



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 AM GMT

PDB ID : 2Y1K
Title : STRUCTURE OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED
BY CBDP (12H SOAK): PHOSPHOSERINE ADDUCT
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Deposited on : 2010-12-08
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

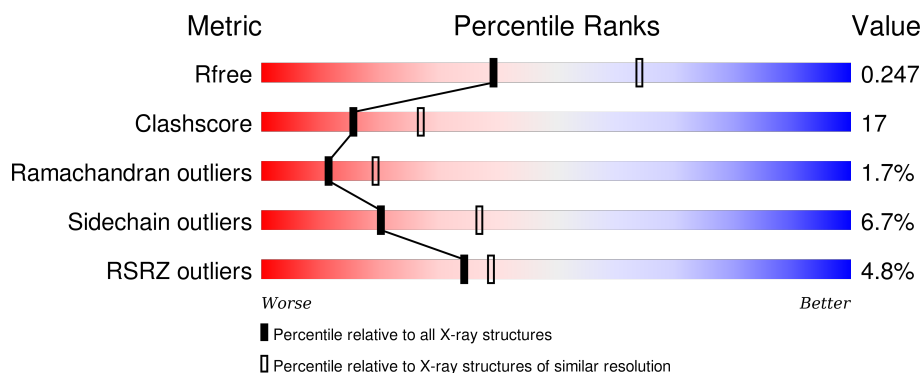
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 ≥ 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	529	

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	SO4	A	1540	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1541	-	-	-	X
4	CL	A	1533	-	-	X	-
7	NAG	A	1542	-	-	X	-
8	FU4	A	1543	-	-	-	X
8	FU4	A	1549	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4597 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 CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	P	S	0	2	0
			4193	2704	705	768	1	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

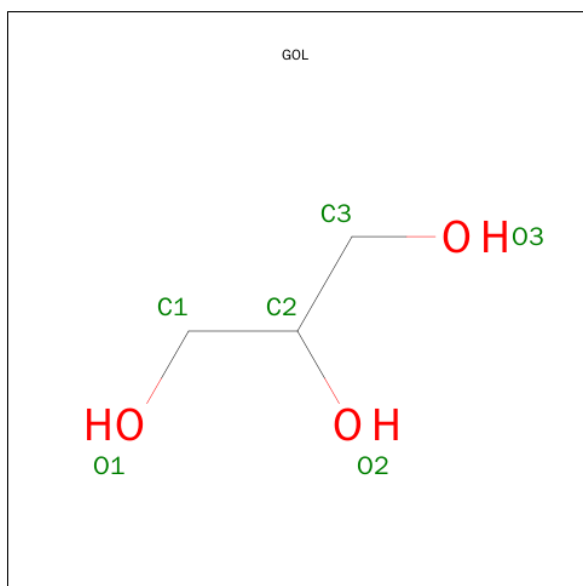
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

