



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:10 PM GMT

PDB ID : 1J06  
Title : Crystal structure of mouse acetylcholinesterase in the apo form  
Authors : Bourne, Y.; Taylor, P.; Radic, Z.; Marchot, P.  
Deposited on : 2002-11-07  
Resolution : 2.35 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

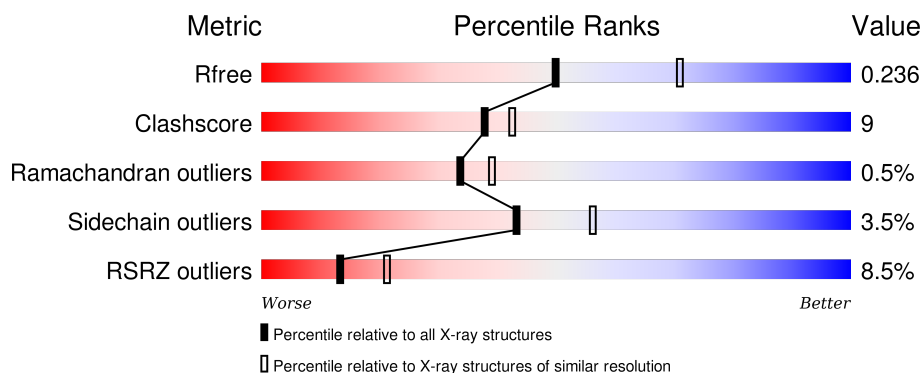
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	543	<div> <div>8%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	B	543	<div> <div>9%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

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
2	NAG	A	544	-	-	-	X
3	NAG	B	601	-	-	-	X
5	P6G	A	901	-	-	-	X
6	AE3	A	902	-	-	-	X
6	AE3	B	903	-	-	-	X
7	PG4	B	904	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8804 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	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	533	Total	C	N	O	S	0	0	0
			4159	2670	718	757	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:  $C_8H_{15}NO_6$ ).



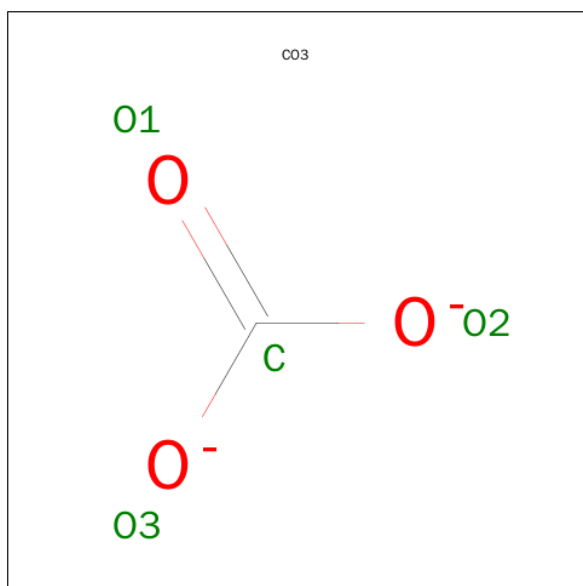
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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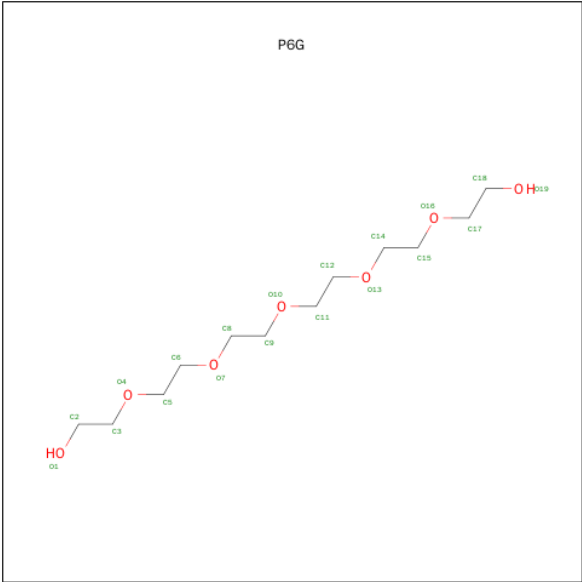
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



