



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:10 PM BST

PDB ID : 1H3X  
Title : CRYSTAL STRUCTURE OF THE HUMAN IGG1 FC-FRAGMENT, GLYC  
OFORM (G0F)2  
Authors : Krapp, S.; Mimura, Y.; Jefferis, R.; Huber, R.; Sonderrmann, P.  
Deposited on : 2002-09-19  
Resolution : 2.44 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

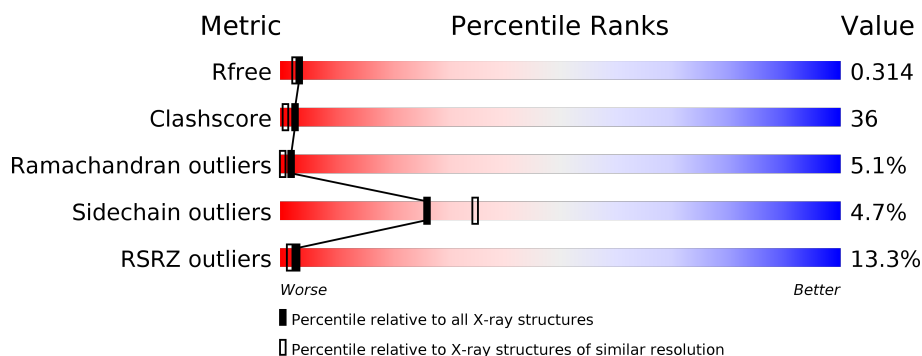
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	A	223	
1	B	223	
2	C	8	
2	D	8	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	-	-	X	X
2	NAG	D	5	X	-	-	-

## 2 Entry composition [i](#)

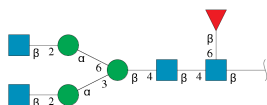
There are 3 unique types of molecules in this entry. The entry contains 3668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	1
			1661	1057	283	314	7			
1	B	207	Total	C	N	O	S	0	0	1
			1655	1054	281	313	7			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			
2	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

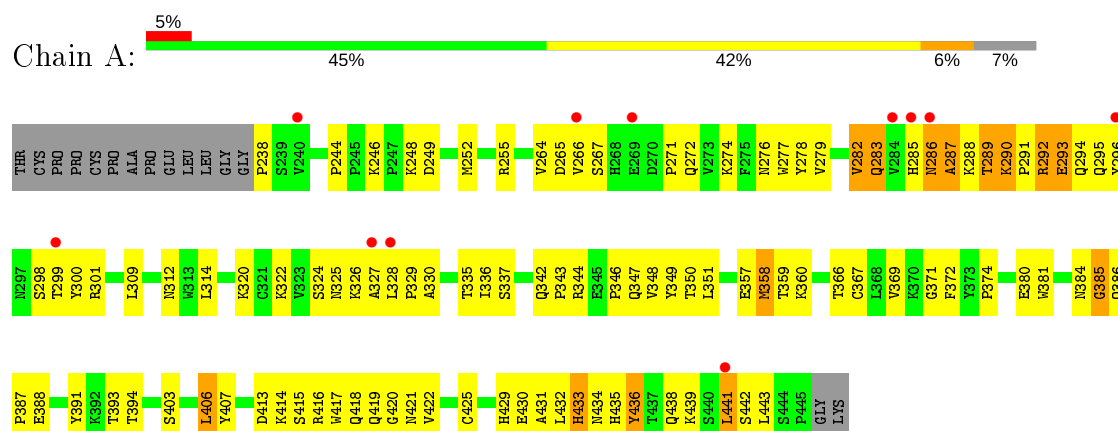
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	79	Total	O	0	0
			79	79		

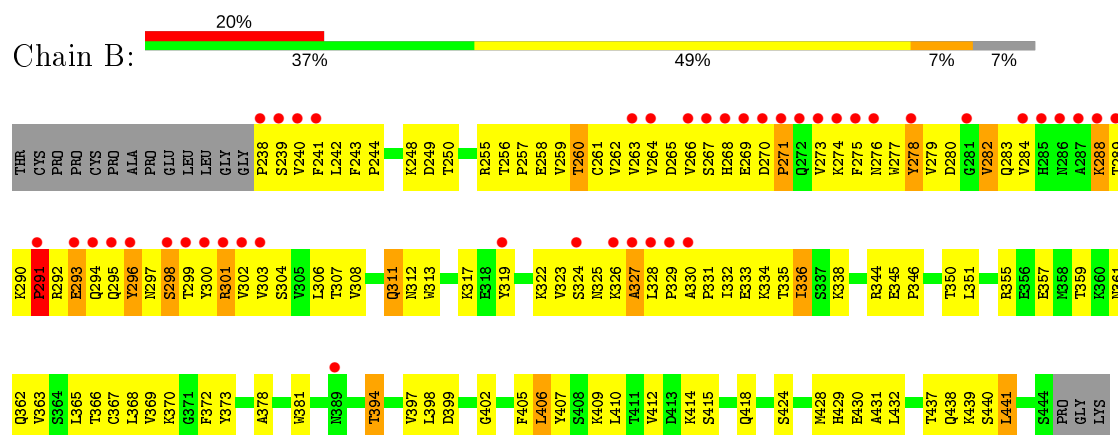
### 3 Residue-property plots [i](#)

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: IG GAMMA-1 CHAIN C REGION



#### • Molecule 1: IG GAMMA-1 CHAIN C REGION



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



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

Chain D:  38% 63%

HA61	HA62	HA63	HA64	HA65	HA66	HA67	FUL8
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.69 Å 80.20 Å 138.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 40.42 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-2.44) 93.8 (40.42-2.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.45 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.278 , 0.339 0.260 , 0.314	Depositor DCC
$R_{free}$ test set	961 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.44	0/1707	0.68	0/2325
1	B	0.38	0/1700	0.64	0/2314
All	All	0.41	0/3407	0.66	0/4639

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	TYR	Sidechain

### 5.2 Too-close contacts

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	A	1661	0	1631	109	0
1	B	1655	0	1625	133	0
2	C	99	0	85	4	0
2	D	99	0	85	14	0
3	A	75	0	0	13	0
3	B	79	0	0	14	0
All	All	3668	0	3426	252	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 36.

