



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1N5M  
Title : Crystal structure of the mouse acetylcholinesterase-gallamine complex  
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.  
Deposited on : 2002-11-06  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

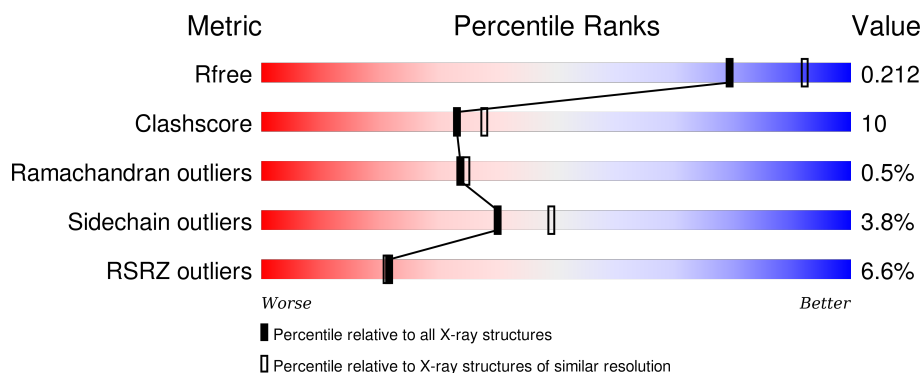
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	541	
1	B	541	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	601	-	-	-	X
5	IOD	A	990	-	-	X	-
6	P6G	A	901	-	-	-	X
7	PG4	B	902	-	-	-	X
8	GMN	A	951	-	X	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8970 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.

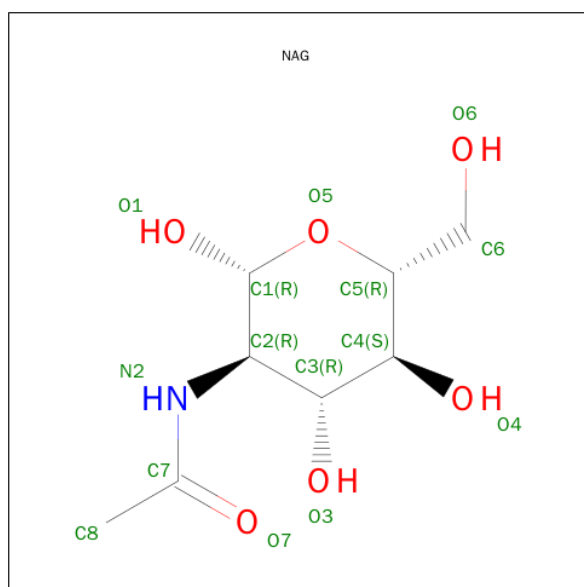
- Molecule 1 is a protein called acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4184	2683	726	761	14			
1	B	531	Total	C	N	O	S	0	0	0
			4143	2662	715	752	14			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

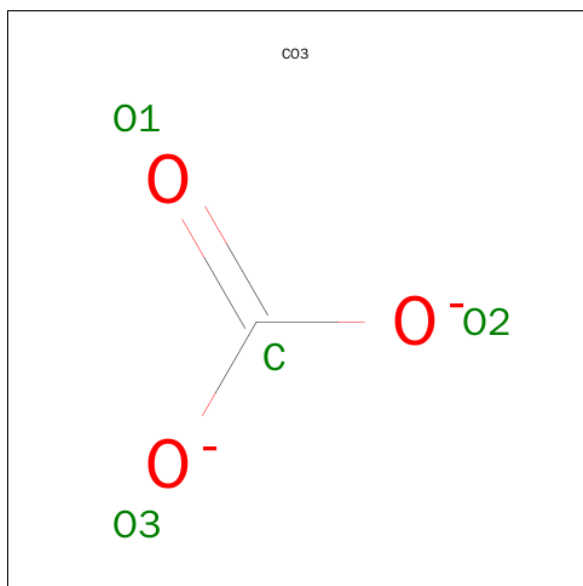
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula:  $\text{CO}_3$ ).