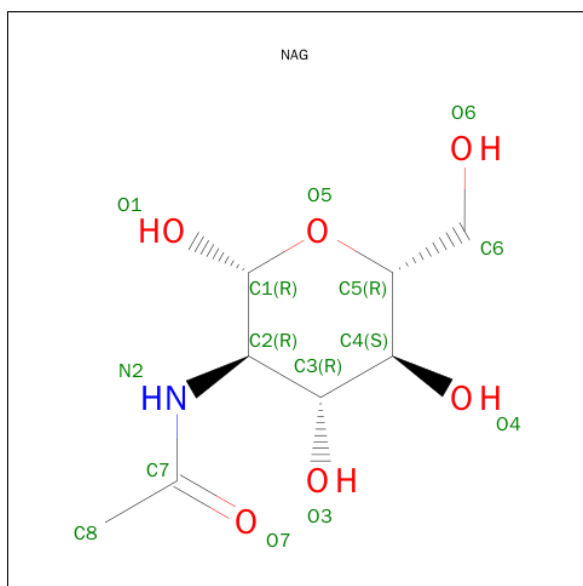


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

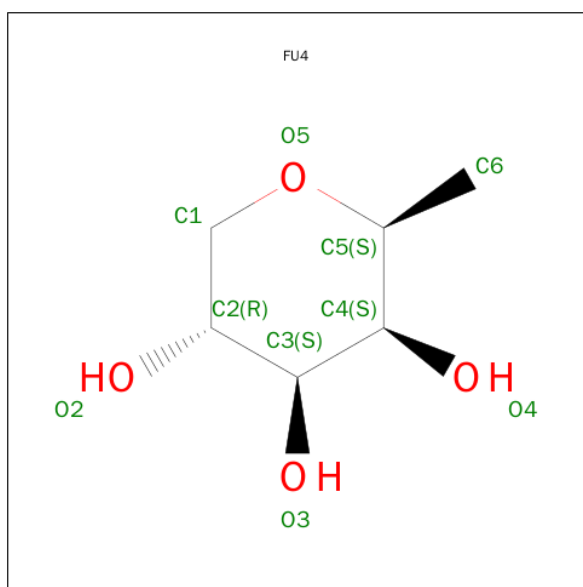
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is SUGAR (2,6-ANHYDRO-1-DEOXY-D-GALACTITOL) (three-letter code: FU4) (formula: $C_6H_{12}O_4$).



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

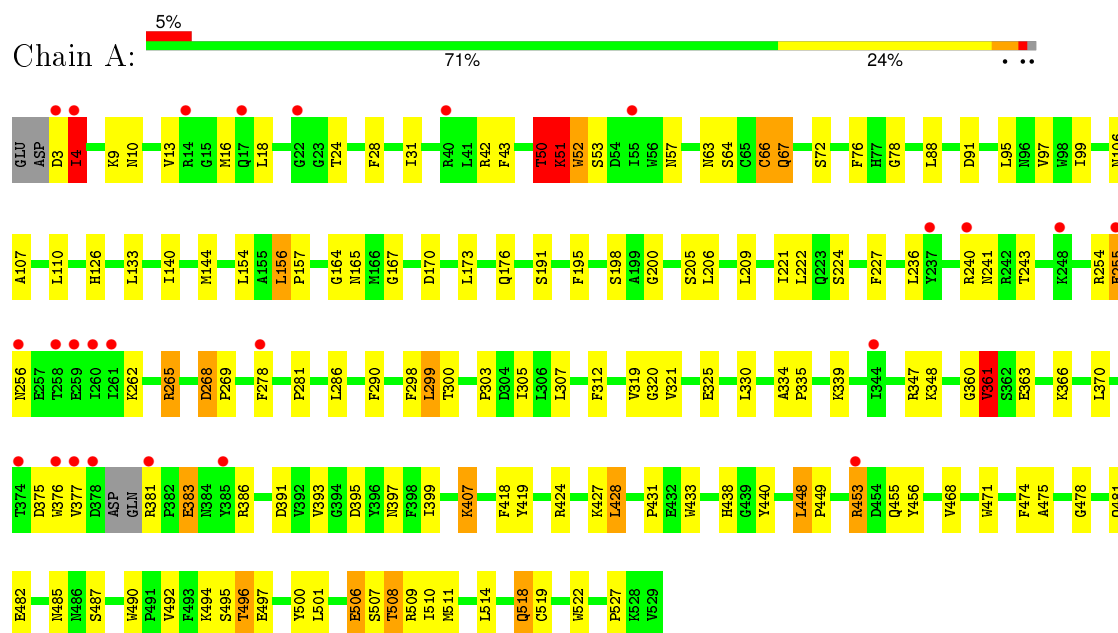
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	229	Total	O	0	0
			229	229		