All (252) 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:D:1:NAG:H61	2:D:2:NAG:HN2	1.05	1.19
2:D:1:NAG:H61	2:D:2:NAG:N2	1.79	0.98
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.44	0.96
1:A:272:GLN:HE22	1:A:326:LYS:HD2	1.35	0.92
1:B:311:GLN:H	1:B:311:GLN:NE2	1.71	0.87
1:A:282:VAL:O	1:A:283:GLN:HB2	1.72	0.87
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.59	0.84
1:B:243:PHE:HB2	1:B:260:THR:HG23	1.60	0.84
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.60	0.83
1:B:291:PRO:HB3	1:B:304:SER:HA	1.60	0.82
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.63	0.80
1:A:314:LEU:HD22	1:A:430:GLU:HG3	1.62	0.79
1:B:289:THR:HG22	1:B:290:LYS:H	1.48	0.79
1:B:263:VAL:O	1:B:301:ARG:HA	1.84	0.78
2:D:6:MAN:O5	2:D:7:NAG:H82	1.81	0.78
1:A:291:PRO:C	1:A:292:ARG:HD2	2.03	0.78
1:A:292:ARG:O	1:A:293:GLU:HB3	1.84	0.76
1:B:429:HIS:CD2	1:B:431:ALA:H	2.03	0.76
1:B:266:VAL:HB	1:B:300:TYR:CB	2.15	0.75
1:A:429:HIS:CD2	1:A:431:ALA:H	2.05	0.75
1:A:296:TYR:CD2	2:C:8:FUL:H2	2.22	0.74
1:A:272:GLN:NE2	1:A:326:LYS:HD2	2.01	0.74
1:B:429:HIS:HD2	1:B:431:ALA:H	1.31	0.74
2:D:1:NAG:C6	2:D:2:NAG:HN2	1.94	0.73
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.69	0.73
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.72
1:B:296:TYR:HE2	2:D:1:NAG:H62	1.53	0.72
1:B:296:TYR:CE2	2:D:1:NAG:H62	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:H	1:B:288:LYS:HD3	1.54	0.71
1:B:409:LYS:HE2	3:B:2041:HOH:O	1.92	0.69
1:A:422:VAL:HG22	1:A:442:SER:OG	1.92	0.68
1:B:270:ASP:N	1:B:271:PRO:HD3	2.09	0.68
1:A:325:ASN:HD21	1:A:327:ALA:HB3	1.58	0.68
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.75	0.68
1:A:418:GLN:HA	1:A:443:LEU:CD2	2.24	0.68
1:A:429:HIS:HD2	1:A:431:ALA:H	1.43	0.67
1:A:325:ASN:ND2	1:A:327:ALA:HB3	2.10	0.67
1:B:290:LYS:HE3	1:B:292:ARG:HH22	1.61	0.66
2:C:2:NAG:H83	2:C:6:MAN:O4	1.96	0.66
1:A:350:THR:HB	1:A:441:LEU:HG	1.77	0.65
1:B:439:LYS:HB2	3:B:2034:HOH:O	1.96	0.64
1:B:332:ILE:HG22	1:B:333:GLU:N	2.13	0.64
1:A:328:LEU:HG	1:A:330:ALA:O	1.98	0.64
1:A:288:LYS:H	1:A:288:LYS:HD2	1.63	0.63
1:A:279:VAL:O	1:A:282:VAL:HG13	1.97	0.63
1:B:258:GLU:HB3	3:B:2017:HOH:O	1.98	0.63
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.79	0.63
1:B:409:LYS:HG2	3:B:2067:HOH:O	1.98	0.63
2:D:4:MAN:H4	2:D:5:NAG:O7	1.98	0.63
1:A:384:ASN:O	1:A:386:GLN:N	2.31	0.63
1:B:355:ARG:HD2	3:B:2038:HOH:O	2.00	0.62
1:A:300:TYR:HA	3:A:2020:HOH:O	1.99	0.61
1:B:394:THR:HG23	1:B:407:TYR:O	2.01	0.60
1:B:406:LEU:C	1:B:406:LEU:HD12	2.22	0.60
1:B:274:LYS:HE2	1:B:276:ASN:HD21	1.67	0.60
1:B:325:ASN:HD22	1:B:326:LYS:H	1.51	0.59
1:B:267:SER:HA	3:B:2007:HOH:O	2.02	0.59
1:A:417:TRP:HH2	1:A:441:LEU:HD22	1.67	0.59
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.85	0.58
1:A:417:TRP:CH2	1:A:441:LEU:HD22	2.37	0.58
1:B:269:GLU:HG2	1:B:269:GLU:O	2.03	0.58
1:A:286:ASN:O	1:A:287:ALA:HB2	2.03	0.58
1:B:279:VAL:HG23	1:B:279:VAL:O	2.03	0.58
1:B:296:TYR:CE1	1:B:301:ARG:HD3	2.38	0.58
1:A:415:SER:O	1:A:419:GLN:HG3	2.04	0.58
1:A:421:ASN:N	1:A:421:ASN:HD22	2.00	0.58
1:A:433:HIS:ND1	1:A:434:ASN:OD1	2.36	0.58
1:B:424:SER:OG	1:B:438:GLN:HG2	2.04	0.58
1:A:344:ARG:HG2	3:A:2035:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HB2	1:B:308:VAL:HB	1.85	0.57
1:B:265:ASP:HA	1:B:299:THR:HB	1.86	0.57
1:B:288:LYS:HE2	1:B:306:LEU:HD11	1.86	0.57
1:B:439:LYS:HE3	1:B:440:SER:O	2.05	0.56
1:A:320:LYS:HG3	1:A:335:THR:HG22	1.87	0.56
1:B:328:LEU:HG	1:B:330:ALA:O	2.05	0.56
1:B:301:ARG:HE	1:B:303:VAL:CG2	2.18	0.56
1:B:311:GLN:H	1:B:311:GLN:CD	2.08	0.56
1:B:270:ASP:OD2	1:B:327:ALA:HB2	2.06	0.55
1:B:325:ASN:ND2	1:B:326:LYS:H	2.04	0.55
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.88	0.55
1:B:241:PHE:CE2	2:D:3:BMA:H3	2.42	0.55
1:B:273:VAL:HG13	3:B:2011:HOH:O	2.07	0.55
1:B:275:PHE:HE1	1:B:302:VAL:HG12	1.72	0.55
1:B:266:VAL:CB	1:B:300:TYR:HB2	2.28	0.54
1:A:289:THR:O	1:A:290:LYS:HB2	2.07	0.54
1:B:240:VAL:O	1:B:334:LYS:HE3	2.08	0.54
