



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2019 – 05:04 PM EST

PDB ID : 6D4M  
Title : Crystal Structure of a Fc Fragment of Rhesus macaque (*Macaca mulatta*) IgG3  
Authors : Gohain, N.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2018-04-18  
Resolution : 3.47 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

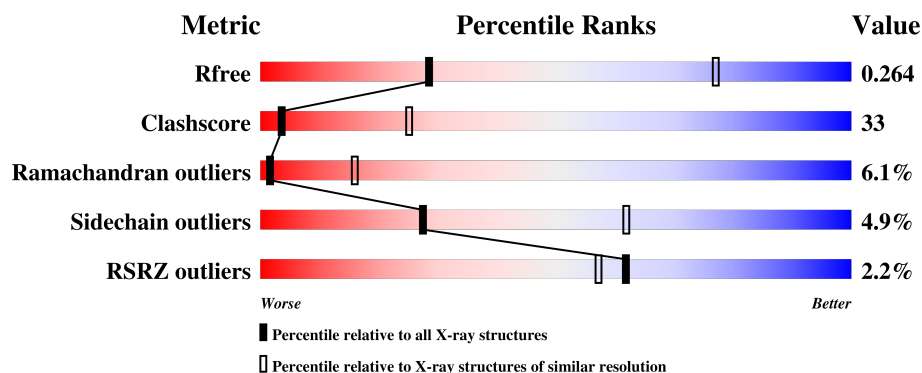
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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))
$R_{free}$	111664	1159 (3.56-3.40)
Clashscore	122126	1235 (3.56-3.40)
Ramachandran outliers	120053	1202 (3.56-3.40)
Sidechain outliers	120020	1203 (3.56-3.40)
RSRZ outliers	108989	1080 (3.56-3.40)

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. 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	224	<div> <div>2%</div> <div>33%</div> <div>55%</div> <div>7%</div> </div>
1	B	224	<div> <div>2%</div> <div>35%</div> <div>52%</div> <div>6%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

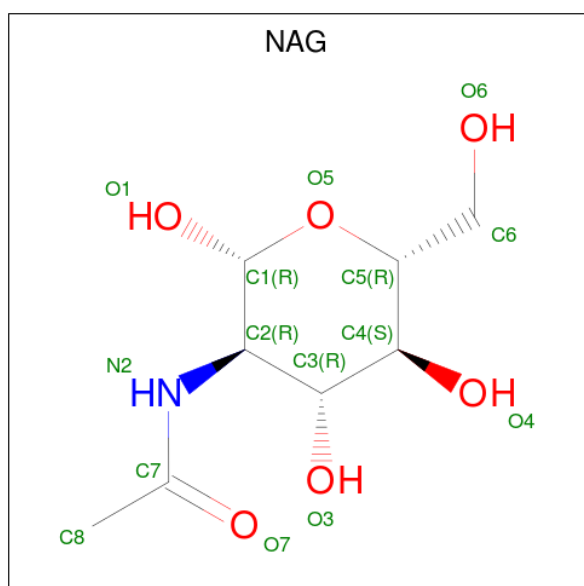
There are 5 unique types of molecules in this entry. The entry contains 3518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fc fragment of IgG3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1658	1052	278	322	6			
1	B	209	Total	C	N	O	S	0	0	0
			1662	1054	279	323	6			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



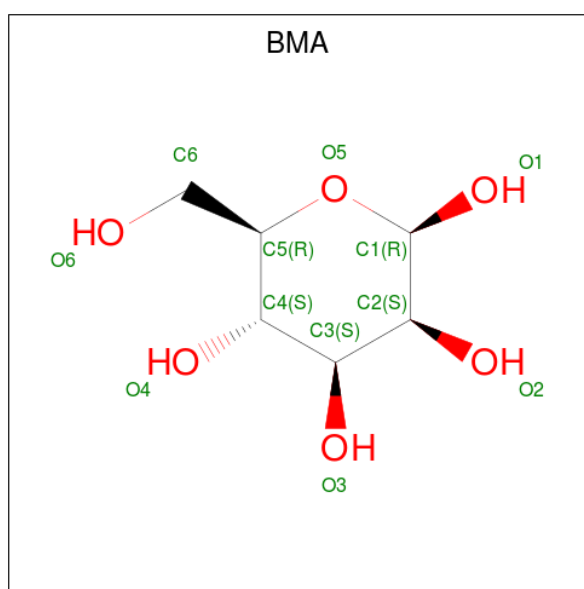
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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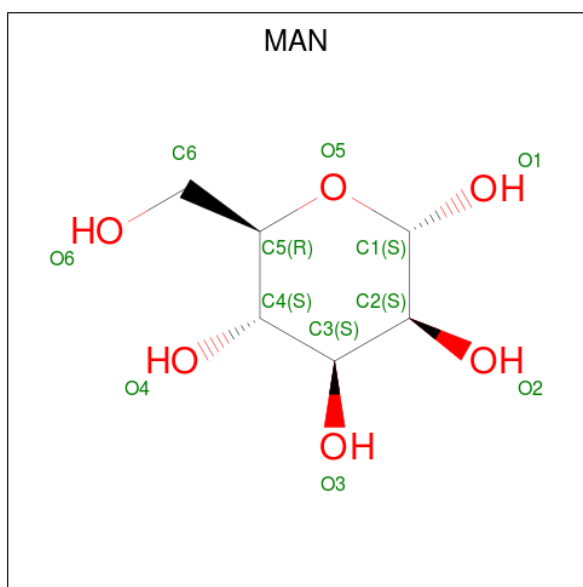
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