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: CHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.77Å 153.77Å 127.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.38 – 2.50 41.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (41.38-2.50) 94.8 (41.38-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.183 , 0.247 0.183 , 0.247	Depositor DCC
R_{free} test set	760 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25337 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, FU4, NAG, SEP, NA, CL, FUC, SO4

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	0.90	1/4306 (0.0%)	0.86	4/5841 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CYS	CB-SG	-5.11	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	361	VAL	N-CA-C	5.39	125.55	111.00
1	A	265	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	448	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	LEU	Peptide

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	4193	0	4093	138	0
2	A	25	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	3	0
5	A	6	0	8	0	0
6	A	24	0	22	4	0
7	A	98	0	91	24	0
8	A	20	0	24	5	0
9	A	229	0	0	38	3
All	All	4597	0	4238	148	3

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 17.

All (148) 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:300:THR:HG22	9:A:2111:HOH:O	1.22	1.31
1:A:391:ASP:O	9:A:2144:HOH:O	1.52	1.26
1:A:475:ALA:HB3	9:A:2179:HOH:O	1.42	1.17
1:A:527:PRO:HD3	9:A:2214:HOH:O	1.46	1.16
7:A:1542:NAG:O6	8:A:1543:FU4:H1C2	1.46	1.15
1:A:522:TRP:O	9:A:2214:HOH:O	1.66	1.10
6:A:1536:NAG:O4	7:A:1538:NAG:C1	2.00	1.09
1:A:475:ALA:CB	9:A:2179:HOH:O	1.98	1.04
1:A:518:GLN:H	1:A:518:GLN:HE21	1.04	1.01
1:A:495:SER:HA	9:A:2192:HOH:O	1.58	1.00
4:A:1533:CL:CL	9:A:2186:HOH:O	2.18	0.98
1:A:241:ASN:HD21	7:A:1547:NAG:H4	1.26	0.97
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.32	0.93
6:A:1536:NAG:HO4	7:A:1538:NAG:C1	1.77	0.93
1:A:522:TRP:C	9:A:2214:HOH:O	2.06	0.92
1:A:381:ARG:N	9:A:2138:HOH:O	2.01	0.92
1:A:424:ARG:NH1	1:A:428:LEU:HD12	1.86	0.92
1:A:514:LEU:O	9:A:2210:HOH:O	1.89	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1536:NAG:O4	7:A:1538:NAG:O5	1.86	0.91
1:A:485:ASN:ND2	7:A:1545:NAG:H2	1.87	0.90
1:A:500:TYR:O	9:A:2199:HOH:O	1.89	0.90
1:A:501:LEU:HA	9:A:2199:HOH:O	1.70	0.89
1:A:240:ARG:HG3	9:A:2076:HOH:O	1.75	0.87
1:A:485:ASN:HD21	7:A:1545:NAG:H2	1.39	0.86
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.59	0.83
1:A:395:ASP:N	9:A:2144:HOH:O	1.82	0.82
1:A:510:ILE:O	9:A:2204:HOH:O	1.96	0.81
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.16	0.80
1:A:256:ASN:ND2	7:A:1546:NAG:C1	2.45	0.80