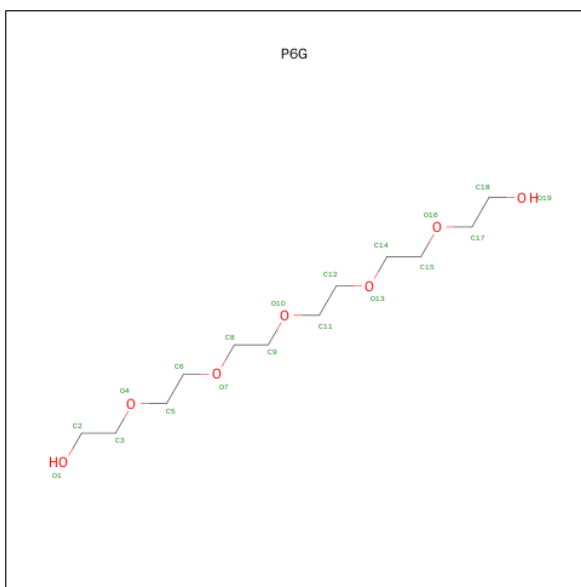


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

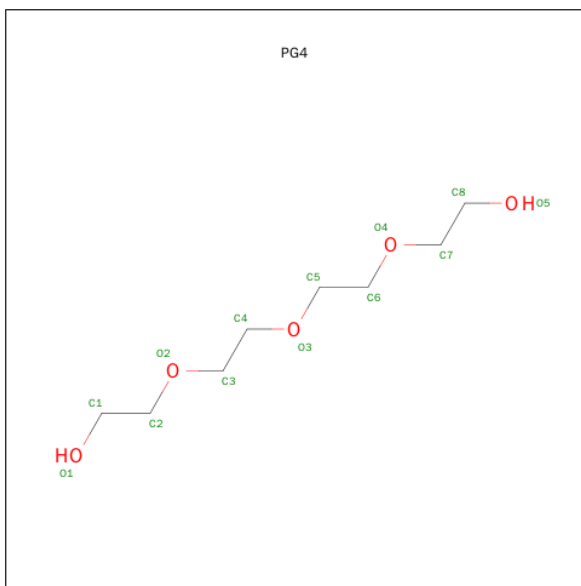
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	I	0	0
			4	4		
5	A	6	Total	I	0	0
			6	6		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $\text{C}_{12}\text{H}_{26}\text{O}_7$ ).



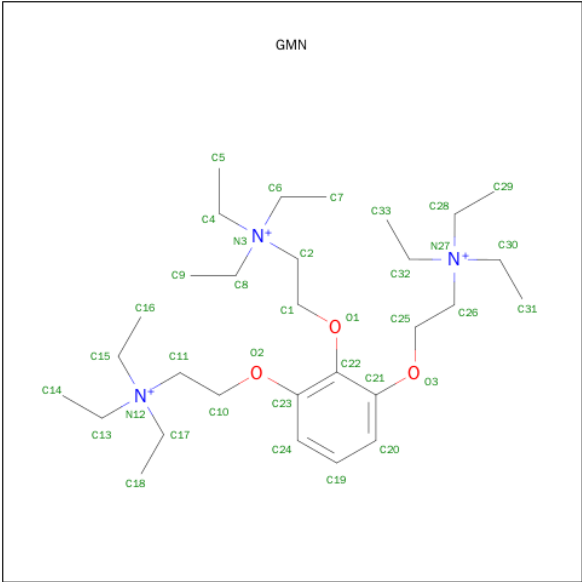
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	8	4		

- Molecule 8 is 2,2',2''-[1,2,3-BENZENE-TRIYLTRIS(OXY)]TRIS[N,N,N-TRIETHYLETHANAMINIUM] (three-letter code: GMN) (formula:  $C_{30}H_{60}N_3O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			9	6	3		