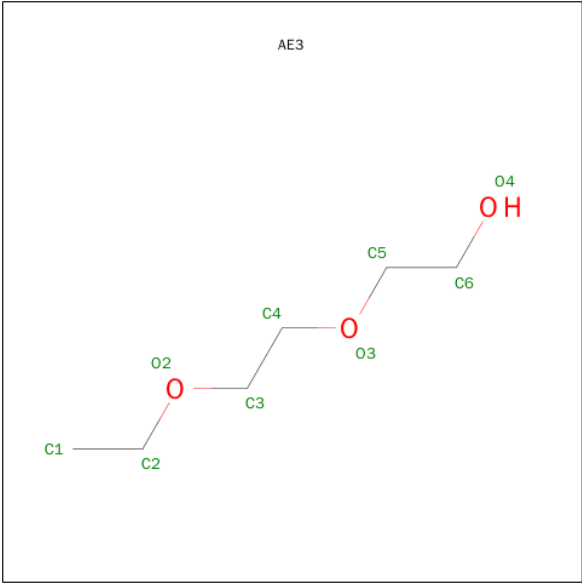
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



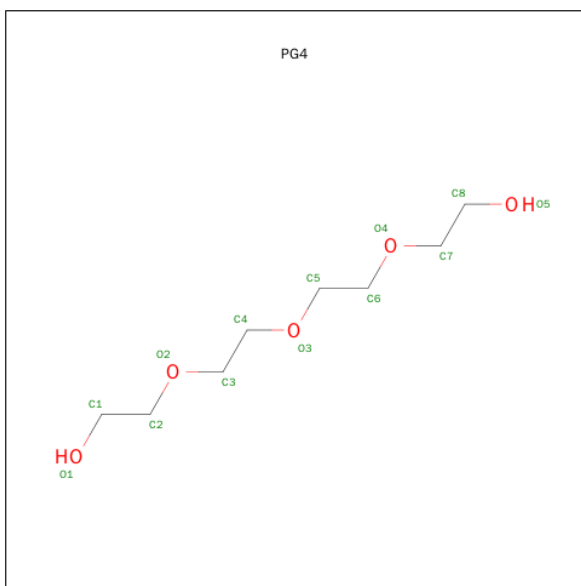
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>).



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

- 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
			11	8	3		

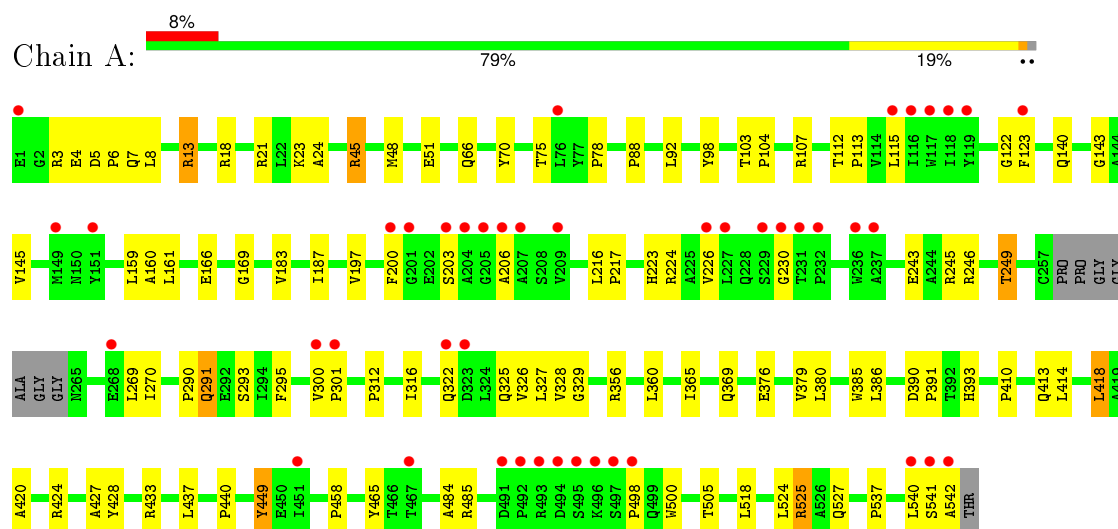
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	210	Total	O	0	0
			210	210		
8	B	150	Total	O	0	0
			150	150		