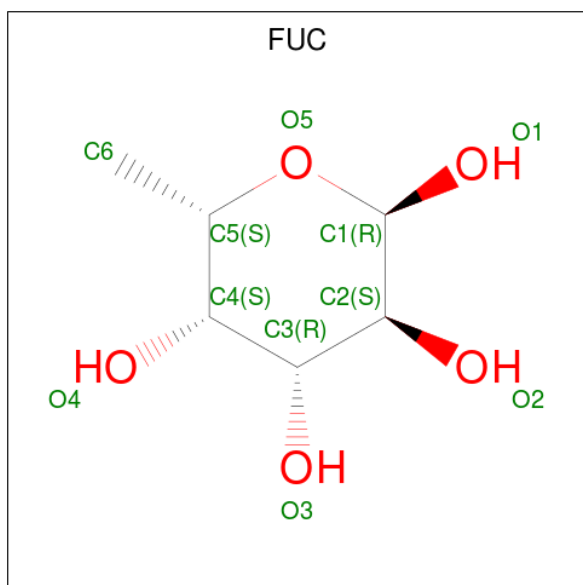
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).

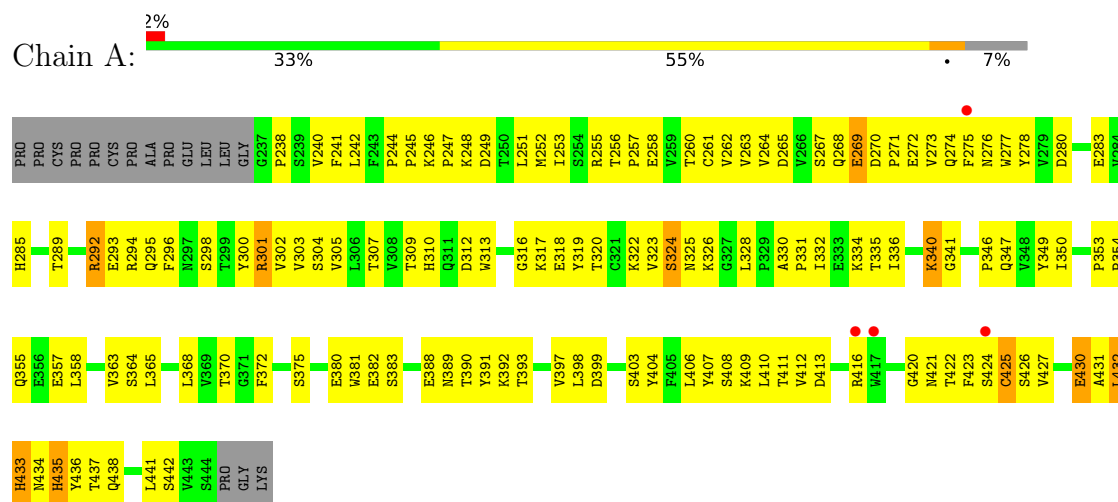


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

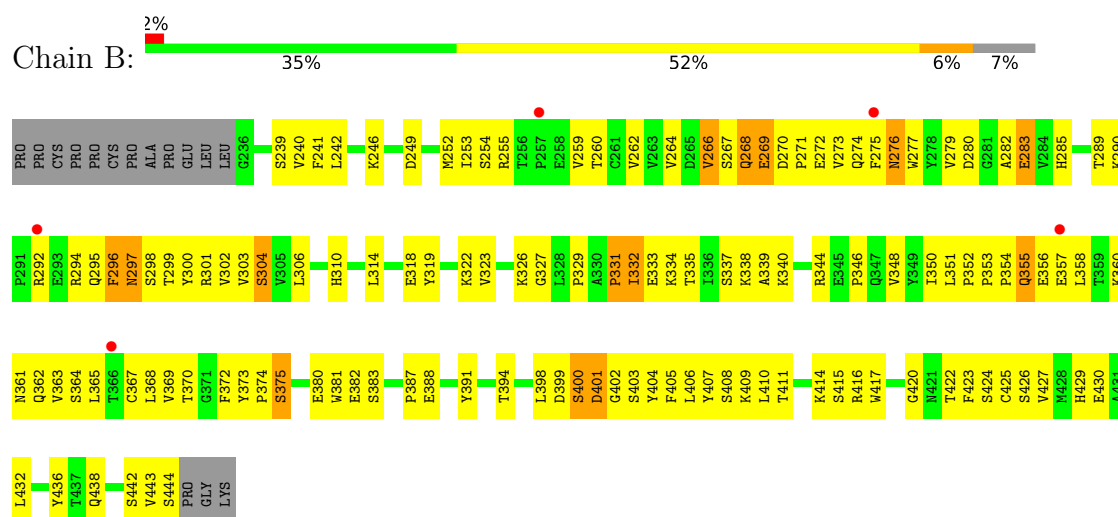
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Fc fragment of IgG3