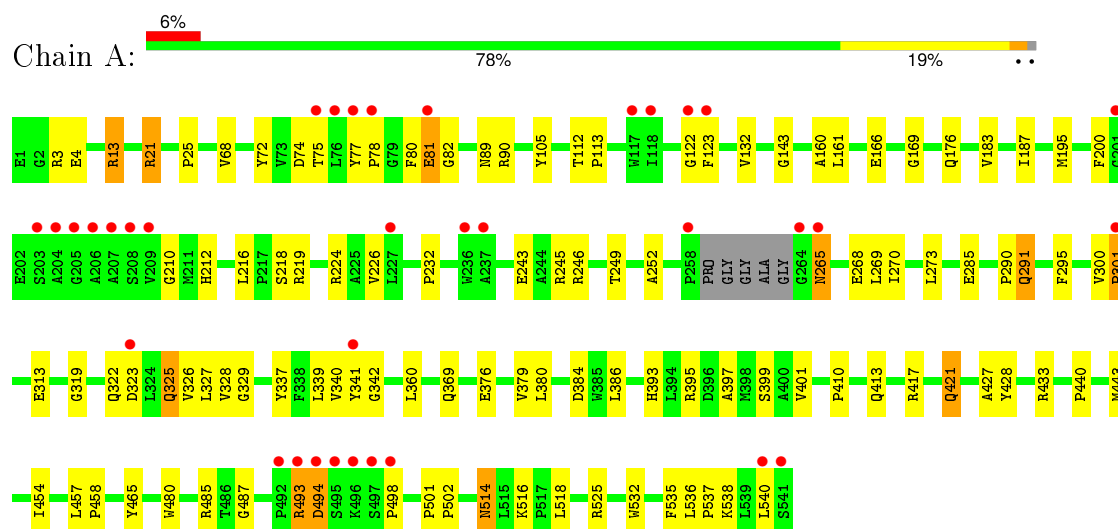
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	302	Total	O	0	0
			302	302		
9	B	249	Total	O	0	0
			249	249		

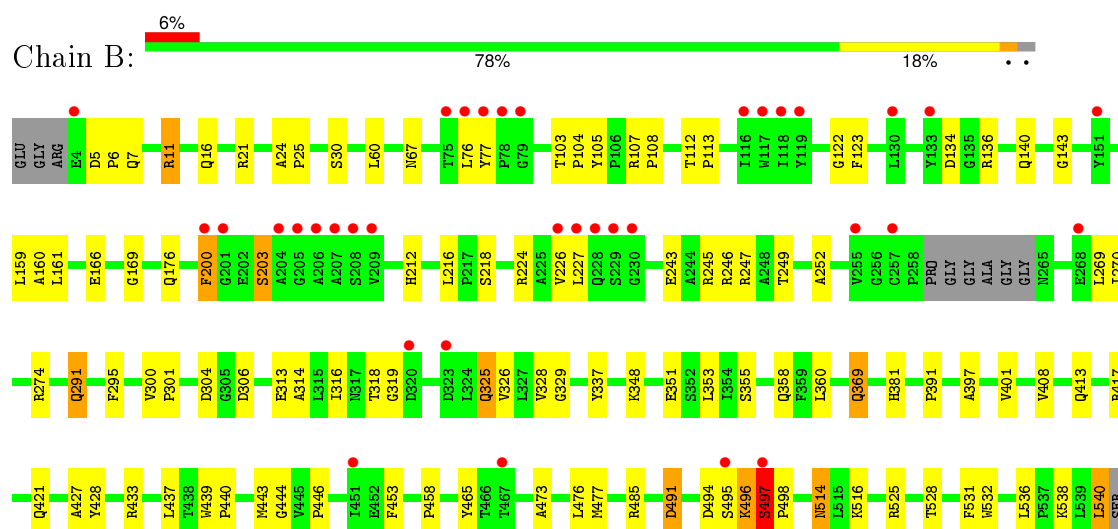
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: acetylcholinesterase



- Molecule 1: acetylcholinesterase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.07Å 110.36Å 227.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 2.20 39.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.04-2.20) 99.0 (39.57-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.74 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198 , 0.213 0.192 , 0.212	Depositor DCC
$R_{free}$ test set	2009 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.833	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100601 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: CO3, GMN, PG4, FUC, P6G, IOD, NAG

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	0.66	0/4308	0.79	2/5885 (0.0%)
1	B	0.62	0/4267	0.77	0/5834
All	All	0.64	0/8575	0.78	2/11719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	395	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	A	4184	0	4069	83	0
1	B	4143	0	4025	87	0
2	A	24	0	22	0	0
3	B	14	0	13	0	0
4	B	4	0	0	1	0
5	A	6	0	0	4	0
5	B	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	19	0	26	2	0
7	B	12	0	15	0	0
8	A	9	0	3	3	0
9	A	302	0	0	11	0
9	B	249	0	0	3	0
All	All	8970	0	8173	170	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 10.

