

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

#### Aug 16, 2023 – 01:13 PM EDT

PDB ID	:	2AJF
Title	:	Structure of SARS coronavirus spike receptor-binding domain complexed with
		its receptor
Authors	:	Li, F.; Li, W.; Farzan, M.; Harrison, S.C.
Deposited on	:	2005-08-01
Resolution	:	2.90  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
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 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain		
1	Δ	507	3%		
1	A	597	66%	30%	•
1	р	507	5%		
	В	597	67%	28%	5%
0	Б	100	8%		
2	E	180	72%	21%	• • •
0	Б	100	8%		_
2	F	180	67%	24%	5% • •
	0				
3	C	3	100%		



Mol	Chain	Length		Quality of chain				
3	D	3	33%	33%	33%			



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	597	Total 4870	C 3115	N 806	O 920	S 29	0	0	0
1	В	597	Total 4870	C 3115	N 806	O 920	S 29	0	0	0

• Molecule 2 is a protein called SARS-coronavirus spike protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	F	E 174	Total	С	Ν	0	S	0	0	0
		174	1403	909	228	259	7	0	0	0
9	F	174	Total	С	Ν	0	S	0	0	0
	Ľ	1/4	1403	909	228	259	7			U

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



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

• Molecule 4 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
4	Δ	1	Total	С	Ν	0	0	Ο
- T	11	1	14	8	1	5	0	0
4	Δ	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	0
4	А	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	0	0
4	В	1	Total	С	Ν	Ο	0	0
	D	I	14	8	1	5	0	0
4	E	1	Total	С	Ν	Ο	0	0
	Ц	I	14	8	1	5	0	0
4	F	1	Total	С	Ν	Ο	0	0
<b>T</b>	T		14	8	1	5		

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Cl 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Cl 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	36	Total O 36 36	0	0
7	В	24	Total O 24 24	0	0
7	Ε	4	Total O 4 4	0	0
7	F	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 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

Cha	in	C
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100%

UAG 1 UAG 2

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

Chain D:	33%	33%	33%
NAG1 NG2 BMA3			



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	82.30Å 119.43Å 113.24Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.97^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.40 - 2.90	Depositor
Resolution (A)	47.39 - 2.81	EDS
% Data completeness	92.4 (47.40-2.90)	Depositor
(in resolution range)	85.9 (47.39-2.81)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.09	Depositor
$< I/\sigma(I) > 1$	$2.95 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.218 , $0.275$	Depositor
$\Pi, \Pi_{free}$	0.213 , $0.270$	DCC
$R_{free}$ test set	2449 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	73.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29 , $80.5$	EDS
L-test for $twinning^2$	$<  L  > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% 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: CL, BMA, NAG, ZN

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	
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.47	0/5007	0.62	0/6803
1	В	0.45	0/5007	0.58	2/6803~(0.0%)
2	Е	0.47	0/1448	0.62	0/1972
2	F	0.44	0/1448	0.60	0/1972
All	All	0.46	0/12910	0.60	2/17550~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	444	LEU	CA-CB-CG	5.95	128.99	115.30
1	В	423	LEU	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4870	0	4639	124	0
1	В	4870	0	4641	124	0
2	Е	1403	0	1326	24	0
2	F	1403	0	1325	31	0
3	С	39	0	34	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	39	0	34	1	0
4	А	42	0	39	2	0
4	В	14	0	13	0	0
4	Е	14	0	13	0	0
4	F	14	0	13	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	А	1	0	0	1	0
6	В	1	0	0	0	0
7	А	36	0	0	3	0
7	В	24	0	0	3	0
7	Е	4	0	0	0	0
7	F	1	0	0	0	0
All	All	12777	0	12077	302	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 12.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.36	1.05
1:A:261:CYS:HB2	1:A:488:VAL:CG2	1.93	0.97
1:B:245:ARG:HG2	1:B:245:ARG:HH21	1.32	0.94
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.48	0.94
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.49	0.93
1:B:589:GLU:OE1	1:B:589:GLU:HA	1.69	0.91
1:B:407:ILE:HD11	1:B:522:GLN:O	1.71	0.91
1:B:371:THR:OG1	7:B:1923:HOH:O	1.88	0.89
1:A:348:ALA:HB1	1:A:379:ILE:HD12	1.53	0.89
2:E:329:PHE:HD1	2:E:329:PHE:H	1.20	0.87
1:A:348:ALA:HB1	1:A:379:ILE:CD1	2.06	0.85
1:B:411:SER:OG	7:B:1906:HOH:O	1.94	0.84
2:F:469:PRO:HA	2:F:471:ALA:H	1.41	0.84
1:B:261:CYS:HB2	1:B:488:VAL:HG22	1.62	0.82
1:B:21:ILE:HA	1:B:24:GLN:HE21	1.45	0.80
1:A:229:THR:HG23	1:A:516:TYR:OH	1.84	0.78
2:E:329:PHE:HB3	2:E:497:VAL:HG21	1.63	0.78
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.68	0.75
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.73	0.72
1:A:310:GLU:HG2	1:A:421:ILE:HD11	1.72	0.72