1:A:288:LYS:O	1:A:289:THR:O	2.24	0.54
1:B:238:PRO:CG	1:B:328:LEU:HD13	2.37	0.54
1:A:414:LYS:HE2	1:A:418:GLN:NE2	2.22	0.54
2:D:6:MAN:C1	2:D:7:NAG:H82	2.37	0.54
1:B:351:LEU:C	1:B:441:LEU:HD11	2.28	0.54
1:A:414:LYS:O	1:A:418:GLN:HG3	2.08	0.54
1:A:300:TYR:HD2	3:A:2011:HOH:O	1.91	0.53
1:A:282:VAL:O	1:A:283:GLN:CB	2.52	0.53
1:A:285:HIS:O	1:A:286:ASN:HB2	2.08	0.53
1:B:322:LYS:HE3	1:B:333:GLU:OE2	2.08	0.53
1:B:262:VAL:HG13	1:B:303:VAL:HG22	1.90	0.53
1:A:296:TYR:HD2	2:C:8:FUL:H2	1.72	0.53
1:A:351:LEU:HB2	1:A:366:THR:HB	1.90	0.52
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.90	0.52
1:B:289:THR:HG22	1:B:290:LYS:N	2.21	0.52
1:B:312:ASN:ND2	1:B:317:LYS:HD2	2.24	0.52
1:A:384:ASN:OD1	1:A:385:GLY:N	2.41	0.52
1:A:393:THR:HG22	1:A:394:THR:O	2.10	0.52
1:A:337:SER:HB2	3:A:2027:HOH:O	2.09	0.52
2:C:5:NAG:O3	2:C:5:NAG:H83	2.09	0.52
1:B:297:ASN:O	1:B:298:SER:HB3	2.09	0.52
1:A:271:PRO:HD2	3:A:2013:HOH:O	2.08	0.52
1:B:296:TYR:HE1	1:B:301:ARG:HD3	1.74	0.52
1:B:249:ASP:O	1:B:257:PRO:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:MAN:HO3	2:D:5:NAG:C1	2.23	0.52
1:B:325:ASN:ND2	1:B:326:LYS:N	2.59	0.51
1:A:429:HIS:O	1:A:435:HIS:HA	2.11	0.51
1:A:350:THR:HB	1:A:441:LEU:CG	2.40	0.51
1:A:436:TYR:CD1	1:A:436:TYR:C	2.84	0.51
1:A:418:GLN:C	1:A:420:GLY:H	2.15	0.50
1:A:443:LEU:O	1:A:443:LEU:HG	2.11	0.50
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.92	0.50
1:A:294:GLN:O	1:A:300:TYR:CD1	2.65	0.50
1:B:291:PRO:CB	1:B:304:SER:HA	2.37	0.50
1:A:380:GLU:O	1:A:425:CYS:HA	2.12	0.50
1:B:406:LEU:HD12	1:B:406:LEU:O	2.12	0.50
1:A:360:LYS:O	1:A:414:LYS:HD2	2.11	0.50
1:B:332:ILE:CG2	1:B:333:GLU:N	2.74	0.50
1:A:246:LYS:HB2	1:A:249:ASP:OD2	2.12	0.50
1:B:249:ASP:C	1:B:257:PRO:HG3	2.32	0.50
1:B:369:VAL:O	1:B:405:PHE:HA	2.12	0.50
1:A:292:ARG:O	1:A:293:GLU:CB	2.58	0.49
1:A:299:THR:HA	3:A:2011:HOH:O	2.11	0.49
1:B:278:TYR:CD1	1:B:278:TYR:N	2.79	0.49
1:B:291:PRO:HB3	1:B:304:SER:CA	2.37	0.49
1:A:248:LYS:O	1:A:255:ARG:HD3	2.13	0.49
1:A:357:GLU:C	1:A:359:THR:H	2.15	0.49
1:A:388:GLU:OE2	1:A:416:ARG:NH2	2.42	0.49
1:B:250:THR:HG22	1:B:257:PRO:HB3	1.94	0.49
1:B:256:THR:HG23	3:B:2003:HOH:O	2.12	0.49
1:A:277:TRP:O	1:A:283:GLN:HB3	2.13	0.49
1:B:292:ARG:O	1:B:293:GLU:HB3	2.12	0.49
1:B:432:LEU:CD1	1:B:437:THR:HG22	2.42	0.48
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.94	0.48
1:A:283:GLN:C	1:A:285:HIS:N	2.63	0.48
1:A:301:ARG:N	3:A:2020:HOH:O	2.46	0.48
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.39	0.48
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.43	0.48
1:B:274:LYS:N	3:B:2011:HOH:O	2.44	0.48
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.47	0.48
1:A:238:PRO:HD3	3:A:2001:HOH:O	2.14	0.48
1:B:312:ASN:HB3	1:B:319:TYR:OH	2.14	0.48
1:A:266:VAL:O	1:A:300:TYR:HB2	2.13	0.48
1:A:358:MET:O	1:A:414:LYS:HE3	2.14	0.47
1:A:388:GLU:HA	1:A:388:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PRO:HB3	1:B:336:ILE:HD11	1.95	0.47
1:B:275:PHE:HZ	1:B:302:VAL:O	1.97	0.47
1:A:414:LYS:HG2	1:A:418:GLN:NE2	2.29	0.47
1:A:371:GLY:HA2	1:A:403:SER:OG	2.14	0.47
1:B:398:LEU:HD11	1:B:402:GLY:HA2	1.95	0.47
1:A:289:THR:CG2	1:A:290:LYS:N	2.78	0.47
2:D:1:NAG:O6	2:D:8:FUL:H63	2.14	0.47
1:A:283:GLN:CD	1:A:287:ALA:HB2	2.34	0.47
1:B:248:LYS:HD2	3:B:2051:HOH:O	2.15	0.47
1:B:296:TYR:HB3	1:B:297:ASN:H	1.34	0.47
1:A:438:GLN:O	1:A:439:LYS:HD3	2.15	0.47
1:B:368:LEU:HD12	1:B:369:VAL:H	1.79	0.47
1:B:350:THR:HB	1:B:441:LEU:HG	1.95	0.47
1:A:288:LYS:H	1:A:288:LYS:CD	2.27	0.47
1:A:380:GLU:HB3	3:A:2047:HOH:O	2.14	0.46
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.50	0.46
1:B:361:ASN:ND2	1:B:362:GLN:HG3	2.31	0.46
1:A:286:ASN:O	1:A:287:ALA:CB	2.63	0.46
1:B:278:TYR:CE2	1:B:284:VAL:HG22	2.50	0.46
1:B:279:VAL:O	1:B:282:VAL:HG22	2.15	0.46
1:B:432:LEU:HD22	1:B:437:THR:HB	1.97	0.46
1:B:294:GLN:NE2	3:B:2016:HOH:O	2.46	0.46
1:B:322:LYS:HG3	1:B:333:GLU:HG2	1.97	0.46