All (170) 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:485:ARG:HG3	9:A:1692:HOH:O	1.62	0.97
1:B:497:SER:HB2	1:B:498:PRO:C	1.90	0.92
1:B:30:SER:HB2	1:B:103:THR:HG22	1.54	0.88
1:A:313:GLU:HG2	9:A:1700:HOH:O	1.71	0.88
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.54	0.86
1:A:245:ARG:O	1:A:249:THR:HG23	1.78	0.82
1:B:245:ARG:O	1:B:249:THR:HG23	1.78	0.82
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.62	0.81
1:A:72:TYR:CE1	8:A:951:GMN:H19	2.15	0.81
1:B:369:GLN:HG2	9:B:1828:HOH:O	1.81	0.79
1:A:21:ARG:NH2	5:A:991:IOD:I	2.87	0.78
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.69	0.75
1:B:497:SER:HB2	1:B:498:PRO:O	1.87	0.75
1:A:72:TYR:HE1	8:A:951:GMN:H19	1.54	0.72
1:B:203:SER:OG	4:B:904:CO3:C	2.38	0.72
1:A:376:GLU:HG2	1:B:538:LYS:HE3	1.72	0.71
1:A:325:GLN:HE21	1:A:487:GLY:HA3	1.55	0.71
1:B:212:HIS:HD2	1:B:218:SER:OG	1.75	0.68
1:A:13:ARG:NH2	9:A:1625:HOH:O	2.28	0.67
1:B:224:ARG:HD3	1:B:325:GLN:HE21	1.60	0.66
1:A:75:THR:O	1:A:78:PRO:HD3	1.96	0.66
1:A:393:HIS:HB2	9:A:1540:HOH:O	1.97	0.65
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.80	0.64
1:B:514:ASN:ND2	1:B:516:LYS:H	1.94	0.63
1:A:537:PRO:O	1:A:540:LEU:HB3	1.98	0.63
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.32	0.62
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.81	0.62
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LYS:C	1:A:540:LEU:H	2.03	0.61
1:B:514:ASN:HD22	1:B:516:LYS:H	1.48	0.61
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.36	0.61
1:A:433:ARG:HD3	9:A:1542:HOH:O	2.01	0.61
1:B:7:GLN:O	1:B:107:ARG:NH1	2.34	0.60
1:B:224:ARG:HG2	1:B:325:GLN:NE2	2.16	0.60
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.28	0.60
1:A:393:HIS:HD2	9:A:1617:HOH:O	1.86	0.59
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.84	0.59
1:B:514:ASN:HD22	1:B:514:ASN:C	2.07	0.58
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.86	0.58
1:A:413:GLN:O	1:A:417:ARG:HG2	2.03	0.58
1:B:497:SER:HB2	1:B:498:PRO:CA	2.33	0.58
1:B:319:GLY:O	1:B:421:GLN:HG3	2.03	0.58
1:B:495:SER:O	1:B:496:LYS:O	2.23	0.57
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.86	0.57
1:B:30:SER:HB2	1:B:103:THR:CG2	2.29	0.57
1:A:265:ASN:OD1	1:A:268:GLU:HG3	2.05	0.57
1:A:291:GLN:NE2	5:A:990:IOD:I	3.08	0.55
1:B:355:SER:OG	1:B:358:GLN:HG3	2.07	0.55
1:B:224:ARG:HD3	1:B:325:GLN:NE2	2.22	0.55
1:A:212:HIS:HD2	1:A:218:SER:OG	1.92	0.53
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.24	0.53
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.90	0.53
1:A:243:GLU:CD	1:A:246:ARG:NH1	2.62	0.53
1:A:77:TYR:OH	1:A:340:VAL:HG11	2.07	0.53
1:A:75:THR:HG22	1:A:75:THR:O	2.09	0.52
1:B:514:ASN:HD22	1:B:516:LYS:N	2.08	0.52
1:B:313:GLU:OE2	1:B:316:ILE:HD11	2.09	0.52
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.90	0.52
1:A:195:MET:HE3	9:A:1679:HOH:O	2.09	0.52
1:B:538:LYS:C	1:B:540:LEU:H	2.14	0.51
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.91	0.51
1:B:413:GLN:O	1:B:417:ARG:HG2	2.10	0.51