1:A:347:ARG:NH1	9:A:2129:HOH:O	1.93	0.79
1:A:106:ASN:HD21	7:A:1542:NAG:C1	1.97	0.78
7:A:1544:NAG:H61	9:A:2224:HOH:O	1.85	0.77
7:A:1542:NAG:O6	8:A:1543:FU4:C1	2.33	0.74
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.69	0.73
1:A:518:GLN:H	1:A:518:GLN:NE2	1.84	0.72
1:A:496:THR:N	9:A:2192:HOH:O	2.01	0.72
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.25	0.72
1:A:495:SER:CA	9:A:2192:HOH:O	2.24	0.71
1:A:485:ASN:HD21	7:A:1545:NAG:H62	1.54	0.70
1:A:485:ASN:HD21	7:A:1545:NAG:C2	2.05	0.70
1:A:241:ASN:ND2	7:A:1547:NAG:H4	2.06	0.68
1:A:51:LYS:O	1:A:52:TRP:HB3	1.93	0.68
1:A:107:ALA:HB3	1:A:140:ILE:HD12	1.74	0.68
1:A:106:ASN:CG	7:A:1542:NAG:H83	2.16	0.66
1:A:485:ASN:ND2	7:A:1545:NAG:H62	2.12	0.65
1:A:157:PRO:O	9:A:2078:HOH:O	2.14	0.65
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.78	0.64
1:A:330:LEU:O	1:A:334:ALA:HB3	1.97	0.64
1:A:509:ARG:NH1	1:A:509:ARG:HG2	2.10	0.64
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.79	0.63
1:A:50:THR:O	1:A:51:LYS:HB3	1.99	0.63
1:A:256:ASN:HD21	7:A:1546:NAG:C1	2.11	0.62
1:A:510:ILE:HA	9:A:2199:HOH:O	2.01	0.61
1:A:361:VAL:O	1:A:366:LYS:NZ	2.33	0.61
1:A:106:ASN:ND2	7:A:1542:NAG:H83	2.16	0.60
1:A:28:PHE:HB3	1:A:31:ILE:HD11	1.82	0.60
1:A:64:SER:O	1:A:88:LEU:HA	2.02	0.59
1:A:383:GLU:CD	1:A:383:GLU:H	2.05	0.59
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.07	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:SEP:HA	1:A:224:SER:O	2.01	0.59
7:A:1548:NAG:H5	8:A:1549:FU4:O2	2.03	0.59
1:A:52:TRP:HD1	1:A:53:SER:O	1.86	0.58
1:A:205:SER:HB3	1:A:222:LEU:CD2	2.33	0.57
1:A:508:THR:HB	9:A:2200:HOH:O	2.04	0.57
1:A:424:ARG:CZ	1:A:428:LEU:HD12	2.33	0.57
1:A:66:CYS:O	1:A:67:GLN:HB3	2.05	0.57
1:A:95:LEU:HD12	1:A:95:LEU:C	2.25	0.57
1:A:240:ARG:HA	9:A:2076:HOH:O	2.05	0.57
6:A:1536:NAG:O3	7:A:1538:NAG:H61	2.04	0.56
1:A:518:GLN:HE21	1:A:518:GLN:N	1.89	0.56
1:A:319:VAL:O	1:A:418:PHE:HA	2.06	0.55
1:A:126:HIS:HB2	9:A:2008:HOH:O	2.05	0.55
1:A:222:LEU:N	1:A:222:LEU:HD12	2.22	0.55
1:A:10:ASN:HB3	1:A:52:TRP:CZ3	2.42	0.54
1:A:492:VAL:CG2	1:A:494:LYS:HE2	2.37	0.54
1:A:508:THR:HG21	4:A:1533:CL:CL	2.45	0.54
7:A:1542:NAG:C6	8:A:1543:FU4:H1C2	2.36	0.53
1:A:255:GLU:HG2	1:A:256:ASN:H	1.73	0.53
1:A:509:ARG:NH1	1:A:509:ARG:CG	2.70	0.53
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.44	0.53
1:A:254:ARG:NE	9:A:2101:HOH:O	2.27	0.52
1:A:347:ARG:NH2	1:A:370:LEU:HD21	2.24	0.51
1:A:3:ASP:C	1:A:4:ILE:HG13	2.31	0.51
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.45	0.51
1:A:485:ASN:ND2	7:A:1545:NAG:C2	2.65	0.51
1:A:154:LEU:HD12	1:A:290:PHE:CE1	2.45	0.51
1:A:471:TRP:O	9:A:2179:HOH:O	2.20	0.50
1:A:221:ILE:C	1:A:222:LEU:HD12	2.31	0.50