#### • Molecule 1: Fc fragment of IgG3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.87Å 65.87Å 89.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.11 – 3.47 35.11 – 3.47	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.11-3.47) 94.9 (35.11-3.47)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???), REFMAC	Depositor
R, $R_{free}$	0.249 , 0.270 0.250 , 0.264	Depositor DCC
$R_{free}$ test set	293 reflections (5.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 89.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l 0.308 for h,-h-k,-l 0.098 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: FUC, 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	0.32	0/1705	0.55	0/2329
1	B	0.32	0/1709	0.56	0/2334
All	All	0.32	0/3414	0.56	0/4663

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1658	0	1607	115	1
1	B	1662	0	1610	123	1
2	A	56	0	49	2	0
2	B	56	0	49	1	0
3	A	11	0	8	0	0
3	B	11	0	8	1	0
4	A	22	0	18	0	0
4	B	22	0	18	0	0
5	A	10	0	10	0	0
5	B	10	0	10	1	0
All	All	3518	0	3387	231	2

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 33.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:PRO:O	1:A:325:ASN:ND2	1.84	1.10
1:A:273:VAL:HG12	1:A:325:ASN:HB2	1.53	0.90
1:B:363:VAL:HG23	1:B:414:LYS:HB2	1.57	0.87
1:B:240:VAL:HG21	1:B:332:ILE:HG12	1.57	0.86
1:A:273:VAL:HG12	1:A:325:ASN:CB	2.07	0.84
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.59	0.82
1:B:416:ARG:HH21	1:B:423:PHE:HE1	1.22	0.81
1:A:317:LYS:HB2	1:A:319:TYR:HE2	1.45	0.81
1:A:364:SER:HA	1:A:410:LEU:O	1.80	0.81
1:B:363:VAL:CG2	1:B:414:LYS:HB2	2.12	0.80
1:B:273:VAL:HB	1:B:323:VAL:HG13	1.63	0.78
1:A:340:LYS:HE3	1:A:341:GLY:H	1.49	0.77
1:B:348:VAL:HG22	1:B:369:VAL:HG22	1.66	0.77
1:B:422:THR:HA	1:B:442:SER:HB3	1.67	0.77
1:B:416:ARG:NH2	1:B:423:PHE:HE1	1.85	0.75
1:B:240:VAL:HG11	1:B:332:ILE:HD13	1.69	0.75
1:B:442:SER:OG	1:B:443:VAL:N	2.17	0.75
1:A:365:LEU:O	1:A:409:LYS:HA	1.86	0.75
1:B:275:PHE:HB3	1:B:277:TRP:HE1	1.52	0.75
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.69	0.74
1:A:409:LYS:NZ	1:A:411:THR:OG1	2.21	0.74
1:B:314:LEU:HA	1:B:338:LYS:HE2	1.70	0.74
1:B:268:GLN:HG2	1:B:269:GLU:H	1.53	0.73
1:B:271:PRO:HD2	1:B:326:LYS:HB3	1.70	0.73
1:B:242:LEU:HD22	1:B:334:LYS:HB3	1.69	0.72
1:A:317:LYS:HB2	1:A:319:TYR:CE2	2.24	0.72
1:B:403:SER:OG	1:B:404:TYR:N	2.20	0.71
1:A:241:PHE:O	1:A:262:VAL:HB	1.91	0.71
1:A:242:LEU:HD11	1:A:336:ILE:HG21	1.73	0.71
1:A:273:VAL:CG1	1:A:325:ASN:HB2	2.21	0.70
1:A:349:TYR:HB3	1:B:354:PRO:HG3	1.71	0.70
1:B:249:ASP:HA	1:B:255:ARG:HD3	1.72	0.70
1:A:253:ILE:HA	1:A:310:HIS:CE1	2.27	0.69
1:A:264:VAL:HG11	2:A:501:NAG:H5	1.75	0.69
1:A:397:VAL:HG21	1:B:394:THR:HA	1.75	0.68
1:B:331:PRO:O	1:B:333:GLU:N	2.23	0.68
1:B:372:PHE:N	1:B:403:SER:OG	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.29	0.67
1:A:268:GLN:O	1:A:270:ASP:N	2.27	0.67
1:A:355:GLN:HA	1:A:358:LEU:HD12	1.76	0.67
1:B:268:GLN:OE1	1:B:268:GLN:N	2.21	0.66
1:B:367:CYS:HB3	1:B:408:SER:HB3	1.76	0.66
1:A:422:THR:HB	1:A:442:SER:HB3	1.78	0.66
1:B:275:PHE:HB3	1:B:277:TRP:NE1	2.11	0.64
1:A:264:VAL:HG12	1:A:265:ASP:H	1.63	0.64
1:A:347:GLN:HB2	1:A:370:THR:HG23	1.79	0.64
1:A:347:GLN:HB3	1:A:349:TYR:CE2	2.34	0.63
1:A:309:THR:OG1	1:A:312:ASP:OD2	2.17	0.63
1:A:430:GLU:O	1:A:435:HIS:ND1	2.32	0.63
1:A:257:PRO:HD3	1:A:310:HIS:CE1	2.34	0.62
1:A:410:LEU:HG	1:A:412:VAL:HG13	1.80	0.62
1:B:399:ASP:HB2	1:B:405:PHE:HD1	1.62	0.62
1:B:400:SER:O	1:B:402:GLY:N	2.28	0.62
1:A:268:GLN:N	1:A:268:GLN:OE1	2.33	0.62
1:B:266:VAL:HG12	1:B:267:SER:H	1.64	0.62
1:A:324:SER:O	1:A:324:SER:OG	2.17	0.61
1:A:434:ASN:O	1:A:436:TYR:N	2.33	0.61
1:A:392:LYS:O	1:A:408:SER:OG	2.14	0.60
1:A:262:VAL:HG22	1:A:303:VAL:HG12	1.84	0.60
1:B:416:ARG:NH2	1:B:423:PHE:CE1	2.59	0.60
1:B:252:MET:SD	1:B:253:ILE:N	2.75	0.59