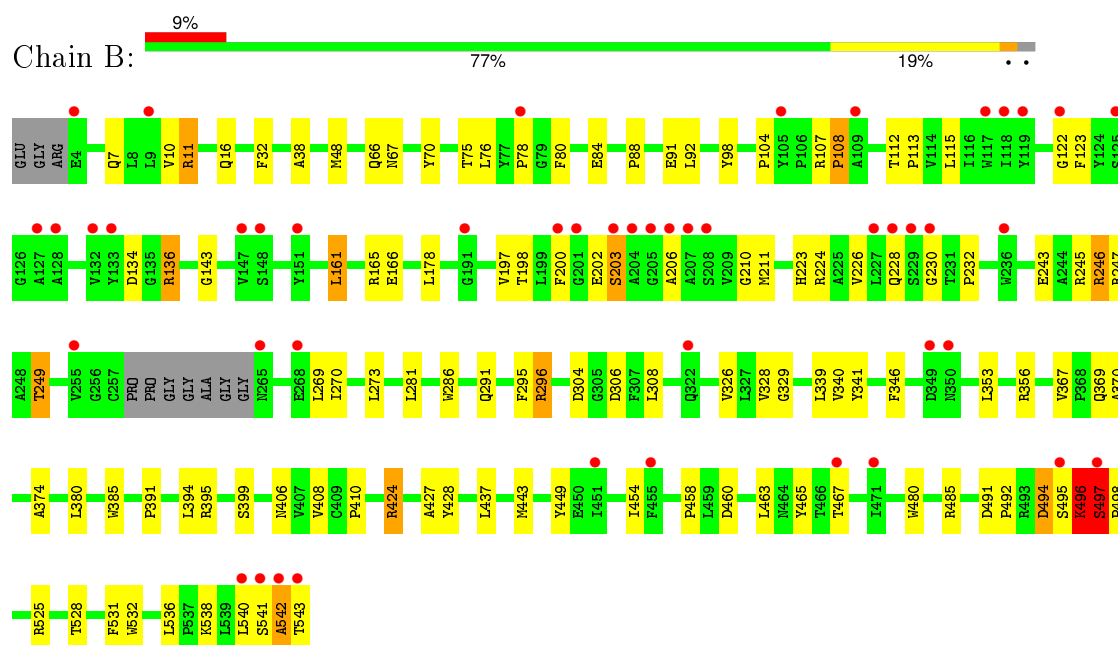
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	79.20Å 111.97Å 226.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 39.84 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.35) 99.0 (39.84-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 2.34Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.232 0.210 , 0.236	Depositor DCC
$R_{free}$ test set	1690 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 83956 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AE3, NAG, CO3, PG4, FUC, P6G

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	0.69	0/4300	0.80	0/5875
1	B	0.61	0/4282	0.78	1/5851 (0.0%)
All	All	0.65	0/8582	0.79	1/11726 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LEU	N-CA-C	-5.82	95.28	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	TYR	Sidechain
1	B	70	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	4177	0	4063	72	0
1	B	4159	0	4046	85	0
2	A	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
5	A	19	0	26	1	0
6	A	9	0	14	0	0
6	B	9	0	14	2	0
7	B	11	0	12	0	0
8	A	210	0	0	6	0
8	B	150	0	0	2	0
All	All	8804	0	8223	154	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 9.