1:A:514:ASN:HD22	1:A:516:LYS:H	1.58	0.51
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.93	0.51
1:A:339:LEU:HD11	1:A:399:SER:HA	1.93	0.51
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.93	0.51
1:B:497:SER:CB	1:B:498:PRO:CA	2.89	0.50
1:B:328:VAL:O	1:B:427:ALA:HA	2.11	0.50
1:A:112:THR:HG21	1:A:143:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG21	1:B:143:GLY:O	2.11	0.50
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.44	0.50
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.47	0.50
1:B:319:GLY:O	1:B:421:GLN:CG	2.60	0.50
1:B:314:ALA:O	1:B:318:THR:HG23	2.12	0.50
1:A:25:PRO:HD3	9:A:1598:HOH:O	2.12	0.50
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.47	0.50
1:B:122:GLY:O	1:B:123:PHE:HB2	2.12	0.49
1:B:444:GLY:O	1:B:446:PRO:HD3	2.13	0.49
1:A:291:GLN:HE22	1:A:369:GLN:NE2	2.11	0.49
1:A:74:ASP:HB2	9:A:1587:HOH:O	2.13	0.49
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.43	0.48
1:A:176:GLN:OE1	1:A:212:HIS:HE1	1.96	0.48
1:B:433:ARG:CZ	1:B:437:LEU:HD23	2.43	0.48
1:A:340:VAL:O	1:A:340:VAL:HG12	2.12	0.47
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.97	0.47
1:B:243:GLU:O	1:B:247:ARG:HG3	2.15	0.47
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.49	0.47
1:A:369:GLN:HB2	9:A:1754:HOH:O	2.14	0.47
1:A:493:ARG:HB2	1:A:494:ASP:H	1.51	0.47
1:B:491:ASP:CB	1:B:494:ASP:HB3	2.45	0.47
1:A:540:LEU:HD12	1:A:540:LEU:C	2.35	0.47
1:B:76:LEU:HG	1:B:77:TYR:CE2	2.50	0.47
1:A:89:ASN:O	1:A:90:ARG:NH1	2.42	0.47
1:B:351:GLU:OE2	1:B:351:GLU:HA	2.14	0.46
1:A:433:ARG:NH2	1:A:440:PRO:O	2.48	0.46
1:A:74:ASP:OD1	1:A:341:TYR:HE2	1.98	0.46
5:A:1463:IOD:I	8:A:951:GMN:O3	3.03	0.46
1:A:81:GLU:HB2	9:A:1548:HOH:O	2.15	0.46
1:B:514:ASN:HD21	1:B:516:LYS:HB2	1.81	0.46
1:A:328:VAL:O	1:A:427:ALA:HA	2.15	0.46
1:A:252:ALA:HA	1:A:273:LEU:HD21	1.97	0.45
1:A:21:ARG:HG3	1:A:105:TYR:CE1	2.52	0.45
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.31	0.45
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.51	0.45
1:A:337:TYR:HA	1:A:443:MET:HE1	1.98	0.45
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.98	0.45
1:A:122:GLY:O	1:A:123:PHE:HB2	2.15	0.45
1:A:300:VAL:HB	1:A:301:PRO:CD	2.46	0.45
1:A:319:GLY:O	1:A:421:GLN:CG	2.65	0.45
1:B:103:THR:HG23	1:B:104:PRO:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:SER:O	1:B:496:LYS:C	2.55	0.45
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.99	0.45
1:A:514:ASN:ND2	1:A:516:LYS:H	2.14	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.98	0.45
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.52	0.45
1:B:67:ASN:ND2	9:B:1617:HOH:O	2.46	0.45
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.85	0.44
1:A:384:ASP:OD1	1:A:384:ASP:C	2.55	0.44
1:A:322:GLN:O	1:A:323:ASP:HB2	2.17	0.44
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.52	0.44
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.44
1:A:200:PHE:CB	1:A:226:VAL:HB	2.48	0.44
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.16	0.44
1:A:210:GLY:HA3	1:A:232:PRO:HD3	1.98	0.44