1:A:339:LYS:O	1:A:431:PRO:HG3	2.11	0.50
1:A:508:THR:CG2	4:A:1533:CL:CL	2.97	0.49
1:A:106:ASN:ND2	7:A:1542:NAG:C1	2.72	0.49
1:A:255:GLU:CD	1:A:255:GLU:H	2.15	0.49
1:A:482:GLU:OE1	1:A:487:SER:OG	2.31	0.48
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.95	0.48
1:A:133:LEU:HD23	1:A:468:VAL:HG13	1.94	0.48
1:A:455:GLN:N	9:A:2173:HOH:O	2.46	0.48
1:A:18:LEU:O	1:A:24:THR:HA	2.14	0.48
1:A:449:PRO:HA	1:A:456:TYR:CD2	2.48	0.48
1:A:4:ILE:N	1:A:4:ILE:HD12	2.29	0.48
1:A:206:LEU:HB3	1:A:298:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.79	0.47
1:A:97:VAL:HG12	1:A:99:ILE:HG23	1.96	0.47
1:A:506:GLU:HB2	1:A:507:SER:H	1.47	0.47
1:A:164:GLY:O	1:A:165:ASN:HB2	2.15	0.47
1:A:424:ARG:HH12	1:A:428:LEU:HD12	1.76	0.47
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.51	0.46
1:A:13:VAL:HG12	1:A:52:TRP:HZ2	1.81	0.46
1:A:386:ARG:CZ	1:A:433:TRP:HB2	2.46	0.46
1:A:173:LEU:HA	1:A:173:LEU:HD12	1.71	0.46
1:A:325:GLU:O	1:A:438:HIS:HB2	2.15	0.46
1:A:527:PRO:CD	9:A:2214:HOH:O	2.29	0.46
1:A:377:VAL:HG23	9:A:2137:HOH:O	2.16	0.46
1:A:227:PHE:CD1	1:A:227:PHE:C	2.88	0.46
1:A:492:VAL:HG23	1:A:494:LYS:HE2	1.99	0.45
1:A:299:LEU:HD21	1:A:303:PRO:HD3	1.99	0.45
1:A:395:ASP:CB	9:A:2144:HOH:O	2.65	0.44
1:A:448:LEU:N	1:A:449:PRO:CD	2.80	0.44
1:A:76:PHE:CE2	1:A:78:GLY:HA3	2.52	0.44
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.32	0.44
1:A:474:PHE:O	1:A:478:GLY:N	2.51	0.44
1:A:393:VAL:O	1:A:397:ASN:HB2	2.16	0.44
1:A:191:SER:HB2	8:A:1543:FU4:H3	1.99	0.43
1:A:57:ASN:HD21	7:A:1544:NAG:C1	2.31	0.43
1:A:198:SEP:C	1:A:200:GLY:N	2.79	0.43
1:A:519:CYS:HB3	9:A:2150:HOH:O	2.18	0.43
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.84	0.43
1:A:487:SER:HB2	9:A:2182:HOH:O	2.17	0.43
1:A:265:ARG:NE	9:A:2102:HOH:O	2.37	0.43
1:A:481:GLN:HA	9:A:2183:HOH:O	2.19	0.42
1:A:42:ARG:O	1:A:43:PHE:HB2	2.19	0.42
1:A:427:LYS:O	1:A:428:LEU:C	2.56	0.42
1:A:240:ARG:CA	9:A:2076:HOH:O	2.66	0.42
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.55	0.42
1:A:492:VAL:HG21	1:A:494:LYS:HE2	2.02	0.42
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.85	0.42
1:A:407:LYS:HE3	1:A:407:LYS:HB2	1.41	0.42
1:A:255:GLU:HG2	1:A:256:ASN:N	2.32	0.41
1:A:50:THR:O	1:A:51:LYS:CB	2.65	0.41
1:A:300:THR:CG2	9:A:2111:HOH:O	2.10	0.41
1:A:268:ASP:O	1:A:269:PRO:C	2.59	0.41
1:A:428:LEU:HD23	1:A:440:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.56	0.41
1:A:255:GLU:CG	1:A:256:ASN:H	2.34	0.41
1:A:347:ARG:HH22	1:A:370:LEU:HD21	1.86	0.41
1:A:167:GLY:O	1:A:170:ASP:HB2	2.21	0.41
1:A:475:ALA:HB2	9:A:2179:HOH:O	1.94	0.40
1:A:63:ASN:HB2	1:A:91:ASP:O	2.22	0.40
1:A:453:ARG:H	1:A:453:ARG:HG2	1.43	0.40