1:B:432:LEU:HD11	1:B:437:THR:HG22	1.98	0.46
1:B:308:VAL:HG11	1:B:313:TRP:HB2	1.97	0.46
1:A:295:GLN:HA	3:A:2020:HOH:O	2.15	0.46
1:B:344:ARG:O	1:B:372:PHE:HA	2.16	0.46
1:A:296:TYR:HD1	3:A:2020:HOH:O	1.97	0.46
1:B:300:TYR:O	1:B:301:ARG:HB2	2.16	0.45
1:B:300:TYR:O	1:B:301:ARG:CB	2.64	0.45
1:B:345:GLU:HA	1:B:431:ALA:HB3	1.98	0.45
1:A:278:TYR:CD1	1:A:278:TYR:N	2.85	0.45
1:B:242:LEU:HD13	1:B:336:ILE:HG22	1.98	0.45
1:B:269:GLU:C	1:B:271:PRO:HD3	2.36	0.45
1:A:374:PRO:O	1:A:429:HIS:HE1	2.00	0.45
1:A:265:ASP:HA	1:A:299:THR:HB	1.98	0.45
1:A:421:ASN:N	1:A:421:ASN:ND2	2.64	0.45
1:B:238:PRO:CB	1:B:328:LEU:HD13	2.47	0.45
1:B:326:LYS:C	1:B:328:LEU:H	2.20	0.45
1:B:406:LEU:C	1:B:406:LEU:CD1	2.84	0.45
1:A:244:PRO:HB3	1:A:336:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LYS:HE3	1:B:292:ARG:HH12	1.82	0.45
1:B:323:VAL:HG12	1:B:324:SER:N	2.32	0.44
1:B:415:SER:HB3	3:B:2068:HOH:O	2.17	0.44
1:A:291:PRO:O	1:A:292:ARG:HD2	2.17	0.44
1:A:347:GLN:NE2	1:A:349:TYR:OH	2.50	0.44
1:B:239:SER:HB3	1:B:264:VAL:CG2	2.47	0.44
1:B:258:GLU:HA	1:B:308:VAL:HG23	1.99	0.44
1:A:309:LEU:O	1:A:312:ASN:N	2.51	0.44
1:B:279:VAL:O	1:B:280:ASP:HB2	2.17	0.44
1:B:265:ASP:OD2	2:D:1:NAG:H3	2.17	0.44
1:A:278:TYR:HA	1:A:282:VAL:O	2.18	0.44
1:B:301:ARG:HG2	1:B:303:VAL:HG23	1.99	0.43
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.98	0.43
1:B:265:ASP:HA	1:B:299:THR:CB	2.47	0.43
1:B:363:VAL:HG22	1:B:412:VAL:O	2.18	0.43
3:A:2037:HOH:O	1:B:351:LEU:HD22	2.17	0.43
1:A:348:VAL:O	1:A:439:LYS:HG3	2.19	0.43
1:B:238:PRO:HB2	1:B:328:LEU:HD13	2.01	0.43
1:B:278:TYR:HE2	1:B:284:VAL:HG22	1.83	0.43
1:B:414:LYS:O	1:B:418:GLN:HG3	2.18	0.43
1:B:338:LYS:NZ	1:B:430:GLU:OE2	2.52	0.42
1:A:287:ALA:O	1:A:288:LYS:C	2.56	0.42
1:A:384:ASN:CG	1:A:385:GLY:H	2.22	0.42
1:B:357:GLU:C	1:B:359:THR:H	2.23	0.42
1:B:368:LEU:HD12	1:B:369:VAL:N	2.34	0.42
1:B:291:PRO:O	1:B:292:ARG:HB3	2.19	0.42
1:A:264:VAL:O	1:A:265:ASP:HB2	2.18	0.42
1:B:266:VAL:HB	1:B:300:TYR:CD2	2.54	0.42
1:A:394:THR:HA	1:B:397:VAL:HG21	2.02	0.42
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.83	0.42
1:A:386:GLN:HG3	1:A:387:PRO:HD2	2.02	0.42
1:A:283:GLN:C	1:A:285:HIS:H	2.23	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.87	0.42
1:A:369:VAL:HB	1:A:406:LEU:HD12	2.02	0.42
1:B:296:TYR:OH	1:B:301:ARG:NH1	2.46	0.42
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.94	0.42
1:A:336:ILE:HG12	1:A:337:SER:N	2.35	0.42
1:B:350:THR:HB	1:B:441:LEU:CD1	2.50	0.42
1:B:307:THR:HA	3:B:2017:HOH:O	2.20	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CH2	2.55	0.41
1:A:391:TYR:C	1:A:391:TYR:CD2	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:HD2	3:B:2031:HOH:O	2.20	0.41
1:A:274:LYS:HE2	1:A:324:SER:HB2	2.02	0.41
1:B:335:THR:O	1:B:336:ILE:HB	2.21	0.41
2:D:4:MAN:O3	2:D:5:NAG:C1	2.66	0.41
1:A:417:TRP:HH2	1:A:441:LEU:CD2	2.33	0.41
1:B:276:ASN:HB3	1:B:278:TYR:CE1	2.56	0.41
1:A:328:LEU:HD12	1:A:329:PRO:CD	2.50	0.41
1:B:273:VAL:HB	1:B:302:VAL:HG21	2.03	0.41
1:B:325:ASN:HD22	1:B:326:LYS:N	2.15	0.41
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.41
1:B:296:TYR:HE2	2:D:8:FUL:H2	1.86	0.41
1:A:238:PRO:HD2	3:A:2002:HOH:O	2.21	0.41
1:B:311:GLN:N	1:B:311:GLN:NE2	2.53	0.41
1:A:394:THR:HG23	1:A:407:TYR:O	2.22	0.40
1:B:268:HIS:O	1:B:271:PRO:CG	2.68	0.40
1:B:351:LEU:HB2	1:B:366:THR:HB	2.03	0.40
1:A:439:LYS:HD3	1:A:439:LYS:HA	1.91	0.40
1:B:350:THR:HB	1:B:441:LEU:CG	2.51	0.40
1:A:432:LEU:O	1:A:435:HIS:N	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/223 (92%)	175 (85%)	20 (10%)	11 (5%)	2	0
1	B	205/223 (92%)	178 (87%)	17 (8%)	10 (5%)	2	0
All	All	411/446 (92%)	353 (86%)	37 (9%)	21 (5%)	2	0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	287	ALA
1	A	289	THR
1	A	433	HIS
1	B	298	SER
1	B	301	ARG
1	A	267	SER
1	A	298	SER
1	B	271	PRO
1	A	293	GLU
1	B	282	VAL
1	B	291	PRO
1	B	293	GLU
1	A	286	ASN
1	A	358	MET
1	A	385	GLY
1	B	283	GLN
1	B	295	GLN
1	B	327	ALA
1	B	336	ILE
1	A	290	LYS