1:A:413:ASP:OD2	1:A:416:ARG:NE	2.35	0.59
1:B:239:SER:HB3	1:B:264:VAL:HG23	1.82	0.59
1:B:302:VAL:HG12	1:B:303:VAL:H	1.67	0.59
1:B:267:SER:HB2	1:B:270:ASP:OD2	2.03	0.59
1:A:257:PRO:HD3	1:A:310:HIS:NE2	2.17	0.59
1:B:367:CYS:HB2	1:B:381:TRP:HZ2	1.67	0.59
1:A:280:ASP:OD1	1:A:318:GLU:N	2.35	0.58
1:A:353:PRO:HD3	1:A:365:LEU:HD21	1.85	0.58
1:B:436:TYR:OH	1:B:438:GLN:OE1	2.15	0.58
1:A:244:PRO:HB3	1:A:336:ILE:HD11	1.85	0.58
1:B:294:ARG:O	1:B:295:GLN:NE2	2.37	0.58
1:A:253:ILE:HA	1:A:310:HIS:NE2	2.19	0.57
1:A:293:GLU:N	1:A:301:ARG:O	2.37	0.57
1:B:351:LEU:O	1:B:365:LEU:HD23	2.04	0.57
1:B:260:THR:HA	1:B:304:SER:O	2.04	0.57
1:A:283:GLU:HG2	1:A:285:HIS:HE1	1.70	0.57
1:B:372:PHE:HE1	1:B:375:SER:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:O	1:B:335:THR:OG1	2.14	0.56
1:B:350:ILE:HD11	1:B:425:CYS:H	1.71	0.56
1:A:246:LYS:HD3	1:A:248:LYS:HE3	1.88	0.56
1:B:241:PHE:CE2	3:B:503:BMA:H2	2.41	0.56
1:B:268:GLN:CD	1:B:268:GLN:H	2.06	0.55
1:B:322:LYS:HD2	1:B:331:PRO:HB2	1.89	0.55
1:B:270:ASP:O	1:B:292:ARG:NH1	2.40	0.55
1:B:360:LYS:HG2	1:B:362:GLN:O	2.06	0.55
1:B:382:GLU:HG3	1:B:387:PRO:HA	1.89	0.55
1:A:249:ASP:CG	1:A:255:ARG:HD3	2.27	0.55
1:B:249:ASP:OD1	1:B:255:ARG:HB2	2.07	0.55
1:B:259:VAL:HB	1:B:306:LEU:HB3	1.89	0.54
1:A:280:ASP:OD2	1:A:317:LYS:HB3	2.08	0.54
1:B:276:ASN:HB2	1:B:322:LYS:HE3	1.89	0.54
1:A:397:VAL:HG21	1:B:394:THR:HG22	1.90	0.54
1:B:295:GLN:O	1:B:298:SER:N	2.41	0.53
1:A:381:TRP:CZ2	1:A:408:SER:HB3	2.44	0.53
1:A:273:VAL:HG12	1:A:325:ASN:HB3	1.87	0.53
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.91	0.52
1:B:246:LYS:HG3	1:B:249:ASP:HB2	1.90	0.52
1:B:363:VAL:O	1:B:411:THR:HA	2.08	0.52
1:B:401:ASP:OD1	1:B:401:ASP:N	2.43	0.52
1:B:364:SER:HA	1:B:410:LEU:O	2.10	0.52
1:A:381:TRP:CE3	1:A:410:LEU:HB2	2.44	0.52
1:A:273:VAL:HG11	1:A:323:VAL:HG13	1.90	0.52
1:A:350:ILE:HD11	1:A:425:CYS:HB2	1.92	0.52
1:A:433:HIS:ND1	1:A:434:ASN:OD1	2.43	0.52
1:B:253:ILE:HA	1:B:310:HIS:NE2	2.25	0.51
1:A:382:GLU:OE2	1:A:426:SER:OG	2.25	0.51
1:A:426:SER:HB3	1:A:436:TYR:CE1	2.46	0.51
1:A:399:ASP:HB3	1:A:403:SER:O	2.11	0.51
1:B:346:PRO:HG2	1:B:432:LEU:HD21	1.93	0.51
1:A:349:TYR:CB	1:B:354:PRO:HG3	2.41	0.50
1:A:372:PHE:HE2	1:A:375:SER:HA	1.76	0.50
1:A:409:LYS:HB2	1:B:407:TYR:OH	2.11	0.50
1:B:354:PRO:HD2	1:B:357:GLU:OE1	2.12	0.50
1:B:346:PRO:HG3	1:B:429:HIS:HD2	1.77	0.50
1:B:374:PRO:HD2	1:B:429:HIS:HE1	1.76	0.50
1:A:263:VAL:HB	1:A:302:VAL:HG22	1.93	0.50
1:A:383:SER:HA	1:A:423:PHE:HD1	1.77	0.50
1:B:394:THR:OG1	1:B:407:TYR:O	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HA	1:A:310:HIS:CE1	2.47	0.49
1:A:292:ARG:HA	1:A:302:VAL:HG12	1.93	0.49
1:A:425:CYS:O	1:A:438:GLN:HA	2.12	0.49
1:A:278:TYR:HB2	1:A:320:THR:OG1	2.12	0.49
1:B:355:GLN:N	1:B:355:GLN:OE1	2.45	0.49
1:B:275:PHE:HE2	1:B:289:THR:HG23	1.77	0.49
1:A:364:SER:HB2	1:A:409:LYS:HG3	1.94	0.49
1:A:325:ASN:OD1	1:A:326:LYS:O	2.30	0.49
1:A:247:PRO:O	1:A:251:LEU:HG	2.13	0.49
1:B:363:VAL:HG21	1:B:414:LYS:HB2	1.93	0.48
1:A:245:PRO:HG3	1:A:257:PRO:HB2	1.95	0.48
1:A:289:THR:HG23	1:A:304:SER:HB2	1.95	0.48
1:A:398:LEU:HD12	1:A:399:ASP:H	1.78	0.48
1:A:422:THR:OG1	1:A:423:PHE:N	2.46	0.48
1:B:253:ILE:HA	1:B:310:HIS:CE1	2.48	0.48
1:A:380:GLU:C	1:A:381:TRP:HD1	2.17	0.48
1:B:297:ASN:OD1	1:B:299:THR:OG1	2.27	0.48
1:B:290:LYS:HE2	1:B:303:VAL:HG21	1.96	0.48
1:B:398:LEU:HD12	1:B:403:SER:O	2.14	0.48
1:A:275:PHE:CD1	1:A:304:SER:HB3	2.49	0.48
1:B:368:LEU:HD13	1:B:407:TYR:CE1	2.49	0.48
1:A:252:MET:O	1:A:310:HIS:NE2	2.46	0.48
1:B:369:VAL:HB	1:B:406:LEU:HD12	1.95	0.47
1:B:277:TRP:CZ3	1:B:306:LEU:HD22	2.49	0.47
1:A:278:TYR:O	1:A:320:THR:OG1	2.32	0.47
1:A:258:GLU:HB3	1:A:305:VAL:HG13	1.97	0.47
1:B:383:SER:HB3	1:B:423:PHE:CD1	2.50	0.47
1:B:361:ASN:O	1:B:414:LYS:HB3	2.15	0.47
1:A:294:ARG:O	1:A:295:GLN:NE2	2.41	0.46