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.72	0.71
1:B:209:VAL:HG23	1:B:216:ASP:HA	1.73	0.70
1:B:24:GLN:HG3	1:B:83:TYR:HE2	1.57	0.70
1:B:294:THR:O	1:B:298:VAL:HG23	1.94	0.68
1:B:47:SER:HA	1:B:62:MET:HG2	1.73	0.68
1:A:320:LEU:CD1	1:A:380:GLN:HG2	2.20	0.67
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.75	0.67
1:B:111:ASP:O	1:B:115:ARG:HB3	1.93	0.67
1:B:315:PHE:HB2	7:B:1907:HOH:O	1.93	0.67
1:A:529:LEU:HD21	1:A:554:LEU:HD13	1.77	0.67
1:A:126:ILE:HD11	1:A:176:LEU:HD22	1.77	0.66
1:B:168:TRP:O	1:B:172:VAL:HG22	1.94	0.66
1:B:240:LEU:O	1:B:244:VAL:HG13	1.95	0.66
1:A:248:LEU:HD21	1:A:278:LEU:HD23	1.77	0.66
1:A:462:MET:HE3	1:A:468:ILE:HD11	1.78	0.66
1:B:440:LEU:HD13	1:B:444:LEU:CD2	2.25	0.66
1:B:524:GLN:HE22	1:B:579:MET:HA	1.61	0.65
1:B:245:ARG:HH21	1:B:245:ARG:CG	2.08	0.65
1:A:597:ASP:O	1:A:600:LYS:HB2	1.95	0.65
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.77	0.65
2:F:323:CYS:N	2:F:348:CYS:SG	2.70	0.65
1:A:261:CYS:HB2	1:A:488:VAL:HG23	1.79	0.64
1:B:126:ILE:HA	1:B:129:THR:HG22	1.80	0.64
1:A:229:THR:OG1	1:A:581:VAL:HB	1.98	0.63
1:B:419:LYS:HD2	1:B:428:PHE:HB3	1.80	0.63
1:A:225:ASP:O	1:A:229:THR:HG22	1.99	0.63
1:A:320:LEU:HD13	1:A:380:GLN:CG	2.23	0.62
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.64	0.62
1:A:248:LEU:HD21	1:A:278:LEU:CD2	2.28	0.62
1:B:553:LYS:HE3	1:B:573:VAL:O	2.00	0.61
2:E:329:PHE:HD1	2:E:329:PHE:N	1.96	0.61
1:A:455:MET:HE2	1:A:481:LYS:HG2	1.81	0.61
2:E:395:ARG:HH11	2:E:395:ARG:HB2	1.65	0.61
1:A:72:PHE:O	1:A:76:GLN:HG2	2.01	0.60
1:B:499:ASP:N	1:B:500:PRO:HD2	2.17	0.60
1:A:296:ALA:HA	1:A:299:ASP:HB2	1.85	0.59
1:B:351:LEU:HD11	1:B:357:ARG:HD3	1.84	0.59
1:A:269:ASP:OD2	1:A:272:GLY:N	2.31	0.59
2:E:323:CYS:N	2:E:348:CYS:SG	2.76	0.59
1:B:294:THR:HG23	1:B:365:THR:HA	1.84	0.58
2:F:469:PRO:HA	2:F:471:ALA:N	2.15	0.58