### 5.3.2 Protein sidechains ⓘ

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	A	193/206 (94%)	187 (97%)	6 (3%)	40	52
1	B	192/206 (93%)	180 (94%)	12 (6%)	18	23
All	All	385/412 (93%)	367 (95%)	18 (5%)	26	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	VAL
1	A	292	ARG
1	A	406	LEU

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Mol	Chain	Res	Type
1	A	413	ASP
1	A	436	TYR
1	A	441	LEU
1	B	255	ARG
1	B	260	THR
1	B	278	TYR
1	B	288	LYS
1	B	291	PRO
1	B	296	TYR
1	B	311	GLN
1	B	370	LYS
1	B	394	THR
1	B	399	ASP
1	B	406	LEU
1	B	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	283	GLN
1	A	311	GLN
1	A	325	ASN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	A	429	HIS
1	B	272	GLN
1	B	276	ASN
1	B	283	GLN
1	B	286	ASN
1	B	311	GLN
1	B	312	ASN
1	B	325	ASN
1	B	342	GLN
1	B	361	ASN
1	B	389	ASN
1	B	390	ASN
1	B	419	GLN

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Mol	Chain	Res	Type
1	B	429	HIS
1	B	434	ASN
1	B	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

16 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.58	0	17,19,21	1.18	2 (11%)
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.70	0
2	BMA	C	3	2	11,11,12	0.53	0	15,15,17	0.55	0
2	MAN	C	4	2	11,11,12	0.48	0	15,15,17	0.60	0
2	NAG	C	5	2	14,14,15	0.50	0	17,19,21	0.62	0
2	MAN	C	6	2	11,11,12	0.45	0	15,15,17	0.67	0
2	NAG	C	7	2	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
2	FUL	C	8	2	10,10,11	0.63	0	14,14,16	0.57	0
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
2	BMA	D	3	2	11,11,12	0.40	0	15,15,17	0.53	0
2	MAN	D	4	2	11,11,12	0.78	0	15,15,17	0.69	0
2	NAG	D	5	2	14,14,15	0.70	0	17,19,21	0.58	0
2	MAN	D	6	2	11,11,12	0.54	0	15,15,17	0.65	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	7	2	14,14,15	0.52	0	17,19,21	0.77	1 (5%)
2	FUL	D	8	2	10,10,11	0.65	0	14,14,16	0.91	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	NAG	C	7	2	-	0/6/23/26	0/1/1/1
2	FUL	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	NAG	D	5	2	1/1/5/7	5/6/23/26	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
2	NAG	D	7	2	-	4/6/23/26	0/1/1/1
2	FUL	D	8	2	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	-2.64	107.15	111.02
2	C	7	NAG	C2-N2-C7	-2.27	119.68	122.90
2	D	6	MAN	C1-O5-C5	2.26	115.26	112.19
2	C	1	NAG	C1-O5-C5	2.21	115.19	112.19
2	D	7	NAG	C2-N2-C7	-2.16	119.83	122.90
2	D	8	FUL	C3-C4-C5	2.15	113.11	109.77
2	D	1	NAG	C1-O5-C5	2.05	114.97	112.19
2	D	2	NAG	C2-N2-C7	-2.02	120.02	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	5	NAG	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	C	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	5	NAG	C1-C2-N2-C7
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	D	7	NAG	C8-C7-N2-C2
2	D	7	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	6	MAN	O5-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6
2	D	7	NAG	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	4	MAN	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
2	D	5	NAG	C4-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 18 short contacts:

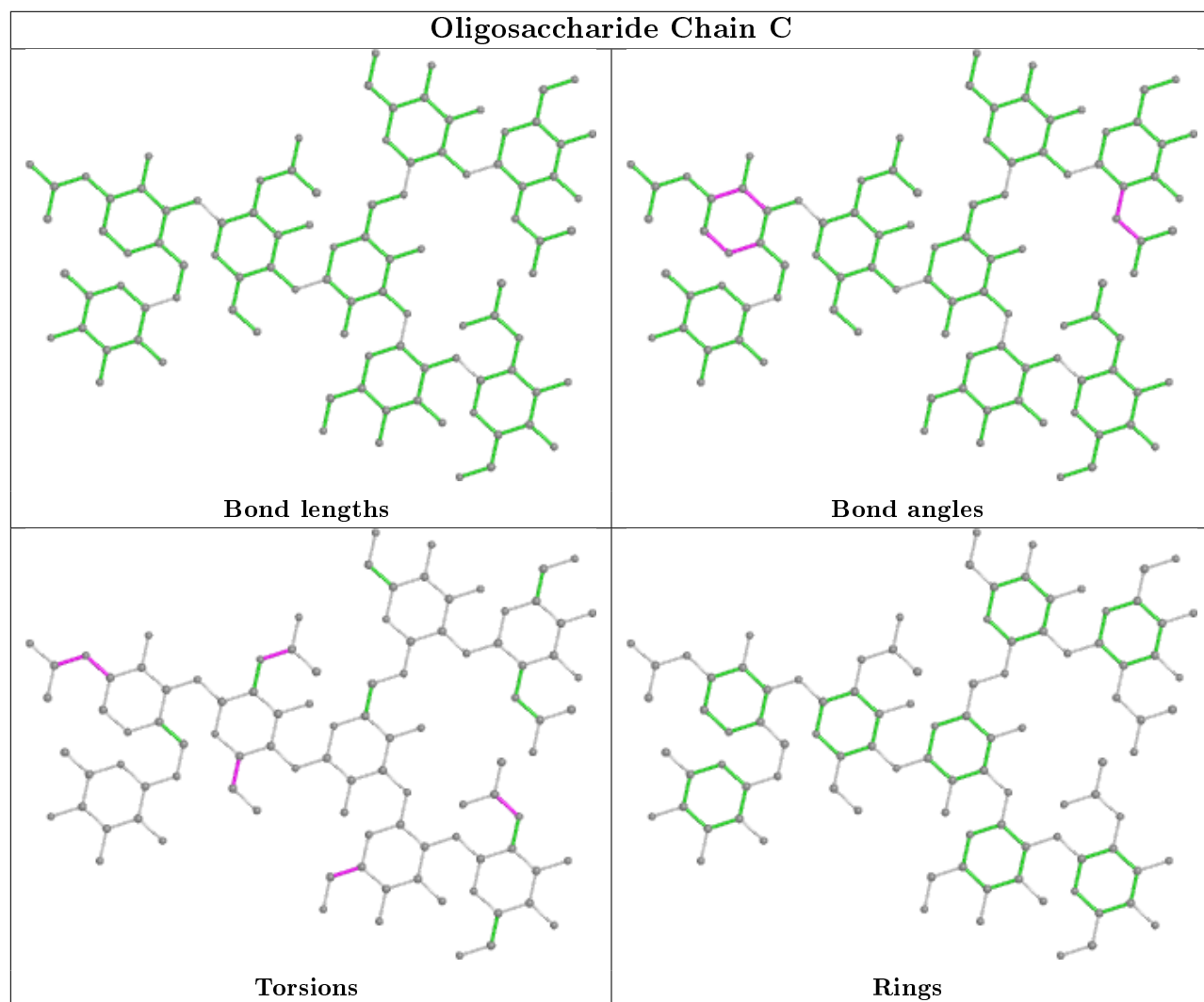
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	7	0