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.51	0.46
1:B:318:GLU:HG2	1:B:337:SER:HB2	1.96	0.46
1:A:289:THR:HA	1:A:304:SER:HA	1.98	0.46
1:A:273:VAL:HG11	1:A:323:VAL:CG1	2.46	0.46
1:B:274:GLN:O	1:B:323:VAL:HA	2.14	0.46
1:B:296:PHE:C	1:B:298:SER:H	2.18	0.46
1:B:362:GLN:O	1:B:363:VAL:HG23	2.16	0.46
1:A:368:LEU:HD12	1:A:407:TYR:CE1	2.50	0.46
1:A:427:VAL:HB	1:A:437:THR:HG22	1.98	0.46
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.97	0.46
1:A:242:LEU:HB2	1:A:260:THR:O	2.16	0.46
1:A:388:GLU:O	1:A:391:TYR:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLU:HG2	1:B:410:LEU:HD11	1.99	0.45
1:A:238:PRO:HD2	1:A:328:LEU:HG	1.97	0.45
1:B:318:GLU:OE1	1:B:337:SER:HB2	2.16	0.45
1:B:352:PRO:HA	1:B:365:LEU:CD2	2.46	0.45
1:B:399:ASP:HB2	1:B:405:PHE:CD1	2.48	0.45
1:B:273:VAL:CB	1:B:323:VAL:HG13	2.41	0.45
1:A:267:SER:OG	1:A:268:GLN:OE1	2.25	0.45
1:A:274:GLN:N	1:A:324:SER:OG	2.46	0.45
1:B:262:VAL:HG12	1:B:264:VAL:HG13	1.99	0.45
1:B:283:GLU:O	1:B:285:HIS:NE2	2.49	0.45
1:B:417:TRP:CZ2	1:B:443:VAL:HG22	2.52	0.45
1:A:301:ARG:HG2	1:A:302:VAL:N	2.31	0.45
1:B:337:SER:OG	1:B:338:LYS:N	2.50	0.45
1:B:292:ARG:HB3	1:B:300:TYR:CD1	2.52	0.45
1:B:372:PHE:CE1	1:B:404:TYR:HB2	2.53	0.44
1:B:344:ARG:HB2	1:B:373:TYR:H	1.82	0.44
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.78	0.44
1:A:313:TRP:C	1:A:316:GLY:H	2.21	0.44
1:A:350:ILE:HD11	1:A:425:CYS:CB	2.47	0.44
1:B:295:GLN:HB2	1:B:299:THR:OG1	2.17	0.44
1:A:349:TYR:HE1	1:B:356:GLU:HG2	1.82	0.44
1:A:430:GLU:O	1:A:432:LEU:N	2.49	0.44
1:B:279:VAL:H	1:B:282:ALA:H	1.65	0.44
1:B:301:ARG:NH1	2:B:502:NAG:H81	2.32	0.44
1:B:279:VAL:HG22	1:B:319:TYR:CD2	2.53	0.44
1:B:338:LYS:O	1:B:340:LYS:N	2.51	0.44
1:B:414:LYS:O	1:B:417:TRP:HB3	2.18	0.43
1:A:325:ASN:OD1	1:A:326:LYS:C	2.57	0.43
1:B:290:LYS:HE2	1:B:303:VAL:CG2	2.48	0.43
1:A:436:TYR:CE2	1:A:438:GLN:HB3	2.53	0.43
1:B:279:VAL:HG22	1:B:319:TYR:HD2	1.83	0.43
1:B:369:VAL:HG21	1:B:427:VAL:HG11	2.00	0.43
1:A:275:PHE:CG	1:A:304:SER:HB3	2.53	0.43
1:B:370:THR:HG22	1:B:405:PHE:HB2	2.00	0.43
1:A:393:THR:HG23	1:A:407:TYR:O	2.19	0.43
1:B:255:ARG:HG2	1:B:255:ARG:H	1.59	0.43
1:B:270:ASP:OD2	1:B:327:GLY:HA2	2.19	0.43
1:B:239:SER:HB3	1:B:264:VAL:CG2	2.49	0.43
1:B:372:PHE:CE1	1:B:375:SER:HA	2.53	0.42
1:A:268:GLN:HG3	1:A:300:TYR:CE2	2.54	0.42
1:A:275:PHE:HZ	1:A:302:VAL:HG23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ALA:HB1	1:A:331:PRO:HD2	2.00	0.42
1:A:375:SER:HB3	1:A:404:TYR:CD1	2.54	0.42
1:B:425:CYS:O	1:B:438:GLN:HB2	2.18	0.42
1:A:382:GLU:OE2	1:A:424:SER:OG	2.18	0.42
1:B:381:TRP:HA	1:B:424:SER:O	2.19	0.42
1:A:382:GLU:HG2	1:A:424:SER:HB3	2.02	0.42
1:B:270:ASP:CG	1:B:327:GLY:HA2	2.40	0.42
1:A:268:GLN:HG3	1:A:300:TYR:HE2	1.85	0.42
1:B:422:THR:CA	1:B:442:SER:HB3	2.44	0.42
1:A:270:ASP:O	1:A:325:ASN:ND2	2.52	0.42
1:A:256:THR:OG1	1:A:307:THR:HB	2.19	0.42
1:B:367:CYS:HB2	1:B:381:TRP:CE2	2.55	0.42
1:A:340:LYS:HE3	1:A:341:GLY:N	2.25	0.42
1:A:312:ASP:O	1:A:317:LYS:HG2	2.20	0.42
1:A:407:TYR:OH	1:B:409:LYS:HB2	2.20	0.41
1:B:353:PRO:HG3	1:B:364:SER:O	2.20	0.41
1:B:382:GLU:CG	1:B:387:PRO:HA	2.49	0.41
1:B:296:PHE:HB2	5:B:508:FUC:H63	2.02	0.41
1:A:296:PHE:C	1:A:298:SER:H	2.23	0.41
1:A:319:TYR:O	1:A:335:THR:HA	2.21	0.41
1:B:275:PHE:HB3	1:B:277:TRP:CD1	2.55	0.41
1:A:241:PHE:HZ	2:A:505:NAG:H82	1.85	0.41
1:B:276:ASN:OD1	1:B:276:ASN:N	2.53	0.41
1:A:240:VAL:HB	1:A:332:ILE:HG21	2.02	0.41
1:A:275:PHE:CZ	1:A:302:VAL:HG23	2.56	0.41
1:A:322:LYS:HG3	1:A:323:VAL:N	2.35	0.40
1:A:357:GLU:HB3	1:A:363:VAL:HG13	2.03	0.40
1:B:338:LYS:HE3	1:B:338:LYS:HB3	1.89	0.40
1:B:344:ARG:HG3	1:B:373:TYR:HB3	2.04	0.40
1:B:380:GLU:HB2	1:B:426:SER:OG	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLN:OE1	1:B:444:SER:OG[1_565]	2.09	0.11
1:A:334:LYS:NZ	1:A:413:ASP:OD2[2_554]	2.16	0.04

