
4	Н	4	MAN	O5-C5-C6-O6
4	Н	1	NAG	C4-C5-C6-O6
4	Н	3	BMA	O5-C5-C6-O6
4	Н	5	MAN	O5-C5-C6-O6
4	Н	2	NAG	C1-C2-N2-C7
4	Н	2	NAG	C4-C5-C6-O6
4	Н	2	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	5	MAN	C1-C2-C3-C4-C5-O5
4	Н	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Н	1	NAG	1	0
4	Н	2	NAG	1	0

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











# 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
INIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	А	2401	1	14,14,15	0.53	0	$17,\!19,\!21$	0.52	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
6	NAG	А	2401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	2401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	1265/1467~(86%)	0.03	28 (2%)	62	52	73, 137, 194, 330	1 (0%)
2	В	217/223~(97%)	0.42	15 (6%)	16	13	30, 172, 220, 233	0
3	С	213/213~(100%)	0.36	14 (6%)	18	14	99, 156, 232, 243	0
All	All	1695/1903~(89%)	0.12	57 (3%)	45	36	30, 142, 212, 330	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	34	THR	7.1
1	А	28	ASP	4.6
1	А	26	HIS	4.3
2	В	186	SER	4.1
1	А	44	SER	3.8
2	В	10	GLU	3.8
3	С	133	CYS	3.7
1	А	2202	THR	3.7
1	А	33	ALA	3.7
1	А	27	VAL	3.5
1	А	29	THR	3.3
3	С	130	SER	3.2
1	А	16	TYR	3.2
2	В	20	ILE	3.1
1	А	31	PHE	3.0
2	В	220	ARG	3.0
1	А	173	LEU	3.0
1	А	22	LEU	3.0
3	С	207	SER	2.9
3	С	134	PHE	2.9
1	А	25	LEU	2.8
2	В	126	PRO	2.7
2	B	34	MET	2.7



Mol	Chain	Res	Type	RSRZ
1	А	2198	ASN	2.7
1	А	557	GLU	2.7
2	В	121	ALA	2.7
1	А	2269	HIS	2.6
2	В	11	LEU	2.6
1	А	35	ALA	2.6
3	С	194	GLU	2.6
2	В	157	VAL	2.5
1	А	2270	GLN	2.5
3	С	200	LYS	2.5
3	С	192	THR	2.5
1	А	32	PRO	2.3
2	В	114	THR	2.3
1	А	2191	THR	2.3
1	А	48	LYS	2.3
2	В	159	LEU	2.3
1	А	1704	GLU	2.2
1	А	63	ALA	2.2
2	В	187	SER	2.2
3	С	143	ILE	2.2
3	С	21	MET	2.2
1	А	332	GLU	2.2
3	С	152	SER	2.1
1	А	2318	ALA	2.1
3	С	140	PRO	2.1
1	А	1851	LEU	2.1
3	С	103	ILE	2.1
2	В	48	MET	2.1
3	С	201	THR	2.1
2	В	119	SER	2.0
2	В	204	VAL	2.0
1	А	2201	ALA	2.0
3	С	141	LYS	2.0
1	А	30	ARG	2.0

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# 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	$B-factors(A^2)$	Q<0.9
4	BMA	Н	3	11/12	0.70	0.21	179,186,197,202	0
5	NAG	D	2	14/15	0.71	0.31	194,209,214,215	0
4	MAN	Н	4	11/12	0.78	0.39	171,188,202,202	0
4	NAG	Н	2	14/15	0.88	0.17	150,171,185,185	0
5	NAG	D	1	14/15	0.89	0.21	164,200,213,214	0
4	MAN	Н	5	11/12	0.89	0.20	167,182,186,189	0
4	NAG	Н	1	14/15	0.90	0.23	138,150,158,160	0

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







## 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
6	NAG	А	2401	14/15	0.80	0.25	167,182,194,195	0
9	ZN	А	2404	1/1	0.96	0.23	137,137,137,137	0
7	CU	А	2402	1/1	0.98	0.26	133,133,133,133	0
8	CA	А	2403	1/1	0.99	0.20	141,141,141,141	0



# 6.5 Other polymers (i)

There are no such residues in this entry.