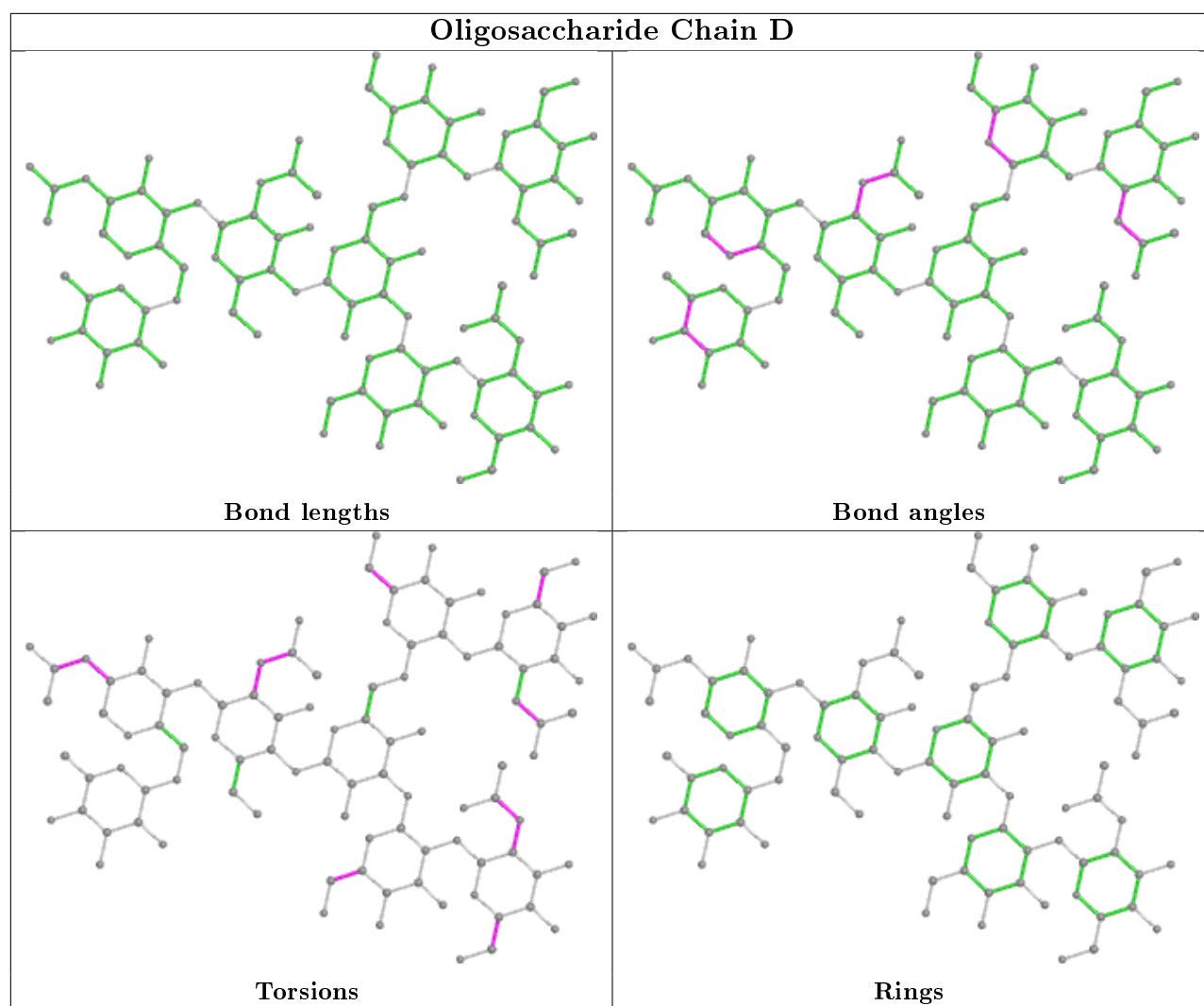
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	NAG	1	0
2	D	6	MAN	2	0
2	D	3	BMA	1	0
2	C	8	FUL	2	0
2	C	2	NAG	1	0
2	D	5	NAG	3	0
2	D	4	MAN	3	0
2	D	7	NAG	2	0
2	D	8	FUL	2	0
2	D	2	NAG	3	0
2	C	6	MAN	1	0

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](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/223 (93%)	0.59	11 (5%) 26 23	19, 39, 70, 85	0
1	B	207/223 (92%)	1.20	44 (21%) 0 0	17, 49, 100, 100	0
All	All	415/446 (93%)	0.89	55 (13%) 3 2	17, 43, 99, 100	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	HIS	9.6
1	B	286	ASN	8.5
1	B	300	TYR	8.4
1	B	272	GLN	7.4
1	B	296	TYR	6.9
1	B	289	THR	5.1
1	B	276	ASN	5.1
1	B	295	GLN	5.0
1	B	299	THR	5.0
1	B	240	VAL	4.8
1	B	239	SER	4.4
1	B	284	VAL	4.4
1	B	273	VAL	4.1
1	B	324	SER	4.0
1	B	293	GLU	3.8
1	B	303	VAL	3.6
1	B	302	VAL	3.4
1	B	294	GLN	3.4
1	B	328	LEU	3.3
1	B	266	VAL	3.2
1	B	238	PRO	3.1
1	A	327	ALA	3.1
1	B	326	LYS	3.1
1	B	291	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	3.0
1	B	327	ALA	3.0
1	A	266	VAL	2.9
1	B	263	VAL	2.9
1	B	267	SER	2.9
1	B	275	PHE	2.9
1	B	270	ASP	2.9
1	B	268	HIS	2.9
1	B	241	PHE	2.8
1	B	271	PRO	2.8
1	B	269	GLU	2.8
1	B	319	TYR	2.8
1	A	285	HIS	2.8
1	B	298	SER	2.6
1	A	286	ASN	2.5
1	B	274	LYS	2.5
1	B	278	TYR	2.5
1	B	264	VAL	2.4
1	A	269	GLU	2.4
1	B	288	LYS	2.3
1	A	441	LEU	2.3
1	B	287	ALA	2.2
1	B	330	ALA	2.2
1	B	301	ARG	2.1
1	A	240	VAL	2.1
1	A	296	TYR	2.1
1	A	299	THR	2.0
1	A	328	LEU	2.0
1	B	329	PRO	2.0
1	B	389	ASN	2.0
1	B	281	GLY	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](#)

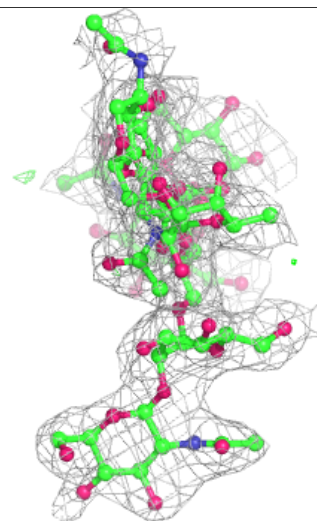
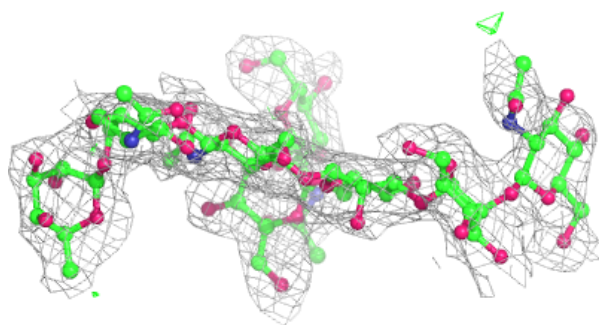
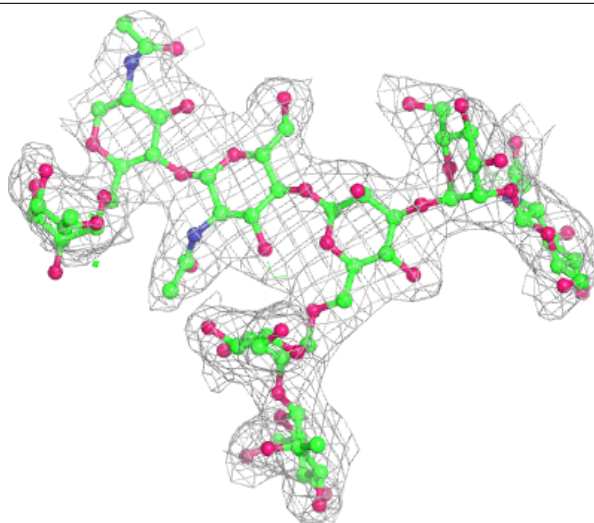
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