All (154) 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:48:MET:HE3	1:A:166:GLU:HA	1.29	1.09
1:B:48:MET:HE1	1:B:166:GLU:HA	1.32	1.09
1:A:197:VAL:H	1:A:223:HIS:HD2	1.14	0.94
1:B:197:VAL:H	1:B:223:HIS:HD2	1.03	0.93
1:A:485:ARG:HG3	8:A:1107:HOH:O	1.70	0.92
1:B:497:SER:HB2	1:B:498:PRO:O	1.72	0.90
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.73	0.88
1:B:245:ARG:O	1:B:249:THR:HG23	1.80	0.82
1:B:197:VAL:H	1:B:223:HIS:CD2	1.94	0.80
1:B:497:SER:HB2	1:B:498:PRO:C	2.02	0.79
1:A:197:VAL:H	1:A:223:HIS:CD2	1.99	0.78
1:A:245:ARG:O	1:A:249:THR:HG23	1.85	0.77
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.73	0.70
1:B:424:ARG:HG3	1:B:424:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.55	0.70
1:A:203:SER:OG	4:A:951:CO3:C	2.39	0.70
1:B:112:THR:HG21	1:B:143:GLY:O	1.92	0.69
1:A:48:MET:CE	1:A:166:GLU:HA	2.18	0.66
1:B:203:SER:OG	4:B:952:CO3:C	2.43	0.66
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.29	0.65
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.79	0.64
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.31	0.64
1:B:48:MET:CE	1:B:166:GLU:HA	2.18	0.62
1:A:376:GLU:HG2	1:B:538:LYS:NZ	2.15	0.61
1:A:376:GLU:HG2	1:B:538:LYS:CE	2.29	0.61
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.83	0.61
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.83	0.60
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.83	0.60
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.37	0.60
1:A:88:PRO:HD3	8:A:1062:HOH:O	2.01	0.59
1:A:433:ARG:HD3	8:A:1080:HOH:O	2.02	0.59
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.84	0.58
1:A:161:LEU:HD12	1:A:270:ILE:CG1	2.32	0.58
1:A:112:THR:HG21	1:A:143:GLY:O	2.03	0.58
1:B:374:ALA:HB2	1:B:540:LEU:HD21	1.86	0.57
1:B:11:ARG:NH1	1:B:16:GLN:HG2	2.19	0.57
1:B:495:SER:O	1:B:496:LYS:O	2.23	0.57
1:A:13:ARG:NH2	8:A:1029:HOH:O	2.38	0.57
1:A:537:PRO:O	1:A:540:LEU:HB3	2.04	0.57
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.86	0.56
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.88	0.56
1:B:11:ARG:HH12	1:B:16:GLN:CG	2.20	0.54
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.38	0.54
1:A:245:ARG:O	1:A:249:THR:CG2	2.55	0.54
1:B:437:LEU:HD11	1:B:449:TYR:CD2	2.43	0.53
1:B:80:PHE:O	1:B:84:GLU:HG2	2.09	0.53
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.90	0.53
1:A:541:SER:O	1:A:542:ALA:CB	2.57	0.53
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.44	0.52
1:B:424:ARG:CG	1:B:424:ARG:HH11	2.20	0.52
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.09	0.52
1:A:541:SER:O	1:A:542:ALA:HB2	2.10	0.52
1:B:340:VAL:HG11	1:B:443:MET:CE	2.40	0.51
1:A:420:ALA:HB2	1:A:505:THR:HG21	1.92	0.51
1:B:122:GLY:O	1:B:123:PHE:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.93	0.51
1:A:75:THR:O	1:A:78:PRO:HD3	2.11	0.51
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.75	0.51
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.93	0.51
1:A:527:GLN:HE21	5:A:901:P6G:H21	1.77	0.50
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.26	0.50
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.47	0.50
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.46	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.12	0.49
1:B:67:ASN:OD1	1:B:91:GLU:HB2	2.11	0.49
1:B:243:GLU:O	1:B:247:ARG:HG3	2.13	0.49
1:B:11:ARG:NH1	1:B:16:GLN:CG	2.74	0.49
1:B:104:PRO:HG2	1:B:108:PRO:HD3	1.94	0.49
1:A:216:LEU:HB3	1:A:217:PRO:HD3	1.94	0.49
1:A:161:LEU:HD12	1:A:270:ILE:CD1	2.42	0.49
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.95	0.48
1:B:541:SER:O	1:B:542:ALA:HB2	2.13	0.48
1:B:369:GLN:HB2	8:B:988:HOH:O	2.12	0.48
1:A:380:LEU:HD22	1:A:385:TRP:CZ2	2.49	0.48
1:A:498:PRO:HG2	1:A:518:LEU:HB2	1.96	0.48
1:A:5:ASP:HB3	1:A:8:LEU:HD12	1.96	0.48
1:A:312:PRO:O	1:A:316:ILE:HG23	2.14	0.48
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.49	0.47