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:223:ILE:O	1:A:227:GLU:HG3	2.03	0.58
1:B:21:ILE:HA	1:B:24:GLN:NE2	2.18	0.58
1:B:51:ASN:HD22	1:B:343:VAL:HG11	1.68	0.58
1:A:233:ILE:HD11	1:A:584:LEU:HD23	1.86	0.57
2:F:403:GLY:HA2	2:F:407:ASP:CG	2.24	0.57
2:E:325:PHE:HB3	2:E:329:PHE:HE1	1.70	0.56
2:F:323:CYS:HB2	2:F:324:PRO:HD3	1.87	0.56
1:B:134:ASN:HB3	1:B:137:ASN:HB3	1.87	0.56
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.87	0.56
1:B:176:LEU:HA	1:B:179:LEU:HD12	1.87	0.56
1:B:290:ASN:OD1	1:B:292:ASP:HB3	2.06	0.56
1:A:245:ARG:NH2	7:A:1572:HOH:O	2.40	0.55
1:A:418:LEU:HB3	1:A:424:LEU:HB2	1.88	0.55
1:B:288:LYS:HB3	1:B:289:PRO:HD2	1.88	0.55
1:B:540:HIS:HA	1:B:587:TYR:CE1	2.41	0.55
2:F:418:GLY:HA3	2:F:499:LEU:O	2.07	0.55
1:B:338:ASN:C	1:B:340:GLN:H	2.09	0.54
1:B:433:GLU:O	1:B:437:ASN:OD1	2.24	0.54
1:A:146:PRO:O	1:A:148:LEU:N	2.40	0.54
1:B:348:ALA:HB1	1:B:379:ILE:HD13	1.90	0.54
1:A:144:LEU:HA	1:A:148:LEU:HB3	1.90	0.54
1:B:459:TRP:O	1:B:463:VAL:HG23	2.08	0.54
1:A:267:LEU:HD13	7:A:1551:HOH:O	2.08	0.54
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.54
1:A:499:ASP:N	1:A:500:PRO:HD2	2.23	0.53
1:A:489:GLU:O	1:A:489:GLU:HG2	2.08	0.53
1:B:557:MET:HA	1:B:560:LEU:HD22	1.89	0.53
1:B:597:ASP:O	1:B:600:LYS:HD2	2.08	0.53
1:A:134:ASN:HB3	1:A:137:ASN:H	1.73	0.53
1:B:386:ALA:HA	1:B:393:ARG:HD3	1.91	0.53
1:A:407:ILE:HD13	1:A:407:ILE:N	2.22	0.53
1:B:520:LEU:HD22	1:B:579:MET:CE	2.39	0.53
1:B:389:PRO:HG2	1:B:392:LEU:HB2	1.91	0.53
1:B:611:SER:HB2	1:B:614:ALA:HB3	1.89	0.53
1:A:457:GLU:HA	1:A:457:GLU:OE1	2.08	0.53
1:A:245:ARG:NH1	1:A:605:GLY:O	2.42	0.52
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.92	0.52
1:B:315:PHE:CE2	1:B:376:MET:HG2	2.44	0.52
1:A:455:MET:CE	1:A:481:LYS:HG2	2.39	0.52
1:A:420:SER:HB2	4:A:1546:NAG:H61	1.91	0.52
2:F:455:ILE:HG22	2:F:455:ILE:O	2.10	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:146:PRO:O	1:B:148:LEU:N	2.43	0.52
1:B:538:PRO:HB2	1:B:540:HIS:CE1	2.45	0.52
2:F:385:ASP:HB2	2:F:498:VAL:HB	1.92	0.51
2:E:425:THR:HG21	2:E:495:ARG:HD2	1.92	0.51
2:E:403:GLY:O	2:E:405:ILE:N	2.43	0.51
1:B:407:ILE:HG23	1:B:526:GLN:NE2	2.25	0.51
1:B:440:LEU:HD13	1:B:444:LEU:HD22	1.93	0.50
1:B:521:TYR:O	1:B:522:GLN:C	2.49	0.50
1:A:85:LEU:HB3	1:A:101:GLN:HE22	1.77	0.50
1:A:379:ILE:O	1:A:382:ASP:HB2	2.12	0.50
1:A:573:VAL:HG23	1:A:574:VAL:HG13	1.92	0.50
1:B:51:ASN:ND2	1:B:343:VAL:HG11	2.26	0.50
2:F:403:GLY:O	2:F:405:ILE:N	2.45	0.50
1:A:560:LEU:O	1:A:563:SER:HB3	2.11	0.50
1:A:201:ASP:O	1:A:219:ARG:HD2	2.12	0.50
1:A:229:THR:HG23	1:A:516:TYR:HH	1.74	0.50
1:A:414:THR:O	1:A:418:LEU:HD22	2.12	0.50
2:E:337:VAL:HG22	2:E:389:VAL:HG12	1.93	0.50
1:A:21:ILE:HA	1:A:24:GLN:HE21	1.77	0.49
1:B:407:ILE:HG23	1:B:526:GLN:HE22	1.76	0.49
2:F:402:THR:HG23	3:D:3:BMA:H4	1.94	0.49
1:B:21:ILE:HA	1:B:24:GLN:HG2	1.93	0.49
1:A:233:ILE:HD11	1:A:584:LEU:CD2	2.42	0.49
1:B:261:CYS:CB	1:B:488:VAL:HG22	2.40	0.49
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.94	0.49
1:A:402:GLU:OE2	1:A:402:GLU:HA	2.12	0.49
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.77	0.49
1:A:505:HIS:CD2	1:A:505:HIS:H	2.31	0.49
1:B:348:ALA:HB1	1:B:379:ILE:CD1	2.43	0.49
2:E:329:PHE:N	2:E:329:PHE:CD1	2.68	0.49
1:B:225:ASP:O	1:B:229:THR:HB	2.13	0.49
1:B:31:LYS:HE3	1:B:35:GLU:OE1	2.13	0.48
2:E:337:VAL:CG2	2:E:389:VAL:HG12	2.43	0.48
1:B:203:TRP:CZ3	1:B:511:SER:HA	2.49	0.48
1:B:320:LEU:HD13	1:B:380:GLN:CG	2.39	0.48
1:A:338:ASN:HD22	1:A:339:VAL:HG23	1.77	0.48
1:B:388:GLN:HE21	1:B:388:GLN:HA	1.77	0.48
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.96	0.48
2:F:342:ARG:HG3	2:F:385:ASP:OD1	2.14	0.48
2:F:323:CYS:HB2	2:F:324:PRO:CD	2.44	0.48
2:F:417:MET:CE	2:F:417:MET:HA	2.44	0.48



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.95	0.48
2:F:329:PHE:HZ	2:F:355:LEU:HD23	1.79	0.47
2:F:409:ASN:OD1	2:F:440:TYR:HB2	2.14	0.47
1:A:351:LEU:HD12	1:A:351:LEU:N	2.28	0.47
1:A:351:LEU:HD11	1:A:357:ARG:HG2	1.96	0.47
1:A:55:THR:HG22	1:A:57:GLU:H	1.79	0.47
1:A:312:GLU:N	1:A:376:MET:HE1	2.29	0.47
1:B:520:LEU:HD21	1:B:581:VAL:HG23	1.96	0.47
2:E:341:GLU:O	2:E:385:ASP:HA	2.15	0.47
2:E:395:ARG:HH11	2:E:395:ARG:CB	2.27	0.47
2:F:329:PHE:HB3	2:F:497:VAL:HG21	1.96	0.47
1:A:599:ASN:HA	1:A:602:SER:HB2	1.97	0.47
1:B:375:GLU:OE1	1:B:375:GLU:HA	2.13	0.47
1:B:231:GLU:OE1	1:B:234:LYS:HE2	2.15	0.47
1:A:245:ARG:HG2	7:A:1572:HOH:O	2.13	0.47
1:B:305:GLN:O	1:B:309:LYS:HB2	2.14	0.47
1:B:440:LEU:O	1:B:444:LEU:HD22	2.15	0.47
1:B:245:ARG:HG2	1:B:245:ARG:NH2	2.13	0.47
2:F:356:TYR:OH	2:F:370:SER:O	2.33	0.46
1:A:324:THR:O	1:A:327:PHE:HB3	2.16	0.46
1:B:415:PRO:O	1:B:419:LYS:HB2	2.15	0.46
2:F:390:LYS:HG2	2:F:490:GLY:O	2.15	0.46
1:B:50:TYR:HE1	1:B:54:ILE:HG23	1.81	0.46
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.98	0.46
1:B:47:SER:HA	1:B:62:MET:CG	2.41	0.46
1:B:501:ALA:O	1:B:507:SER:HB3	2.16	0.46
1:A:199:TYR:HB3	1:A:464:PHE:CD1	2.51	0.45
1:A:457:GLU:HG3	1:A:513:ILE:HB	1.98	0.45
1:B:237:TYR:CE2	1:B:451:PRO:HG2	2.52	0.45
2:E:390:LYS:HG2	2:E:490:GLY:O	2.16	0.45
1:A:407:ILE:HD11	1:A:522:GLN:O	2.15	0.45
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.76	0.45
1:A:456:LEU:C	1:A:456:LEU:HD13	2.36	0.45
1:B:53:ASN:HD22	1:B:340:GLN:HG3	1.81	0.45
1:B:245:ARG:NH1	1:B:605:GLY:O	2.49	0.45
1:A:597:ASP:HA	1:A:600:LYS:NZ	2.30	0.45
1:A:323:MET:HE3	1:A:376:MET:SD	2.57	0.45
2:F:392:ASP:O	2:F:395:ARG:HD3	2.17	0.45
1:B:60:GLN:O	1:B:64:ASN:HB2	2.16	0.45
1:A:168:TRP:O	1:A:172:VAL:HG22	2.17	0.45
1:A:252:TYR:CD2	1:A:266:LEU:HD13	2.51	0.45