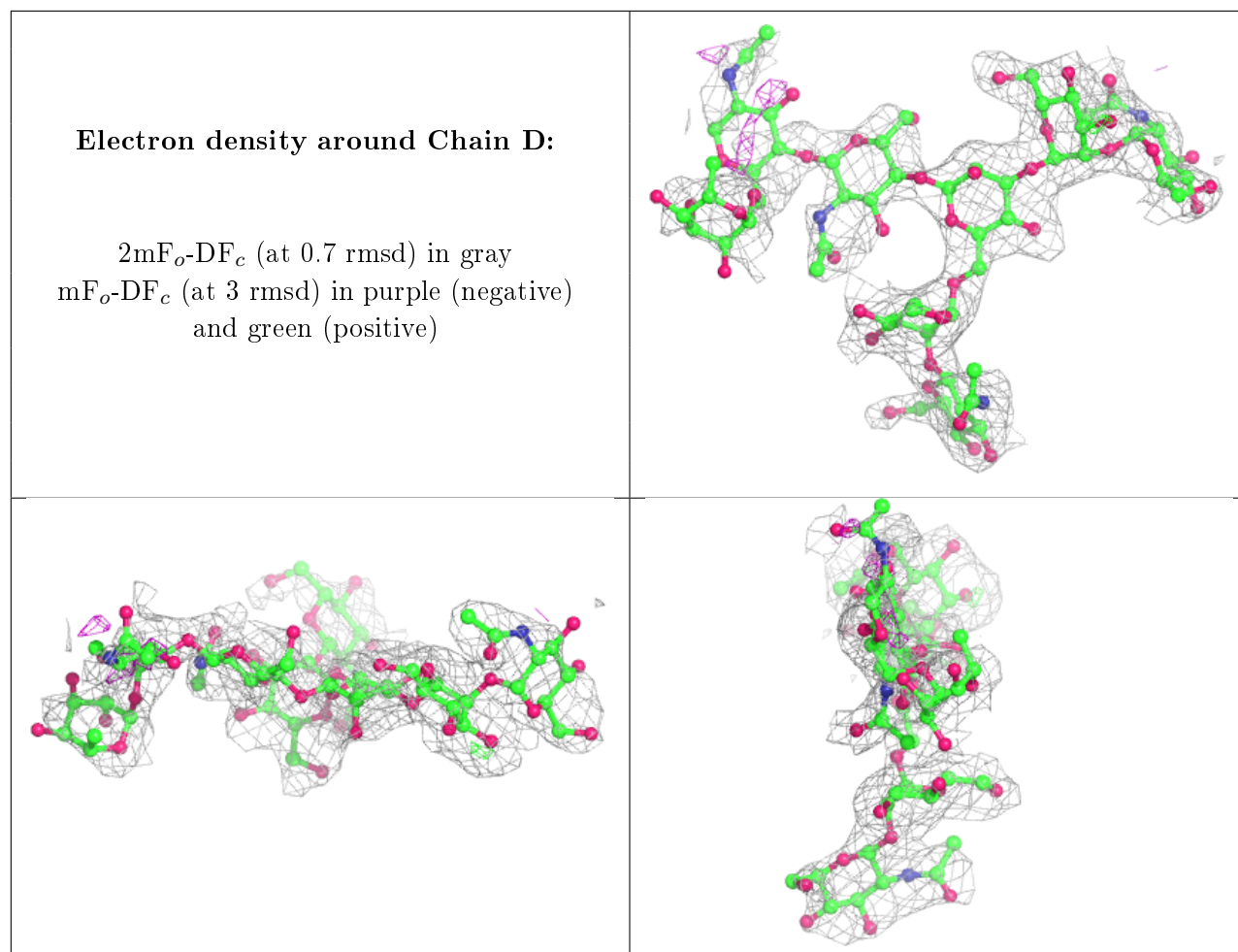
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	1	14/15	0.58	0.54	98,99,100,100	0
2	NAG	D	5	14/15	0.64	0.27	93,95,96,97	0
2	MAN	D	4	11/12	0.64	0.20	78,82,85,89	0
2	FUL	C	8	10/11	0.69	0.24	64,67,69,69	0
2	NAG	D	2	14/15	0.71	0.33	92,97,98,99	0
2	NAG	D	7	14/15	0.72	0.26	77,79,83,83	0
2	NAG	C	5	14/15	0.74	0.24	77,81,82,82	0
2	BMA	D	3	11/12	0.78	0.18	82,85,87,89	0
2	MAN	D	6	11/12	0.81	0.14	78,79,80,80	0
2	FUL	D	8	10/11	0.82	0.42	98,100,100,100	0
2	NAG	C	7	14/15	0.84	0.21	57,61,64,64	0
2	MAN	C	4	11/12	0.85	0.17	61,64,67,72	0
2	NAG	C	1	14/15	0.88	0.21	46,56,61,62	0
2	BMA	C	3	11/12	0.92	0.15	45,47,50,55	0
2	NAG	C	2	14/15	0.93	0.16	42,45,47,48	0
2	MAN	C	6	11/12	0.95	0.15	43,47,48,51	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.

**Electron density around Chain C:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.