All (3) 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)
9:A:2089:HOH:O	9:A:2091:HOH:O[7_556]	1.50	0.70
9:A:2204:HOH:O	9:A:2208:HOH:O[7_556]	1.56	0.64
9:A:2198:HOH:O	9:A:2207:HOH:O[7_556]	2.11	0.09

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	522/529 (99%)	480 (92%)	33 (6%)	9 (2%)	11 19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	281	PRO
1	A	361	VAL
1	A	496	THR
1	A	4	ILE
1	A	50	THR
1	A	52	TRP

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	360	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	449/453 (99%)	418 (93%)	31 (7%)	19	35

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

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	16	MET
1	A	50	THR
1	A	51	LYS
1	A	72	SER
1	A	110	LEU
1	A	144	MET
1	A	176	GLN
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	278	PHE
1	A	286	LEU
1	A	299	LEU
1	A	305	ILE
1	A	348	LYS
1	A	363[A]	GLU
1	A	363[B]	GLU
1	A	375	ASP
1	A	376	TRP
1	A	383	GLU

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Mol	Chain	Res	Type
1	A	407	LYS
1	A	428	LEU
1	A	453	ARG
1	A	497	GLU
1	A	506	GLU
1	A	508	THR
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	241	ASN
1	A	485	ASN
1	A	518	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SEP	A	198	1	8,9,10	3.16	2 (25%)	8,12,14	2.00	4 (50%)

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
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O2P	3.59	1.67	1.54
1	A	198	SEP	P-OG	7.74	1.86	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O-C-CA	-2.95	117.82	125.49
1	A	198	SEP	OG-P-O1P	-2.50	100.77	107.14
1	A	198	SEP	O3P-P-O1P	-2.22	103.43	110.58
1	A	198	SEP	O3P-P-O2P	2.22	115.84	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

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	$\# Z > 2$
6	NAG	A	1536	1,6	14,14,15	0.93	0	15,19,21	2.03	5 (33%)
6	FUC	A	1539	6	10,10,11	0.85	0	14,14,16	2.02	4 (28%)

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	NAG	A	1536	1,6	-	0/6/23/26	0/1/1/1
6	FUC	A	1539	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1536	NAG	C3-C4-C5	-2.13	106.48	110.20
6	A	1536	NAG	O5-C5-C6	2.26	112.24	107.35
6	A	1536	NAG	C6-C5-C4	2.66	119.56	113.02
6	A	1536	NAG	C8-C7-N2	3.13	122.10	116.11
6	A	1539	FUC	O5-C5-C6	3.34	111.65	106.13
6	A	1539	FUC	C2-C3-C4	3.36	116.75	111.04
6	A	1539	FUC	C1-O5-C5	3.56	117.88	112.38
6	A	1539	FUC	C1-C2-C3	3.75	113.98	109.54
6	A	1536	NAG	C2-N2-C7	3.86	128.00	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1536	NAG	4	0