## 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	206/224 (92%)	153 (74%)	45 (22%)	8 (4%)	3	27
1	B	207/224 (92%)	151 (73%)	39 (19%)	17 (8%)	1	10
All	All	413/448 (92%)	304 (74%)	84 (20%)	25 (6%)	1	16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLU
1	B	339	ALA
1	B	358	LEU
1	B	401	ASP
1	A	390	THR
1	A	430	GLU
1	A	431	ALA
1	B	266	VAL
1	B	272	GLU
1	B	280	ASP
1	B	332	ILE
1	B	420	GLY
1	A	435	HIS
1	B	268	GLN
1	B	283	GLU
1	B	331	PRO
1	B	430	GLU
1	A	433	HIS
1	B	329	PRO
1	B	415	SER
1	A	354	PRO
1	B	297	ASN
1	B	400	SER
1	B	296	PHE
1	A	420	GLY



### 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%)	181 (94%)	12 (6%)	20	55
1	B	193/206 (94%)	186 (96%)	7 (4%)	38	70
All	All	386/412 (94%)	367 (95%)	19 (5%)	27	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	GLU
1	A	272	GLU
1	A	292	ARG
1	A	301	ARG
1	A	324	SER
1	A	340	LYS
1	A	389	ASN
1	A	406	LEU
1	A	421	ASN
1	A	425	CYS
1	A	432	LEU
1	A	441	LEU
1	B	254	SER
1	B	269	GLU
1	B	276	ASN
1	B	304	SER
1	B	355	GLN
1	B	375	SER
1	B	391	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	347	GLN
1	A	421	ASN