1:A:376:GLU:O	1:A:380:LEU:HG	2.17	0.44
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.00	0.44
1:B:337:TYR:HA	1:B:443:MET:CE	2.47	0.44
1:B:176:GLN:OE1	1:B:212:HIS:HE1	2.00	0.44
1:A:498:PRO:HG2	1:A:518:LEU:HB2	2.00	0.44
1:B:252:ALA:HB2	1:B:269:LEU:HD21	1.99	0.44
1:A:514:ASN:C	1:A:514:ASN:HD22	2.20	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.18	0.43
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.01	0.43
1:B:224:ARG:HH11	1:B:325:GLN:HE22	1.65	0.42
1:A:457:LEU:N	1:A:458:PRO:CD	2.82	0.42
1:A:397:ALA:O	1:A:401:VAL:HG23	2.19	0.42
1:A:219:ARG:HD2	1:A:219:ARG:HA	1.78	0.42
1:B:473:ALA:O	1:B:477:MET:HG3	2.19	0.42
1:B:5:ASP:HA	1:B:6:PRO:HD2	1.89	0.42
1:B:397:ALA:O	1:B:401:VAL:HG23	2.20	0.42
1:B:11:ARG:NH1	1:B:16:GLN:CG	2.83	0.42
1:A:428:TYR:CD1	1:A:428:TYR:C	2.93	0.42
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.02	0.42
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.19	0.42
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.55	0.42
6:A:901:P6G:H182	1:B:381:HIS:HE1	1.85	0.42
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.49	0.42
1:B:291:GLN:NE2	5:B:1335:IOD:I	3.23	0.42
1:B:536:LEU:HA	1:B:536:LEU:HD23	1.76	0.41
1:B:159:LEU:HD23	1:B:159:LEU:C	2.41	0.41
1:A:535:PHE:CE2	6:A:901:P6G:H112	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:TRP:CE3	1:A:536:LEU:HD12	2.55	0.41
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.03	0.41
1:B:21:ARG:HG3	1:B:105:TYR:CE1	2.56	0.41
1:A:290:PRO:HD2	5:A:990:IOD:I	2.90	0.41
1:B:439:TRP:HB3	1:B:440:PRO:HD2	2.02	0.41
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.50	0.41
1:B:227:LEU:HB2	1:B:328:VAL:HG12	2.02	0.41
1:A:337:TYR:HA	1:A:443:MET:CE	2.51	0.41
1:B:274:ARG:HD3	9:B:1782:HOH:O	2.20	0.41
1:A:77:TYR:OH	1:A:340:VAL:CG1	2.69	0.40
1:B:160:ALA:HB2	1:B:169:GLY:HA2	2.02	0.40
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.03	0.40
1:B:76:LEU:HG	1:B:77:TYR:CD2	2.57	0.40
1:B:107:ARG:HA	1:B:108:PRO:HD3	1.96	0.40
1:B:514:ASN:ND2	1:B:516:LYS:N	2.63	0.40
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.53	0.40
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.80	0.40
1:A:501:PRO:HA	1:A:502:PRO:HD3	1.94	0.40
1:B:269:LEU:C	1:B:269:LEU:HD23	2.42	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	Percentiles	
1	A	532/541 (98%)	514 (97%)	15 (3%)	3 (1%)	30	29
1	B	527/541 (97%)	509 (97%)	16 (3%)	2 (0%)	39	42
All	All	1059/1082 (98%)	1023 (97%)	31 (3%)	5 (0%)	34	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	ASP
1	B	497	SER
1	B	496	LYS
1	A	493	ARG
1	A	342	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	440/442 (100%)	423 (96%)	17 (4%)	39	48
1	B	436/442 (99%)	420 (96%)	16 (4%)	41	50
All	All	876/884 (99%)	843 (96%)	33 (4%)	40	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	21	ARG
1	A	81	GLU
1	A	132	VAL
1	A	216	LEU
1	A	265	ASN
1	A	285	GLU
1	A	291	GLN
1	A	295	PHE
1	A	301	PRO
1	A	325	GLN
1	A	327	LEU
1	A	410	PRO
1	A	421	GLN
1	A	514	ASN
1	A	525	ARG
1	B	11	ARG
1	B	25	PRO