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
2	SO4	A	1531	-	4,4,4	0.63	0	6,6,6	0.45	0
5	GOL	A	1534	-	5,5,5	0.79	0	5,5,5	1.05	0
2	SO4	A	1535	-	4,4,4	0.85	0	6,6,6	3.31	3 (50%)
2	SO4	A	1537	-	4,4,4	0.65	0	6,6,6	0.37	0
7	NAG	A	1538	-	14,14,15	0.60	0	15,19,21	1.30	2 (13%)
2	SO4	A	1540	-	4,4,4	0.78	0	6,6,6	0.41	0
2	SO4	A	1541	-	4,4,4	0.87	0	6,6,6	0.52	0
7	NAG	A	1542	-	14,14,15	0.57	0	15,19,21	1.20	2 (13%)
8	FU4	A	1543	-	10,10,10	0.66	0	14,14,14	1.16	2 (14%)
7	NAG	A	1544	-	14,14,15	0.45	0	15,19,21	1.65	4 (26%)
7	NAG	A	1545	-	14,14,15	0.91	1 (7%)	15,19,21	4.36	10 (66%)
7	NAG	A	1546	-	14,14,15	0.83	0	15,19,21	1.75	3 (20%)
7	NAG	A	1547	-	14,14,15	0.64	0	15,19,21	1.78	4 (26%)
7	NAG	A	1548	-	14,14,15	0.67	0	15,19,21	1.36	2 (13%)
8	FU4	A	1549	-	10,10,10	0.78	0	14,14,14	1.43	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	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1534	-	-	0/4/4/4	0/0/0/0
2	SO4	A	1535	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1537	-	-	0/0/0/0	0/0/0/0
7	NAG	A	1538	-	-	0/6/23/26	0/1/1/1
2	SO4	A	1540	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1541	-	-	0/0/0/0	0/0/0/0
7	NAG	A	1542	-	-	0/6/23/26	0/1/1/1
8	FU4	A	1543	-	-	0/0/17/17	0/1/1/1
7	NAG	A	1544	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1545	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1546	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1547	-	-	0/6/23/26	0/1/1/1
7	NAG	A	1548	-	-	0/6/23/26	0/1/1/1
8	FU4	A	1549	-	-	0/0/17/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1545	NAG	C1-C2	2.15	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1535	SO4	O2-S-O1	-6.91	87.60	109.50
7	A	1545	NAG	C8-C7-N2	-3.31	109.78	116.11
7	A	1545	NAG	C4-C3-C2	-2.72	107.00	111.23
7	A	1545	NAG	O7-C7-C8	-2.66	117.19	122.06
7	A	1544	NAG	O7-C7-C8	-2.64	117.21	122.06
2	A	1535	SO4	O4-S-O1	-2.57	86.23	110.19
7	A	1542	NAG	O7-C7-C8	-2.56	117.36	122.06
7	A	1547	NAG	O3-C3-C4	-2.49	104.73	110.34
7	A	1544	NAG	C4-C3-C2	-2.20	107.80	111.23
8	A	1543	FU4	C3-C4-C5	2.11	113.27	109.72
2	A	1535	SO4	O4-S-O3	2.15	117.72	108.98
7	A	1542	NAG	C8-C7-N2	2.16	120.23	116.11
7	A	1545	NAG	O3-C3-C2	2.16	113.38	109.11
7	A	1548	NAG	C3-C4-C5	2.22	114.06	110.20
7	A	1545	NAG	C3-C4-C5	2.22	114.07	110.20
7	A	1547	NAG	C3-C4-C5	2.29	114.19	110.20
7	A	1544	NAG	C8-C7-N2	2.31	120.52	116.11
7	A	1538	NAG	O5-C5-C6	2.31	112.35	107.35
7	A	1545	NAG	O5-C5-C6	2.44	112.63	107.35
7	A	1538	NAG	C4-C3-C2	2.70	115.42	111.23
7	A	1546	NAG	C3-C4-C5	2.81	115.10	110.20
8	A	1543	FU4	O5-C5-C6	2.87	110.87	106.13
7	A	1546	NAG	C2-N2-C7	2.89	126.75	123.04
7	A	1547	NAG	C1-O5-C5	3.09	116.17	112.25
7	A	1547	NAG	C2-N2-C7	3.23	127.19	123.04
8	A	1549	FU4	O5-C5-C6	3.28	111.55	106.13
7	A	1548	NAG	C4-C3-C2	3.45	116.59	111.23
7	A	1544	NAG	C1-O5-C5	3.64	116.86	112.25
7	A	1545	NAG	C1-O5-C5	3.75	117.00	112.25
7	A	1546	NAG	C4-C3-C2	4.11	117.61	111.23
7	A	1545	NAG	O7-C7-N2	5.46	133.00	121.86
7	A	1545	NAG	C3-C2-N2	5.67	124.13	110.56
7	A	1545	NAG	C2-N2-C7	12.78	139.45	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1538	NAG	4	0
7	A	1542	NAG	7	0
8	A	1543	FU4	4	0
7	A	1544	NAG	2	0
7	A	1545	NAG	6	0
7	A	1546	NAG	2	0
7	A	1547	NAG	2	0
7	A	1548	NAG	1	0
8	A	1549	FU4	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, 95th 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 ²)	Q<0.9
1	A	524/529 (99%)	0.17	25 (4%) 34 39	33, 56, 93, 147	10 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	6.2
1	A	376	TRP	4.7
1	A	377	VAL	3.9
1	A	40	ARG	3.8
1	A	259	GLU	3.8
1	A	255	GLU	3.7
1	A	4	ILE	3.7
1	A	381	ARG	3.4
1	A	261	ILE	3.3
1	A	237	TYR	3.2
1	A	256	ASN	3.2
1	A	17	GLN	3.1
1	A	55	ILE	3.0
1	A	258	THR	2.8
1	A	240	ARG	2.7
1	A	14	ARG	2.6
1	A	453	ARG	2.5
1	A	385	TYR	2.5
1	A	260	ILE	2.1
1	A	248	LYS	2.1
1	A	374	THR	2.1
1	A	344	ILE	2.0
1	A	278	PHE	2.0
1	A	378	ASP	2.0
1	A	22	GLY	2.0