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Mol	Chain	Res	Type
1	B	295	GLN
1	B	429	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	501	1,2,5	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
2	NAG	A	502	3,2	14,14,15	0.94	1 (7%)	17,19,21	1.39	1 (5%)
3	BMA	A	503	2,4	11,11,12	0.74	0	15,15,17	0.98	0
4	MAN	A	504	3,2	11,11,12	0.99	1 (9%)	15,15,17	1.26	1 (6%)
2	NAG	A	505	4	14,14,15	0.45	0	17,19,21	0.92	1 (5%)
4	MAN	A	506	3,2	11,11,12	0.95	0	15,15,17	1.23	1 (6%)
2	NAG	A	507	4	14,14,15	0.58	0	17,19,21	0.49	0
5	FUC	A	508	2	9,10,11	0.82	0	13,14,16	0.92	0
2	NAG	B	501	1,2,5	14,14,15	0.20	0	17,19,21	0.77	1 (5%)
2	NAG	B	502	3,2	14,14,15	0.26	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	B	503	2,4	11,11,12	1.49	2 (18%)	15,15,17	1.82	4 (26%)
4	MAN	B	504	3,2	11,11,12	1.25	1 (9%)	15,15,17	1.20	1 (6%)
2	NAG	B	505	4	14,14,15	0.31	0	17,19,21	0.52	0
4	MAN	B	506	3,2	11,11,12	0.82	0	15,15,17	1.41	1 (6%)
2	NAG	B	507	4	14,14,15	0.21	0	17,19,21	0.79	1 (5%)
5	FUC	B	508	2	9,10,11	1.34	2 (22%)	13,14,16	1.42	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	A	501	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	1/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	4	-	2/6/23/26	0/1/1/1
4	MAN	A	506	3,2	-	1/2/19/22	0/1/1/1
2	NAG	A	507	4	-	2/6/23/26	0/1/1/1
5	FUC	A	508	2	-	-	0/1/1/1
2	NAG	B	501	1,2,5	-	1/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	2/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	2/2/19/22	0/1/1/1
4	MAN	B	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	4	-	2/6/23/26	0/1/1/1
4	MAN	B	506	3,2	-	1/2/19/22	1/1/1/1
2	NAG	B	507	4	-	2/6/23/26	0/1/1/1
5	FUC	B	508	2	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	O5-C1	3.33	1.49	1.43
3	B	503	BMA	O5-C1	-3.24	1.38	1.43
5	B	508	FUC	C1-C2	3.19	1.59	1.52
4	B	504	MAN	O5-C1	-2.96	1.39	1.43
4	A	504	MAN	O5-C1	-2.67	1.39	1.43
3	B	503	BMA	O3-C3	-2.57	1.36	1.43
5	B	508	FUC	C2-C3	2.00	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAG	C1-O5-C5	5.32	119.43	112.20
3	B	503	BMA	C2-C3-C4	4.50	118.70	110.89
4	B	506	MAN	C1-O5-C5	4.19	117.89	112.20
4	A	504	MAN	O2-C2-C3	-3.94	102.47	110.16
5	B	508	FUC	C1-C2-C3	3.85	114.39	109.66
4	B	504	MAN	O2-C2-C3	-3.69	102.95	110.16
4	A	506	MAN	O2-C2-C3	-3.40	103.52	110.16
2	B	507	NAG	C1-O5-C5	2.80	116.00	112.20
3	B	503	BMA	C3-C4-C5	2.72	115.12	110.23
2	A	505	NAG	C1-O5-C5	2.55	115.67	112.20
3	B	503	BMA	C1-C2-C3	2.43	112.65	109.66
2	B	501	NAG	C1-O5-C5	2.40	115.47	112.20
3	B	503	BMA	O3-C3-C4	-2.29	105.03	110.34
2	A	501	NAG	C1-O5-C5	2.26	115.27	112.20