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:111:ASP:HA	1:A:114:LYS:HB2	1.97	0.44
1:B:257:SER:OG	1:B:259:ILE:HD13	2.17	0.44
1:B:275:TRP:O	1:B:278:LEU:HB2	2.17	0.44
1:B:336:PRO:HB2	1:B:340:GLN:HB3	1.99	0.44
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.57	0.44
2:E:385:ASP:O	2:E:497:VAL:HA	2.17	0.44
1:B:233:ILE:HD11	1:B:584:LEU:HD22	2.00	0.44
2:E:455:ILE:CG2	2:E:455:ILE:O	2.65	0.44
2:F:452:GLU:HG2	2:F:453:ARG:H	1.81	0.44
1:A:215:TYR:HB3	1:A:567:THR:OG1	2.17	0.44
1:A:417:HIS:CE1	1:A:545:SER:OG	2.71	0.44
1:B:36:ALA:O	1:B:37:GLU:C	2.55	0.44
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.44
1:A:461:TRP:CH2	1:A:513:ILE:HD12	2.53	0.44
1:A:499:ASP:HB3	6:A:902:CL:CL	2.54	0.44
1:B:526:GLN:HA	1:B:526:GLN:NE2	2.32	0.44
2:E:469:PRO:HA	2:E:471:ALA:N	2.32	0.44
1:B:380:GLN:HA	1:B:383:MET:CE	2.48	0.44
2:E:339:ALA:HA	2:E:455:ILE:HD11	2.00	0.44
1:A:353:LYS:HD2	2:E:487:THR:HG21	2.00	0.44
1:A:514:ARG:HG2	1:A:515:TYR:N	2.33	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.83	0.44
1:A:199:TYR:HD2	1:A:464:PHE:CE1	2.35	0.44
1:B:374:HIS:NE2	1:B:402:GLU:OE1	2.46	0.44
1:A:21:ILE:HD11	1:A:87:GLU:O	2.18	0.43
1:A:555:PHE:O	1:A:559:ARG:HG2	2.18	0.43
1:B:168:TRP:CD1	1:B:502:SER:OG	2.71	0.43
1:B:456:LEU:HD23	1:B:512:PHE:CE1	2.53	0.43
2:F:352:TYR:HD1	2:F:372:THR:HG23	1.83	0.43
1:B:410:LEU:HD22	1:B:522:GLN:HE21	1.83	0.43
1:A:177:ARG:NH1	1:A:495:GLU:HB3	2.34	0.43
1:B:539:LEU:HD23	1:B:587:TYR:HB2	2.01	0.43
1:B:600:LYS:HG2	1:B:601:ASN:ND2	2.33	0.43
2:F:410:TYR:HE2	2:F:412:LEU:HD13	1.83	0.43
2:F:349:VAL:HA	2:F:375:ASN:C	2.38	0.43
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.82	0.43
1:A:474:MET:CE	1:A:499:ASP:H	2.31	0.43
1:B:249:MET:HG2	1:B:256:ILE:HB	1.99	0.43
1:B:568:LEU:HD22	1:B:572:ASN:HD21	1.84	0.43
1:A:243:TYR:CZ	1:A:247:LYS:HE3	2.54	0.43
2:E:324:PRO:O	2:E:328:VAL:HG23	2.19	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:21:ILE:HA	1:A:24:GLN:NE2	2.34	0.43	
1:A:80:ALA:C	1:A:82:MET:H	2.22	0.43	
1:A:146:PRO:HB2	1:A:147:GLY:H	1.63	0.43	
1:B:513:ILE:HD12	1:B:513:ILE:HA	1.92	0.43	
1:A:226:VAL:HG21	1:A:513:ILE:HD11	2.01	0.43	
1:B:397:ASN:C	1:B:399:GLY:H	2.22	0.43	
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.44	0.43	
1:A:97:LEU:O	1:A:101:GLN:HG2	2.18	0.43	
1:B:291:ILE:O	1:B:291:ILE:CG2	2.67	0.43	
1:A:31:LYS:NZ	1:A:76:GLN:OE1	2.51	0.42	
1:A:318:VAL:O	1:A:551:GLY:HA3	2.19	0.42	
1:A:482:ARG:HD3	1:A:608:THR:O	2.19	0.42	
1:A:591:LEU:HG	1:A:595:LEU:HD13	2.01	0.42	
2:E:403:GLY:O	2:E:406:ALA:N	2.51	0.42	
2:F:329:PHE:CD1	2:F:329:PHE:N	2.87	0.42	
1:A:126:ILE:HD11	1:A:176:LEU:CD2	2.47	0.42	
1:A:555:PHE:HA	1:A:558:LEU:HB2	2.01	0.42	
1:A:564:GLU:HB3	1:A:565:PRO:CD	2.49	0.42	
1:B:335:ASP:HA	1:B:336:PRO:HD3	1.89	0.42	
1:B:520:LEU:HD22	1:B:579:MET:HE3	2.01	0.42	
2:F:410:TYR:CE2	2:F:412:LEU:HD13	2.55	0.42	
1:B:270:MET:HB3	1:B:271:TRP:CE3	2.55	0.42	
1:A:35:GLU:OE1	1:A:72:PHE:HE1	2.03	0.42	
1:A:245:ARG:HG2	1:A:245:ARG:HH21	1.83	0.42	
1:B:388:GLN:HB3	1:B:389:PRO:HD2	2.02	0.42	
2:F:337:VAL:HA	2:F:387:PHE:HB2	2.02	0.42	
1:A:407:ILE:N	1:A:407:ILE:CD1	2.78	0.42	
1:A:296:ALA:HA	1:A:299:ASP:CB	2.48	0.42	
1:A:321:PRO:HD2	1:A:380:GLN:OE1	2.19	0.42	
1:A:327:PHE:CE2	1:A:358:ILE:HG13	2.55	0.42	
1:B:557:MET:HG2	1:B:573:VAL:HG21	2.02	0.42	
1:B:111:ASP:O	1:B:115:ARG:CB	2.65	0.42	
1:A:311:ALA:HA	1:A:373:HIS:NE2	2.34	0.41	
1:A:315:PHE:C	1:A:317:SER:N	2.72	0.41	
1:B:96:GLN:HG2	1:B:392:LEU:HD13	2.01	0.41	
1:A:407:ILE:HD12	1:A:407:ILE:HA	1.57	0.41	
1:B:418:LEU:O	1:B:423:LEU:O	2.38	0.41	
1:B:591:LEU:HG	1:B:595:LEU:HD22	2.02	0.41	
1:A:119:ILE:HG23	1:A:179:LEU:HB3	2.02	0.41	
1:A:232:GLU:HB2	1:A:581:VAL:HG11	2.01	0.41	
1:B:257:SER:HA	1:B:258:PRO:HD3	1.87	0.41	