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.49	0.47
1:B:7:GLN:OE1	1:B:107:ARG:N	2.43	0.47
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.96	0.47
1:B:346:PHE:HE2	1:B:395:ARG:HG2	1.80	0.47
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.97	0.47
1:A:393:HIS:HB2	8:A:1033:HOH:O	2.14	0.47
1:B:10:VAL:HG23	1:B:32:PHE:CE2	2.50	0.47
1:A:122:GLY:O	1:A:123:PHE:HB2	2.14	0.47
1:A:369:GLN:HB2	8:A:1027:HOH:O	2.14	0.46
1:A:159:LEU:C	1:A:159:LEU:HD23	2.36	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.51	0.46
1:A:88:PRO:HG2	1:A:92:LEU:HD21	1.97	0.46
1:A:224:ARG:NH1	1:A:224:ARG:HG3	2.29	0.46
1:B:206:ALA:HB3	1:B:230:GLY:HA3	1.97	0.46
1:A:380:LEU:HD22	1:A:385:TRP:HZ2	1.81	0.46
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.98	0.46
1:A:327:LEU:HD11	1:A:500:TRP:CZ2	2.51	0.45
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.51	0.45
1:B:75:THR:O	1:B:78:PRO:HD3	2.17	0.45
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.98	0.45
1:A:45:ARG:CZ	1:A:51:GLU:OE1	2.64	0.45
1:B:367:VAL:HG12	1:B:370:ALA:HB2	1.98	0.45
1:B:339:LEU:HD11	1:B:399:SER:HA	1.99	0.45
1:A:433:ARG:NH2	1:A:440:PRO:O	2.50	0.45
1:B:296:ARG:HG2	8:B:1066:HOH:O	2.16	0.44
1:B:286:TRP:CD2	6:B:903:AE3:H3C1	2.52	0.44
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.99	0.44
1:A:293:SER:HA	1:A:365:ILE:HG23	2.00	0.44
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.00	0.44
1:B:496:LYS:NZ	1:B:496:LYS:HB2	2.33	0.44
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.52	0.44
1:B:528:THR:O	1:B:531:PHE:HB3	2.17	0.44
1:B:536:LEU:HA	1:B:536:LEU:HD23	1.83	0.43
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.78	0.43
1:A:7:GLN:O	1:A:107:ARG:NH1	2.52	0.43
1:B:197:VAL:N	1:B:223:HIS:HD2	1.88	0.43
1:B:202:GLU:HA	1:B:228:GLN:O	2.18	0.43
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.84	0.43
1:B:113:PRO:HG3	1:B:485:ARG:HG2	2.01	0.43
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.01	0.43
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.01	0.43
1:B:497:SER:CB	1:B:498:PRO:C	2.82	0.42
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.49	0.42
1:A:103:THR:HG22	1:A:145:VAL:HG22	2.00	0.42
1:B:161:LEU:CD1	1:B:269:LEU:HD22	2.48	0.42
1:A:376:GLU:HG2	1:B:538:LYS:HE3	2.00	0.42
1:B:76:LEU:HD22	1:B:341:TYR:CE2	2.54	0.42
1:A:243:GLU:CD	1:A:246:ARG:NH1	2.73	0.42
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.66	0.42
1:B:356:ARG:HA	1:B:394:LEU:HD13	2.02	0.42
1:B:107:ARG:HA	1:B:108:PRO:HD3	1.94	0.42
1:A:328:VAL:O	1:A:427:ALA:HA	2.19	0.41
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.41
1:B:491:ASP:HB3	1:B:494:ASP:HB3	2.02	0.41
1:B:496:LYS:HB2	1:B:496:LYS:HZ1	1.85	0.41
1:B:48:MET:HE1	1:B:165:ARG:O	2.21	0.41
1:B:88:PRO:HG2	1:B:92:LEU:HD21	2.02	0.41
1:A:290:PRO:HG2	1:A:291:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.88	0.41
1:B:495:SER:C	1:B:496:LYS:O	2.58	0.41
1:B:104:PRO:CG	1:B:108:PRO:HG3	2.50	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD2	1.96	0.41
1:B:286:TRP:CE2	6:B:903:AE3:H3C1	2.55	0.41
1:B:38:ALA:HB2	1:B:178:LEU:HD23	2.02	0.41
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.02	0.41
1:B:115:LEU:HD23	1:B:198:THR:HB	2.03	0.41
1:A:206:ALA:HB3	1:A:230:GLY:HA3	2.03	0.41
1:B:273:LEU:HA	1:B:273:LEU:HD23	1.93	0.40
1:A:524:LEU:O	1:A:525:ARG:C	2.60	0.40
1:B:454:ILE:HD12	1:B:480:TRP:CE2	2.57	0.40
1:B:380:LEU:HD22	1:B:385:TRP:CZ2	2.57	0.40
1:A:437:LEU:HD11	1:A:449:TYR:CD2	2.57	0.40
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.20	0.40
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.04	0.40
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.95	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	531/543 (98%)	506 (95%)	25 (5%)	0	100	100
1	B	529/543 (97%)	507 (96%)	17 (3%)	5 (1%)	21	22
All	All	1060/1086 (98%)	1013 (96%)	42 (4%)	5 (0%)	34	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	542	ALA