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

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, 95th 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 ²)	Q<0.9
1	SEP	A	198	10/11	0.99	0.19	-	36,40,42,52	0

6.3 Carbohydrates ⓘ

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, 95th 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 ²)	Q<0.9
6	NAG	A	1536	14/15	0.97	0.14	-0.86	47,57,68,68	0
6	FUC	A	1539	10/11	0.94	0.28	-	74,83,92,99	0

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
8	FU4	A	1543	10/10	0.80	0.42	8.80	36,46,58,76	10
8	FU4	A	1549	10/10	0.92	0.51	5.18	64,99,120,122	0
2	SO4	A	1540	5/5	0.83	0.18	2.22	61,68,72,95	5
2	SO4	A	1541	5/5	0.90	0.17	2.16	56,58,71,82	5
5	GOL	A	1534	6/6	0.93	0.25	1.89	54,60,66,79	0
7	NAG	A	1545	14/15	0.87	0.18	0.97	51,89,107,108	0
2	SO4	A	1537	5/5	0.95	0.13	-0.81	78,82,91,97	0
2	SO4	A	1535	5/5	0.95	0.23	-	57,60,66,76	5
7	NAG	A	1542	14/15	0.91	0.17	-	50,87,99,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1531	5/5	0.93	0.24	-	80,83,111,112	0
7	NAG	A	1547	14/15	0.66	0.53	-	81,133,148,149	0
7	NAG	A	1546	14/15	0.79	0.36	-	75,97,112,118	0
7	NAG	A	1538	14/15	0.89	0.18	-	76,94,113,114	0
7	NAG	A	1544	14/15	0.90	0.33	-	64,88,99,121	0
4	CL	A	1533	1/1	0.96	0.11	-	73,73,73,73	0
3	NA	A	1532	1/1	0.93	0.66	-	70,70,70,70	1
7	NAG	A	1548	14/15	0.73	0.55	-	89,106,135,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.