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:281:LEU:HD12	1:B:282:THR:HG23	2.01	0.41
1:A:244:VAL:O	1:A:245:ARG:C	2.57	0.41
2:F:395:ARG:HH11	2:F:395:ARG:HB2	1.86	0.41
1:B:380:GLN:HA	1:B:383:MET:HE2	2.02	0.41
2:F:439:LYS:HG2	2:F:480:ASP:OD1	2.20	0.41
1:B:146:PRO:HB2	1:B:147:GLY:H	1.67	0.41
2:F:387:PHE:CE1	2:F:496:VAL:HB	2.56	0.41
1:A:134:ASN:HB2	1:A:137:ASN:O	2.21	0.41
1:A:145:GLU:HA	1:A:146:PRO:HA	1.81	0.41
1:A:306:ARG:O	1:A:310:GLU:HB2	2.20	0.41
1:A:468:ILE:HD12	1:A:476:LYS:HG3	2.02	0.41
1:A:582:ARG:HE	1:A:582:ARG:HB2	1.45	0.41
1:B:51:ASN:HD22	1:B:343:VAL:CG1	2.32	0.41
1:B:499:ASP:N	1:B:500:PRO:CD	2.84	0.41
1:B:545:SER:O	1:B:546:ASN:HB2	2.20	0.41
2:F:409:ASN:HD22	2:F:409:ASN:N	2.19	0.41
1:A:212:VAL:O	1:A:213:ASP:C	2.60	0.41
1:A:249:MET:HG2	1:A:256:ILE:HB	2.03	0.41
1:B:174:LYS:HA	1:B:496:THR:O	2.20	0.41
1:B:421:ILE:HD13	1:B:421:ILE:HA	1.90	0.41
1:A:271:TRP:CD2	1:A:503:LEU:HD23	2.56	0.40
1:B:53:ASN:ND2	1:B:340:GLN:HE21	2.19	0.40
1:B:478:TRP:O	1:B:482:ARG:HG3	2.21	0.40
1:B:534:LYS:HA	1:B:534:LYS:HD3	1.96	0.40
1:B:535:HIS:CE1	1:B:542:CYS:HA	2.56	0.40
1:A:420:SER:HB2	4:A:1546:NAG:C6	2.51	0.40
1:B:359:LEU:HD13	1:B:359:LEU:C	2.42	0.40
1:B:22:GLU:HG2	1:B:26:LYS:HE3	2.03	0.40
1:B:226:VAL:O	1:B:229:THR:HG22	2.20	0.40
1:B:283:VAL:HA	1:B:284:PRO:HD3	1.90	0.40
1:B:503:LEU:HD23	1:B:504:PHE:H	1.86	0.40
1:A:85:LEU:C	1:A:87:GLU:H	2.25	0.40
1:A:178:PRO:O	1:A:181:GLU:HB2	2.21	0.40
1:A:156:LEU:HD21	1:A:281:LEU:HD11	2.02	0.40
1:A:261:CYS:CB	1:A:488:VAL:HG22	2.36	0.40
2:E:397:ILE:N	2:E:397:ILE:HD12	2.37	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	Perc	entiles
1	А	595/597~(100%)	536 (90%)	55 (9%)	4 (1%)	22	54
1	В	595/597~(100%)	529~(89%)	56~(9%)	10 (2%)	9	31
2	Е	170/180~(94%)	137 (81%)	24 (14%)	9 (5%)	2	6
2	F	170/180~(94%)	143 (84%)	19 (11%)	8 (5%)	2	8
All	All	1530/1554 (98%)	1345 (88%)	154 (10%)	31 (2%)	7	27