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	200	PHE
1	B	203	SER
1	B	216	LEU
1	B	246	ARG
1	B	291	GLN
1	B	295	PHE
1	B	325	GLN
1	B	360	LEU
1	B	369	GLN
1	B	491	ASP
1	B	497	SER
1	B	514	ASN
1	B	540	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	284	HIS
1	A	291	GLN
1	A	325	GLN
1	A	508	GLN
1	A	514	ASN
1	B	212	HIS
1	B	291	GLN
1	B	325	GLN
1	B	514	ASN

### 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 ⓘ

2 carbohydrates 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	542	1,2	14,14,15	0.82	0	15,19,21	1.05	1 (6%)
2	FUC	A	543	2	10,10,11	0.65	0	14,14,16	0.68	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	542	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	543	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	542	NAG	C2-N2-C7	-2.43	119.91	123.04
2	A	543	FUC	C1-O5-C5	2.07	115.58	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	P6G	A	901	-	18,18,18	2.18	6 (33%)	17,17,17	0.95	0
8	GMN	A	951	-	9,9,36	6.06	7 (77%)	12,12,48	2.40	3 (25%)
3	NAG	B	601	1	14,14,15	0.98	1 (7%)	15,19,21	0.95	1 (6%)
7	PG4	B	902	-	11,11,12	2.17	3 (27%)	10,10,11	1.05	0
4	CO3	B	904	-	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	P6G	A	901	-	-	0/16/16/16	0/0/0/0
8	GMN	A	951	-	-	0/0/0/48	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
7	PG4	B	902	-	-	0/9/9/10	0/0/0/0
4	CO3	B	904	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	951	GMN	O2-C23	2.11	1.40	1.36
3	B	601	NAG	C1-C2	2.31	1.55	1.52
6	A	901	P6G	O7-C6	2.55	1.52	1.42
7	B	902	PG4	O3-C4	2.73	1.53	1.42
8	A	951	GMN	C24-C23	2.94	1.44	1.39
6	A	901	P6G	O19-C18	3.10	1.58	1.42
6	A	901	P6G	O16-C15	3.48	1.56	1.42
6	A	901	P6G	O4-C3	3.49	1.56	1.42
7	B	902	PG4	O2-C2	3.69	1.57	1.42
8	A	951	GMN	O3-C21	3.78	1.44	1.36
6	A	901	P6G	O13-C12	3.83	1.58	1.42
6	A	901	P6G	O10-C9	4.25	1.60	1.42
7	B	902	PG4	O4-C6	4.79	1.62	1.42
8	A	951	GMN	C19-C24	5.48	1.50	1.38
8	A	951	GMN	C20-C21	6.47	1.51	1.39
8	A	951	GMN	C23-C22	7.34	1.48	1.39
8	A	951	GMN	C21-C22	13.08	1.55	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	A	951	GMN	C24-C23-C22	-4.91	115.75	120.09
3	B	601	NAG	C1-O5-C5	2.14	114.96	112.25
8	A	951	GMN	C19-C24-C23	2.94	123.81	120.04
8	A	951	GMN	C23-C22-C21	4.62	122.08	119.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	P6G	2	0
8	A	951	GMN	3	0
4	B	904	CO3	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 ⓘ