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Mol	Chain	Res	Type
1	B	496	LYS
1	B	494	ASP
1	B	497	SER
1	B	108	PRO

### 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	439/443 (99%)	423 (96%)	16 (4%)	42	55
1	B	438/443 (99%)	423 (97%)	15 (3%)	44	57
All	All	877/886 (99%)	846 (96%)	31 (4%)	43	56

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	13	ARG
1	A	21	ARG
1	A	23	LYS
1	A	45	ARG
1	A	70	TYR
1	A	249	THR
1	A	291	GLN
1	A	295	PHE
1	A	322	GLN
1	A	356	ARG
1	A	410	PRO
1	A	413	GLN
1	A	418	LEU
1	A	424	ARG
1	A	525	ARG
1	B	11	ARG
1	B	136	ARG
1	B	203	SER

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Mol	Chain	Res	Type
1	B	246	ARG
1	B	249	THR
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	410	PRO
1	B	424	ARG
1	B	467	THR
1	B	496	LYS
1	B	497	SER
1	B	543	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	291	GLN
1	A	527	GLN
1	B	223	HIS
1	B	291	GLN
1	B	499	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	544	1,2	14,14,15	0.96	1 (7%)	15,19,21	1.28	3 (20%)
2	FUC	A	545	2	10,10,11	0.75	0	14,14,16	1.00	2 (14%)

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	544	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	545	2	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	544	NAG	C1-C2	2.41	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	544	NAG	C2-N2-C7	-2.68	119.60	123.04
2	A	544	NAG	C4-C3-C2	-2.32	107.62	111.23
2	A	545	FUC	C1-O5-C5	2.15	115.70	112.38
2	A	545	FUC	C1-C2-C3	2.21	112.15	109.54
2	A	544	NAG	C1-O5-C5	2.32	115.20	112.25