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	146	PRO
1	В	146	PRO
2	Е	402	THR
2	Е	404	VAL
2	Е	416	PHE
1	А	147	GLY
1	В	87	GLU
1	В	110	GLU
1	В	147	GLY
1	В	339	VAL
1	В	519	THR
2	F	370	SER
2	F	402	THR
2	F	404	VAL
1	В	407	ILE
1	В	424	LEU
2	Е	395	ARG
2	F	416	PHE
1	В	213	ASP
1	А	86	GLN
2	Е	368	GLY
2	Е	369	VAL



Mol	Chain	Res	Type
2	Е	370	SER
2	F	369	VAL
2	F	401	GLN
2	Е	401	GLN
2	F	368	GLY
1	А	289	PRO
2	Е	482	GLY
1	В	364	VAL
2	F	470	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	527/527~(100%)	458 (87%)	69~(13%)	4	12
1	В	527/527~(100%)	473 (90%)	54 (10%)	7	22
2	Ε	152/158~(96%)	134 (88%)	18 (12%)	5	16
2	F	152/158~(96%)	137 (90%)	15 (10%)	8	24
All	All	1358/1370~(99%)	1202 (88%)	156 (12%)	5	17

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	20	THR
1	А	21	ILE
1	А	29	LEU
1	А	31	LYS
1	А	37	GLU
1	А	39	LEU
1	А	44	SER
1	А	45	LEU
1	А	60	GLN
1	А	61	ASN
1	А	73	LEU
1	А	79	LEU



Mol	Chain	Res	Type
1	А	81	GLN
1	А	85	LEU
1	А	102	GLN
1	А	107	VAL
1	А	114	LYS
1	А	125	THR
1	А	129	THR
1	А	149	ASN
1	А	171	GLU
1	А	176	LEU
1	А	198	ASP
1	А	209	VAL
1	А	221	GLN
1	А	225	ASP
1	А	234	LYS
1	А	240	LEU
1	А	245	ARG
1	А	259	ILE
1	А	280	SER
1	А	287	GLN
1	А	294	THR
1	А	316	VAL
1	А	343	VAL
1	А	365	THR
1	А	381	TYR
1	А	385	TYR
1	А	394	ASN
1	А	401	HIS
1	А	407	ILE
1	А	410	LEU
1	А	418	LEU
1	А	429	GLN
1	А	436	ILE
1	А	439	LEU
1	А	444	LEU
1	А	445	THR
1	А	457	GLU
1	А	458	LYS
1	А	460	ARG
1	А	473	TRP
1	А	476	LYS
1	А	481	LYS



Mol	Chain	Res	Type
1	А	488	VAL
1	А	514	ARG
1	А	529	LEU
1	А	546	ASN
1	А	549	GLU
1	А	557	MET
1	А	559	ARG
1	А	560	LEU
1	А	563	SER
1	А	570	LEU
1	А	582	ARG
1	А	585	LEU
1	А	597	ASP
1	А	600	LYS
1	А	602	SER
1	В	21	ILE
1	В	29	LEU
1	В	60	GLN
1	В	62	MET
1	В	89	GLN
1	В	95	LEU
1	В	102	GLN
1	В	114	LYS
1	В	136	ASP
1	В	151	ILE
1	В	156	LEU
1	В	227	GLU
1	В	229	THR
1	В	233	ILE
1	В	244	VAL
1	В	245	ARG
1	В	259	ILE
1	В	273	ARG
1	В	276	THR
1	В	278	LEU
1	В	287	GLN
1	В	317	SER
1	В	335	ASP
1	В	341	LYS
1	В	357	ARG
1	В	359	LEU
1	В	381	TYR



Mol	Chain	Res	Type
1	В	385	TYR
1	В	388	GLN
1	В	391	LEU
1	В	401	HIS
1	В	418	LEU
1	В	424	LEU
1	В	429	GLN
1	В	444	LEU
1	В	455	MET
1	В	475	LYS
1	В	488	VAL
1	В	491	VAL
1	В	503	LEU
1	В	511	SER
1	В	526	GLN
1	В	529	LEU
1	В	545	SER
1	В	557	MET
1	В	560	LEU
1	В	568	LEU
1	В	570	LEU
1	В	582	ARG
1	В	585	LEU
1	В	589	GLU
1	В	593	THR
1	В	595	LEU
1	В	600	LYS
2	Е	323	CYS
2	Е	329	PHE
2	Е	330	ASN
2	Е	337	VAL
2	E	348	CYS
2	Е	356	TYR
2	E	369	VAL
2	E	395	ARG
2	Е	416	PHE
2	E	417	MET
2	Е	423	TRP
2	E	431	THR
2	E	433	THR
2	Е	467	CYS
2	Е	470	PRO



