



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:40 pm GMT

PDB ID : 4BBZ  
Title : Structure of human butyrylcholinesterase inhibited by CBDP (2-min soak):  
Cresyl-phosphoserine adduct  
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ridge, O.; Nachon, F.; Weik, M.  
Deposited on : 2012-09-30  
Resolution : 2.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

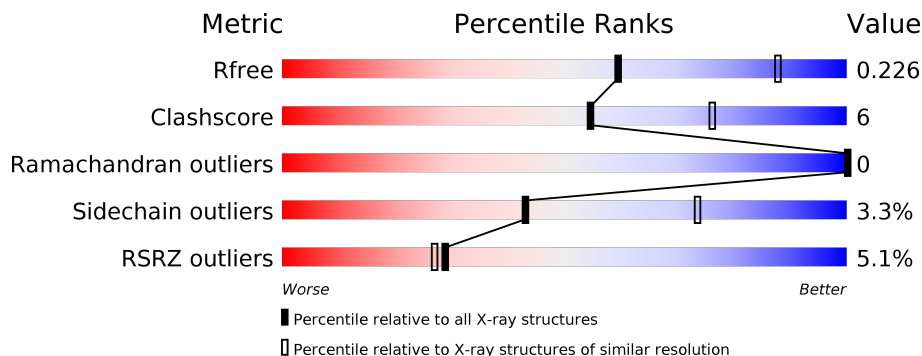
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	529	<div> <div>5%</div> <div>86%</div> <div>12%</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	UNX	A	705	-	-	-	X
2	UNX	A	706	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	712	-	-	-	X
4	NAG	A	580	-	-	-	X
5	NAG	A	560	X	-	-	-
5	FUL	A	562	-	-	-	X
6	SO4	A	703	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4547 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	527	Total	C	N	O	S	2	3	0
			4222	2725	711	771	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 UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	X	0	0
			7	7		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

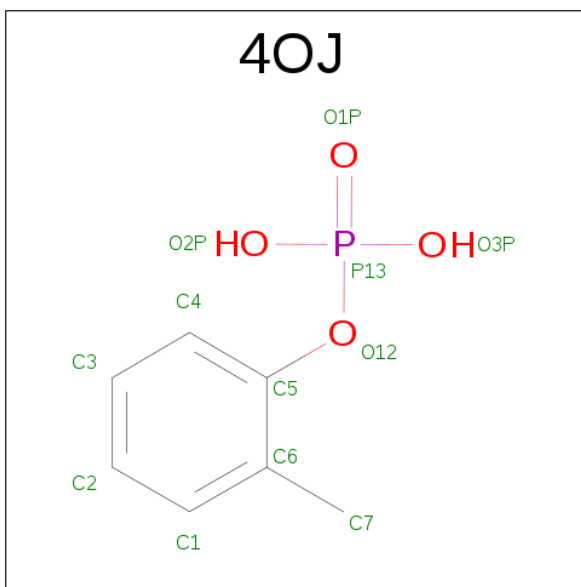


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is (2-METHYLPHENYL) DIHYDROGEN PHOSPHATE (three-letter code: 4OJ) (formula: C<sub>7</sub>H<sub>9</sub>O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			11	7	3	1		

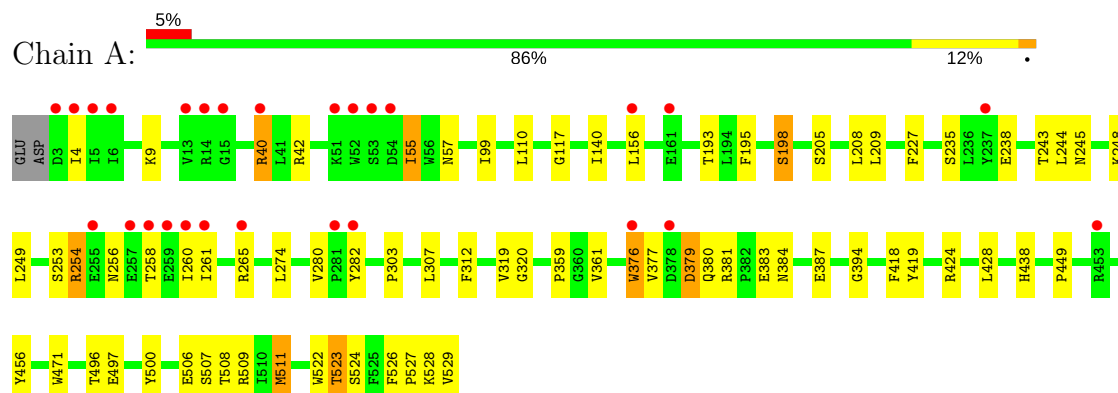
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	139	Total	O	0	0
			139	139		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: CHOLINESTERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.68Å 154.68Å 126.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.69 – 2.70 54.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (54.69-2.70) 98.1 (54.69-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, $R_{free}$	0.166 , 0.225 0.174 , 0.226	Depositor DCC
$R_{free}$ test set	1053 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, UNX, 4OJ, SO4, FUL