### 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	536/541 (99%)	-0.02	35 (6%)	22 22	29, 42, 70, 97	0
1	B	531/541 (98%)	0.09	35 (6%)	22 21	29, 44, 70, 86	0
All	All	1067/1082 (98%)	0.04	70 (6%)	22 21	29, 43, 70, 97	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	6.8
1	A	496	LYS	6.4
1	B	118	ILE	5.0
1	A	497	SER	4.6
1	A	76	LEU	4.6
1	B	117	TRP	4.5
1	A	493	ARG	4.2
1	A	264	GLY	4.0
1	A	494	ASP	3.9
1	A	492	PRO	3.9
1	B	204	ALA	3.8
1	A	341	TYR	3.7
1	A	118	ILE	3.4
1	B	257	CYS	3.3
1	B	200	PHE	3.3
1	A	207	ALA	3.3
1	A	204	ALA	3.3
1	B	201	GLY	3.2
1	A	209	VAL	3.1
1	B	75	THR	3.1
1	A	75	THR	3.1
1	B	227	LEU	3.0
1	B	207	ALA	3.0
1	A	206	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	2.9
1	A	323	ASP	2.9
1	B	133	TYR	2.9
1	B	467	THR	2.8
1	B	119	TYR	2.7
1	B	4	GLU	2.6
1	A	81	GLU	2.6
1	A	78	PRO	2.5
1	A	117	TRP	2.5
1	A	540	LEU	2.5
1	B	79	GLY	2.4
1	B	497	SER	2.4
1	A	236	TRP	2.4
1	A	227	LEU	2.4
1	B	209	VAL	2.4
1	A	258	PRO	2.4
1	A	265	ASN	2.3
1	B	151	TYR	2.3
1	B	226	VAL	2.3
1	A	498	PRO	2.3
1	A	201	GLY	2.3
1	B	206	ALA	2.3
1	B	255	VAL	2.3
1	B	78	PRO	2.2
1	B	451	ILE	2.2
1	B	208	SER	2.2
1	B	205	GLY	2.2
1	B	130	LEU	2.2
1	A	205	GLY	2.2
1	B	230	GLY	2.2
1	B	76	LEU	2.2
1	A	203	SER	2.2
1	B	228	GLN	2.1
1	B	495	SER	2.1
1	B	320	ASP	2.1
1	A	208	SER	2.1
1	B	116	ILE	2.1
1	B	268	GLU	2.1
1	A	237	ALA	2.1
1	A	301	PRO	2.1
1	A	77	TYR	2.1
1	A	541	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	229	SER	2.0
1	A	122	GLY	2.0
1	B	323	ASP	2.0
1	B	77	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	542	14/15	0.78	0.35	-	78,83,88,93	0
2	FUC	A	543	10/11	0.89	0.53	-	95,97,99,99	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	PG4	B	902	12/13	0.66	0.20	5.08	87,89,91,91	0
8	GMN	A	951	9/36	0.80	0.42	3.42	78,79,79,80	9
6	P6G	A	901	19/19	0.86	0.19	3.37	55,67,70,70	0
3	NAG	B	601	14/15	0.53	0.36	3.34	86,89,90,90	0
4	CO3	B	904	4/4	0.84	0.28	1.27	60,61,61,62	0
5	IOD	B	1335	1/1	0.97	0.09	-0.88	51,51,51,51	1
5	IOD	A	1463	1/1	0.99	0.11	-1.38	45,45,45,45	1
5	IOD	A	990	1/1	0.99	0.04	-2.93	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	IOD	B	1590	1/1	0.99	0.09	-3.14	57,57,57,57	1
5	IOD	B	1448	1/1	0.85	0.05	-	93,93,93,93	1
5	IOD	B	1485	1/1	0.95	0.08	-	60,60,60,60	1
5	IOD	A	1243	1/1	0.99	0.10	-	50,50,50,50	1
5	IOD	A	802	1/1	0.99	0.11	-	40,40,40,40	1
5	IOD	A	1367	1/1	0.97	0.04	-	62,62,62,62	1
5	IOD	A	991	1/1	0.83	0.05	-	80,80,80,80	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.