Mol	Chain	Res	Type
2	Е	472	LEU
2	Е	481	TYR
2	Е	485	THR
2	F	329	PHE
2	F	337	VAL
2	F	341	GLU
2	F	348	CYS
2	F	356	TYR
2	F	369	VAL
2	F	373	LYS
2	F	402	THR
2	F	416	PHE
2	F	417	MET
2	F	425	THR
2	F	426	ARG
2	F	431	THR
2	F	481	TYR
2	F	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	24	GLN
1	А	33	ASN
1	А	49	ASN
1	А	101	GLN
1	А	137	ASN
1	А	287	GLN
1	А	338	ASN
1	А	340	GLN
1	А	472	GLN
1	А	493	HIS
1	А	505	HIS
1	А	526	GLN
1	А	580	ASN
1	А	586	ASN
1	А	599	ASN
1	В	24	GLN
1	В	33	ASN
1	В	51	ASN
1	В	53	ASN
1	В	101	GLN



Mol	Chain	Res	Type
1	В	300	GLN
1	В	373	HIS
1	В	388	GLN
1	В	493	HIS
1	B	505	HIS
1	В	524	GLN
1	В	526	GLN
1	В	535	HIS
1	В	556	ASN
1	B	586	ASN
1	В	599	ASN
1	В	601	ASN
2	Е	473	ASN
2	F	473	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)

6 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 Rea			Bo	ond leng	ths	Bond angles							
NIOI	туре	Chain	rtes	rtes	nes	nes	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	3,1	14,14,15	0.48	0	$17,\!19,\!21$	2.04	6 (35%)				
3	NAG	С	2	3	14,14,15	0.33	0	17,19,21	2.62	3 (17%)				
3	BMA	С	3	3	11,11,12	0.62	0	$15,\!15,\!17$	1.12	1 (6%)				
3	NAG	D	1	3,1	14,14,15	0.54	0	17,19,21	0.77	0				



Mal	Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
IVIOI	туре	Chain	nes	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2								
3	NAG	D	2	3	14,14,15	0.48	0	17,19,21	1.18	2 (11%)									
3	BMA	D	3	3	11,11,12	0.63	0	$15,\!15,\!17$	1.44	4 (26%)									

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

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	2	NAG	C1-O5-C5	8.95	124.32	112.19
3	С	1	NAG	C1-O5-C5	5.90	120.18	112.19
3	С	2	NAG	O5-C1-C2	4.29	118.06	111.29
3	D	3	BMA	C1-C2-C3	3.13	113.52	109.67
3	С	3	BMA	C1-O5-C5	3.10	116.39	112.19
3	D	2	NAG	O5-C5-C6	2.85	111.67	107.20
3	D	3	BMA	C1-O5-C5	2.64	115.77	112.19
3	D	3	BMA	O5-C1-C2	2.49	114.61	110.77
3	С	2	NAG	O5-C5-C4	2.40	116.67	110.83
3	D	2	NAG	C3-C4-C5	-2.37	106.01	110.24
3	С	1	NAG	O7-C7-C8	-2.28	117.82	122.06
3	С	1	NAG	C2-N2-C7	2.18	126.00	122.90
3	С	1	NAG	O5-C5-C4	2.16	116.09	110.83
3	С	1	NAG	C3-C4-C5	2.14	114.06	110.24
3	D	3	BMA	O5-C5-C6	2.12	110.53	107.20
3	C	1	NAG	O5-C5-C6	-2.09	103.92	107.20

There are no chirality outliers.

All (17) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	С	1	NAG	C8-C7-N2-C2
3	С	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	С	2	NAG	O5-C5-C6-O6
3	С	1	NAG	O5-C5-C6-O6
3	С	2	NAG	C4-C5-C6-O6
3	С	2	NAG	C8-C7-N2-C2
3	С	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	С	1	NAG	C4-C5-C6-O6
3	С	3	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	1	0

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









### 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	Type	Chain	n Bes Link		Bo	ond leng	ths	Bond angles		
1VIOI	or rype chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
4	NAG	А	1322	1	$14,\!14,\!15$	0.56	0	$17,\!19,\!21$	1.83	1 (5%)
4	NAG	А	1546	1	$14,\!14,\!15$	0.71	0	$17,\!19,\!21$	1.79	3 (17%)
4	NAG	Е	1330	2	$14,\!14,\!15$	0.51	0	$17,\!19,\!21$	1.41	2 (11%)
4	NAG	F	1330	2	14,14,15	0.51	0	$17,\!19,\!21$	2.19	4 (23%)
4	NAG	А	1053	1	14,14,15	0.48	0	$17,\!19,\!21$	1.38	2 (11%)
4	NAG	В	1322	1	14,14,15	0.52	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	А	1322	1	-	3/6/23/26	0/1/1/1
4	NAG	А	1546	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	1330	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1330	2	-	0/6/23/26	0/1/1/1
4	NAG	А	1053	1	-	4/6/23/26	0/1/1/1
4	NAG	В	1322	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (	13)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1322	NAG	C1-O5-C5	6.22	120.62	112.19
4	F	1330	NAG	C1-O5-C5	5.82	120.08	112.19
4	А	1053	NAG	C1-O5-C5	4.34	118.07	112.19
4	F	1330	NAG	C4-C3-C2	-4.33	104.67	111.02



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1546	NAG	C4-C3-C2	-3.95	105.23	111.02
4	F	1330	NAG	C2-N2-C7	-3.94	117.29	122.90
4	А	1546	NAG	C1-O5-C5	3.51	116.95	112.19
4	А	1546	NAG	C3-C4-C5	-3.47	104.06	110.24
4	Ε	1330	NAG	C1-O5-C5	3.44	116.86	112.19
4	В	1322	NAG	C1-O5-C5	2.26	115.26	112.19
4	Ε	1330	NAG	O7-C7-C8	-2.22	117.94	122.06
4	А	1053	NAG	O5-C1-C2	2.15	114.68	111.29
4	F	1330	NAG	C1-C2-N2	2.05	113.99	110.49