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	0.52	2/4352 (0.0%)	0.57	2/5908 (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
5	A	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SER	CB-OG	19.78	1.68	1.42
1	A	198	SER	CA-CB	8.17	1.65	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SER	CA-CB-OG	6.24	128.05	111.20
1	A	198	SER	CB-CA-C	5.41	120.37	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	560	NAG	C1

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4222	0	4121	48	1
2	A	7	0	0	0	0
3	A	24	0	22	1	0
4	A	42	0	39	0	0
5	A	76	0	68	4	0
6	A	25	0	0	0	1
7	A	1	0	0	0	0
8	A	11	0	7	2	0
9	A	139	0	0	2	0
All	All	4547	0	4257	51	1

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 6.

All (51) 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:198:SER:CB	1:A:198:SER:OG	1.68	1.41
1:A:424:ARG:HG3	1:A:428:LEU:HD12	1.67	0.77
5:A:570:NAG:O3	5:A:571:NAG:N2	2.26	0.68
1:A:522:TRP:O	1:A:527:PRO:HD3	1.96	0.66
1:A:117:GLY:N	8:A:1530:4OJ:O2P	2.29	0.65
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.79	0.65
1:A:379:ASP:HB2	1:A:380:GLN:HB2	1.86	0.57
1:A:379:ASP:OD1	1:A:379:ASP:N	2.37	0.57
1:A:198:SER:CB	1:A:198:SER:HG	2.11	0.54
1:A:245:ASN:HD21	5:A:560:NAG:H62	1.72	0.54
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.41	0.54
1:A:379:ASP:H	1:A:381:ARG:N	2.05	0.54
1:A:496:THR:OG1	1:A:497:GLU:OE1	2.26	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.44	0.53
1:A:379:ASP:CB	1:A:380:GLN:HB2	2.39	0.53
1:A:42:ARG:O	1:A:265:ARG:NH1	2.43	0.52
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.95	0.48
1:A:506:GLU:HG2	1:A:507:SER:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HD2	1:A:253:SER:OG	2.14	0.47
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.44	0.47
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.49	0.47
1:A:55:ILE:HD11	1:A:57:ASN:OD1	2.15	0.47
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.47
1:A:198:SER:HG	8:A:1530:4OJ:P13	2.29	0.46
1:A:156:LEU:HA	1:A:156:LEU:HD12	1.71	0.46
1:A:449:PRO:HA	1:A:456:TYR:CD2	2.50	0.46
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.96	0.46
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.80	0.46
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.50	0.45
1:A:110:LEU:HD23	1:A:193:THR:HB	1.97	0.45
1:A:282:TYR:CD1	1:A:359:PRO:HB2	2.52	0.45
3:A:540:NAG:H61	3:A:541:FUL:H2	1.38	0.45
5:A:561:NAG:H3	5:A:562:FUL:H2	1.99	0.45
1:A:526:PHE:O	1:A:529:VAL:HG22	2.16	0.45
1:A:254:ARG:H	1:A:260:ILE:HG12	1.81	0.45
1:A:235:SER:OG	1:A:238:GLU:HG2	2.18	0.44
1:A:379:ASP:H	1:A:380:GLN:C	2.21	0.44
1:A:523:THR:HG21	9:A:2096:HOH:O	2.18	0.43
1:A:249:LEU:HG	5:A:562:FUL:H62	2.01	0.43
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.53	0.43
1:A:376:TRP:CH2	1:A:384:ASN:HB3	2.54	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.55	0.42
1:A:205:SER:O	1:A:208:LEU:HB2	2.20	0.42
1:A:256:ASN:OD1	1:A:258:THR:OG1	2.30	0.41
1:A:244:LEU:O	1:A:248:LYS:HG2	2.20	0.41
1:A:198:SER:HB2	1:A:438:HIS:CE1	2.56	0.41
1:A:524:SER:O	1:A:528:LYS:HE3	2.21	0.41
1:A:40:ARG:O	1:A:265:ARG:NH1	2.54	0.41
1:A:394:GLY:HA3	9:A:2072:HOH:O	2.21	0.40
1:A:383:GLU:O	1:A:387:GLU:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ARG:NH2	6:A:703:SO4:O2[7_555]	2.19	0.01