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	507	NAG	O5-C5-C6-O6
2	B	507	NAG	C4-C5-C6-O6
3	B	503	BMA	O5-C5-C6-O6
2	A	507	NAG	C4-C5-C6-O6
3	B	503	BMA	C4-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	A	507	NAG	O5-C5-C6-O6
2	B	502	NAG	C4-C5-C6-O6
4	B	506	MAN	O5-C5-C6-O6
2	A	502	NAG	O5-C5-C6-O6
2	B	502	NAG	O5-C5-C6-O6
4	A	506	MAN	O5-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	506	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	A	505	NAG	1	0
2	B	502	NAG	1	0
3	B	503	BMA	1	0
5	B	508	FUC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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	208/224 (92%)	-0.09	4 (1%) 66 62	60, 103, 138, 175	0
1	B	209/224 (93%)	0.03	5 (2%) 59 54	72, 108, 145, 164	0
All	All	417/448 (93%)	-0.03	9 (2%) 62 57	60, 106, 140, 175	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	PHE	3.9
1	A	417	TRP	2.9
1	A	416	ARG	2.6
1	B	292	ARG	2.5
1	A	275	PHE	2.4
1	B	366	THR	2.2
1	B	257	PRO	2.2
1	B	357	GLU	2.1
1	A	424	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 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<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(Å <sup>2</sup> )	Q<0.9
2	NAG	B	501	14/15	0.76	0.22	119,123,129,130	0
2	NAG	A	505	14/15	0.82	0.25	105,108,110,110	0
5	FUC	B	508	10/11	0.82	0.23	121,126,130,133	0
2	NAG	B	502	14/15	0.85	0.22	109,115,119,120	0
4	MAN	B	504	11/12	0.90	0.18	92,93,94,95	0
2	NAG	A	502	14/15	0.91	0.20	87,92,101,102	0
2	NAG	B	507	14/15	0.91	0.23	91,96,102,104	0
3	BMA	A	503	11/12	0.91	0.15	94,98,100,102	0
4	MAN	A	504	11/12	0.92	0.22	88,90,95,101	0
2	NAG	A	501	14/15	0.93	0.13	88,95,98,99	0
2	NAG	A	507	14/15	0.93	0.18	105,109,111,114	0
3	BMA	B	503	11/12	0.93	0.12	89,95,103,104	0
5	FUC	A	508	10/11	0.94	0.15	89,93,97,99	0
4	MAN	A	506	11/12	0.94	0.13	100,104,107,107	0
2	NAG	B	505	14/15	0.95	0.13	84,97,104,106	0
4	MAN	B	506	11/12	0.95	0.10	96,99,102,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.