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
4	А	1053	NAG	O7-C7-N2-C2
4	А	1322	NAG	C8-C7-N2-C2
4	А	1322	NAG	O7-C7-N2-C2
4	А	1053	NAG	C8-C7-N2-C2
4	В	1322	NAG	C8-C7-N2-C2
4	А	1546	NAG	O5-C5-C6-O6
4	В	1322	NAG	O7-C7-N2-C2
4	А	1053	NAG	C4-C5-C6-O6
4	А	1546	NAG	C4-C5-C6-O6
4	А	1053	NAG	O5-C5-C6-O6
4	А	1322	NAG	O5-C5-C6-O6
4	E	1330	NAG	C8-C7-N2-C2
4	Е	1330	NAG	O7-C7-N2-C2

All (13) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1546	NAG	2	0

## 5.7 Other polymers (i)

There are no such residues in this entry.



## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	597/597~(100%)	0.14	17 (2%) 53 49	56, 82, 123, 147	0
1	В	597/597~(100%)	0.38	32 (5%) 25 22	56, 82, 123, 148	0
2	Ε	174/180~(96%)	0.45	14 (8%) 12 9	75, 96, 142, 153	0
2	F	174/180~(96%)	0.43	14 (8%) 12 9	76, 96, 142, 152	0
All	All	1542/1554~(99%)	0.30	77 (4%) 28 25	56, 88, 131, 153	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	136	ASP	6.7
1	В	615	ASP	6.5
1	В	140	GLU	5.4
2	Е	501	PHE	5.2
2	F	354	VAL	5.1
1	В	132	VAL	4.4
1	В	193	ALA	4.3
1	В	429	GLN	4.3
2	Е	354	VAL	4.2
1	А	339	VAL	4.2
2	F	350	ALA	4.0
1	А	106	SER	4.0
1	В	339	VAL	3.8
2	Е	352	TYR	3.8
1	В	168	TRP	3.7
1	В	141	CYS	3.7
2	F	364	PHE	3.7
1	В	131	LYS	3.6
1	В	337	GLY	3.4
2	F	443	LEU	3.3
1	В	137	ASN	3.3



Conti	Continued from previous page							
Mol	Chain	Res	Type	RSRZ				

1	В	82	MET	3.2
1	А	615	ASP	3.1
1	А	139	GLN	3.1
2	Е	364	PHE	3.1
1	А	108	LEU	3.1
1	В	89	GLN	3.0
1	В	139	GLN	3.0
2	F	470	PRO	3.0
1	В	491	VAL	2.9
1	В	143	LEU	2.9
2	Е	499	LEU	2.9
1	В	171	GLU	2.8
1	В	135	PRO	2.8
1	А	415	PRO	2.7
2	Е	357	ASN	2.7
1	А	196	TYR	2.7
2	F	344	LYS	2.7
2	Е	372	THR	2.6
2	F	478	LEU	2.6
1	В	59	VAL	2.6
2	Е	500	SER	2.6
1	А	133	CYS	2.5
1	В	194	ASN	2.5
2	Е	382	VAL	2.5
1	В	88	ILE	2.4
1	А	138	PRO	2.4
1	А	86	GLN	2.4
2	F	355	LEU	2.4
1	В	23	GLU	2.4
1	В	338	ASN	2.4
2	F	356	TYR	2.4
1	А	453	THR	2.3
2	Е	410	TYR	2.3
1	В	614	ALA	2.3
1	В	19	SER	2.3
2	Е	421	LEU	2.3
1	В	31	LYS	2.3
2	Е	360	PHE	2.3
1	А	141	CYS	2.2
1	А	57	GLU	2.2
2	F	357	ASN	2.2
1	В	399	GLY	2.2



Mol	Chain	Res	Type	RSRZ
2	F	421	LEU	2.2
1	А	88	ILE	2.2
1	В	129	THR	2.2
2	Е	355	LEU	2.1
1	В	22	GLU	2.1
2	F	442	TYR	2.1
2	F	358	SER	2.1
2	Е	350	ALA	2.1
1	А	58	ASN	2.1
1	В	108	LEU	2.1
1	А	104	GLY	2.0
1	B	85	LEU	2.0
1	А	105	SER	2.0
2	F	476	TRP	2.0

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

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

#### 6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	BMA	С	3	11/12	0.58	0.40	79,80,81,81	0
3	NAG	С	1	14/15	0.82	0.19	79,86,89,93	0
3	BMA	D	3	11/12	0.87	0.28	83,84,84,85	0
3	NAG	С	2	14/15	0.88	0.28	70,75,77,79	0
3	NAG	D	1	14/15	0.89	0.26	93,99,100,102	0
3	NAG	D	2	14/15	0.91	0.28	87,90,91,91	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	$B-factors(A^2)$	Q<0.9
4	NAG	Е	1330	14/15	0.52	0.28	108,109,112,113	0
4	NAG	F	1330	14/15	0.66	0.28	106,107,108,108	0
4	NAG	А	1053	14/15	0.75	0.29	88,89,90,90	0
4	NAG	А	1546	14/15	0.77	0.27	72,74,77,78	0
4	NAG	В	1322	14/15	0.83	0.16	72,74,76,77	0
4	NAG	А	1322	14/15	0.86	0.12	75,77,78,78	0
6	CL	В	1902	1/1	0.86	0.29	115,115,115,115	0
6	CL	А	902	1/1	0.94	0.13	74,74,74,74	0
5	ZN	В	901	1/1	0.98	0.13	84,84,84,84	0
5	ZN	А	901	1/1	0.99	0.12	74,74,74,74	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