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 ⓘ

8 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
3	NAG	A	701	1	14,14,15	0.77	0	15,19,21	0.91	1 (6%)
5	P6G	A	901	-	18,18,18	2.08	6 (33%)	17,17,17	1.12	1 (5%)
6	AE3	A	902	-	8,8,8	1.59	2 (25%)	7,7,7	1.30	1 (14%)
4	CO3	A	951	-	0,3,3	0.00	-	0,3,3	0.00	-
3	NAG	B	601	1	14,14,15	1.01	1 (7%)	15,19,21	0.84	0
6	AE3	B	903	-	8,8,8	1.72	2 (25%)	7,7,7	1.43	1 (14%)
7	PG4	B	904	-	10,10,12	1.89	2 (20%)	9,9,11	0.85	0
4	CO3	B	952	-	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
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	P6G	A	901	-	-	0/16/16/16	0/0/0/0
6	AE3	A	902	-	-	0/6/6/6	0/0/0/0
4	CO3	A	951	-	-	0/0/0/0	0/0/0/0
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
6	AE3	B	903	-	-	0/6/6/6	0/0/0/0
7	PG4	B	904	-	-	0/8/8/10	0/0/0/0
4	CO3	B	952	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	C1-C2	2.12	1.55	1.52
6	A	902	AE3	O2-C3	2.62	1.53	1.42
7	B	904	PG4	O3-C5	2.81	1.54	1.42
5	A	901	P6G	O7-C6	2.88	1.54	1.42
6	B	903	AE3	O2-C3	2.99	1.54	1.42
5	A	901	P6G	O19-C18	3.09	1.58	1.42
6	A	902	AE3	O3-C5	3.32	1.56	1.42
5	A	901	P6G	O4-C3	3.36	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	903	AE3	O3-C5	3.57	1.57	1.42
5	A	901	P6G	O16-C15	3.59	1.57	1.42
5	A	901	P6G	O13-C12	3.70	1.57	1.42
5	A	901	P6G	O10-C9	4.08	1.59	1.42
7	B	904	PG4	O2-C3	4.82	1.62	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	C2-N2-C7	-2.76	119.50	123.04
6	A	902	AE3	O4-C6-C5	2.87	129.76	112.03
6	B	903	AE3	O4-C6-C5	3.07	130.98	112.03
5	A	901	P6G	O1-C2-C3	3.15	131.48	112.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	P6G	1	0
4	A	951	CO3	1	0
6	B	903	AE3	2	0
4	B	952	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	535/543 (98%)	0.18	44 (8%) 14 23	30, 44, 66, 98	0
1	B	533/543 (98%)	0.38	47 (8%) 12 20	35, 49, 71, 99	0
All	All	1068/1086 (98%)	0.28	91 (8%) 13 21	30, 46, 69, 99	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	THR	6.7
1	B	497	SER	5.7
1	B	118	ILE	5.4
1	B	540	LEU	4.7
1	B	117	TRP	4.6
1	A	495	SER	4.5
1	A	118	ILE	4.4
1	B	541	SER	4.3
1	B	204	ALA	4.2
1	B	207	ALA	4.1
1	B	542	ALA	3.9
1	A	493	ARG	3.9
1	B	227	LEU	3.9
1	B	200	PHE	3.7
1	B	119	TYR	3.6
1	A	540	LEU	3.6
1	A	497	SER	3.6
1	A	494	ASP	3.6
1	A	117	TRP	3.4
1	A	230	GLY	3.4
1	B	201	GLY	3.4
1	A	492	PRO	3.4
1	A	496	LYS	3.4
1	A	207	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	236	TRP	3.3
1	B	109	ALA	3.3
1	B	467	THR	3.2
1	B	230	GLY	3.1
1	B	78	PRO	3.1
1	A	206	ALA	3.0
1	A	542	ALA	3.0
1	B	229	SER	3.0
1	A	204	ALA	3.0
1	B	349	ASP	3.0
1	B	203	SER	3.0
1	B	228	GLN	3.0
1	B	206	ALA	2.9
1	B	265	ASN	2.9
1	B	495	SER	2.9
1	A	268	GLU	2.8
1	B	451	ILE	2.8
1	B	255	VAL	2.8
1	A	541	SER	2.8
1	A	1	GLU	2.8
1	B	208	SER	2.8
1	A	229	SER	2.7
1	A	300	VAL	2.7
1	A	119	TYR	2.7
1	B	133	TYR	2.7
1	B	236	TRP	2.7
1	B	205	GLY	2.7
1	B	471	ILE	2.7
1	A	237	ALA	2.7
1	B	151	TYR	2.7
1	A	201	GLY	2.7
1	A	498	PRO	2.7
1	A	231	THR	2.7
1	A	116	ILE	2.6
1	B	4	GLU	2.5
1	B	147	VAL	2.5
1	B	132	VAL	2.4
1	B	268	GLU	2.4
1	A	227	LEU	2.4
1	A	203	SER	2.4
1	A	322	GLN	2.4
1	B	322	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	2.3
1	B	455	PHE	2.3
1	B	191	GLY	2.3
1	A	491	ASP	2.3
1	B	350	ASN	2.3
1	A	209	VAL	2.3
1	A	123	PHE	2.2
1	B	128	ALA	2.2
1	A	151	TYR	2.2
1	A	149	MET	2.2
1	A	451	ILE	2.2
1	B	148	SER	2.2
1	B	125	SER	2.2
1	A	301	PRO	2.2
1	A	226	VAL	2.1
1	A	205	GLY	2.1
1	A	232	PRO	2.1
1	B	9	LEU	2.1
1	B	122	GLY	2.1
1	A	323	ASP	2.1
1	A	76	LEU	2.0
1	A	467	THR	2.0
1	A	115	LEU	2.0
1	A	200	PHE	2.0
1	B	105	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	544	14/15	0.82	0.40	7.93	76,79,85,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FUC	A	545	10/11	0.86	0.53	-	91,93,95,95	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( $\text{\AA}^2$ )	Q<0.9
6	AE3	A	902	9/9	0.80	0.46	7.29	81,82,83,83	0
6	AE3	B	903	9/9	0.68	0.39	5.02	83,87,89,89	0
7	PG4	B	904	11/13	0.83	0.18	3.81	87,88,90,90	0
3	NAG	B	601	14/15	0.62	0.39	3.58	87,89,91,92	0
5	P6G	A	901	19/19	0.92	0.17	2.38	61,71,75,76	0
4	CO3	B	952	4/4	0.91	0.34	1.86	63,64,64,65	0
4	CO3	A	951	4/4	0.91	0.31	1.79	50,50,51,52	0
3	NAG	A	701	14/15	0.85	0.33	-	81,85,88,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.