## 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	528/529 (100%)	495 (94%)	33 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	455/454 (100%)	440 (97%)	15 (3%)	43	73

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	40	ARG
1	A	55	ILE
1	A	195	PHE
1	A	254	ARG
1	A	280	VAL
1	A	361	VAL
1	A	376	TRP
1	A	377	VAL
1	A	379	ASP
1	A	471	TRP
1	A	508	THR

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Mol	Chain	Res	Type
1	A	511	MET
1	A	523	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

8 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$
3	NAG	A	540	1,3	14,14,15	0.47	0	15,19,21	0.76	0
3	FUL	A	541	3	9,10,11	0.95	1 (11%)	13,14,16	1.32	3 (23%)
5	NAG	A	560	1,5	14,14,15	0.48	0	15,19,21	1.05	1 (6%)
5	NAG	A	561	5	14,14,15	0.52	0	15,19,21	2.18	6 (40%)
5	FUL	A	562	5	9,10,11	0.94	0	13,14,16	0.94	0
5	NAG	A	570	1,5	14,14,15	0.65	0	15,19,21	1.76	5 (33%)
5	NAG	A	571	5	14,14,15	0.61	0	15,19,21	1.65	3 (20%)
5	FUL	A	572	5	9,10,11	1.29	2 (22%)	13,14,16	0.95	0

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	540	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	541	3	-	0/0/17/20	0/1/1/1
5	NAG	A	560	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	561	5	-	0/6/23/26	0/1/1/1
5	FUL	A	562	5	-	0/0/17/20	0/1/1/1
5	NAG	A	570	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	571	5	-	0/6/23/26	0/1/1/1
5	FUL	A	572	5	-	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	572	FUL	C4-C3	2.09	1.57	1.52
3	A	541	FUL	C1-C2	2.25	1.57	1.52
5	A	572	FUL	C4-C5	2.44	1.57	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	570	NAG	O5-C1-C2	-3.85	106.11	111.47
5	A	561	NAG	O5-C1-C2	-3.69	106.34	111.47
5	A	561	NAG	C2-N2-C7	-3.08	118.45	122.94
5	A	570	NAG	O3-C3-C2	-2.83	103.32	109.39
5	A	561	NAG	C4-C3-C2	-2.67	107.11	111.02
5	A	570	NAG	C3-C4-C5	-2.07	106.57	110.22
5	A	561	NAG	C1-C2-N2	2.20	114.25	110.49
3	A	541	FUL	C1-C2-C3	2.22	112.46	109.65
5	A	571	NAG	C2-N2-C7	2.23	126.19	122.94
3	A	541	FUL	O5-C1-C2	2.31	114.40	110.79
5	A	570	NAG	O6-C6-C5	2.33	119.17	111.34
5	A	560	NAG	C1-O5-C5	2.49	115.60	112.17
3	A	541	FUL	C1-O5-C5	2.62	118.20	112.39
5	A	570	NAG	C4-C3-C2	2.86	115.22	111.02
5	A	571	NAG	C3-C4-C5	2.97	115.45	110.22
5	A	561	NAG	C3-C4-C5	3.05	115.59	110.22
5	A	571	NAG	C4-C3-C2	3.78	116.55	111.02
5	A	561	NAG	C1-O5-C5	4.66	118.59	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	560	NAG	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	540	NAG	1	0
3	A	541	FUL	1	0
5	A	560	NAG	1	0
5	A	561	NAG	1	0
5	A	562	FUL	2	0
5	A	570	NAG	1	0
5	A	571	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic and 7 are unknown - leaving 9 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	$\# Z  > 2$
8	4OJ	A	1530	1	8,11,12	0.68	0	11,14,17	1.02	0
4	NAG	A	550	1	14,14,15	0.52	0	15,19,21	1.32	1 (6%)
4	NAG	A	580	1	14,14,15	0.54	0	15,19,21	0.90	1 (6%)
4	NAG	A	590	1	14,14,15	0.42	0	15,19,21	0.62	0
6	SO4	A	700	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	A	701	-	4,4,4	0.15	0	6,6,6	0.07	0
6	SO4	A	702	-	4,4,4	0.18	0	6,6,6	0.14	0
6	SO4	A	703	-	4,4,4	0.09	0	6,6,6	0.23	0
6	SO4	A	704	-	4,4,4	0.15	0	6,6,6	0.16	0

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
8	4OJ	A	1530	1	-	0/2/4/5	0/1/1/1
4	NAG	A	550	1	-	1/6/23/26	0/1/1/1
4	NAG	A	580	1	-	0/6/23/26	0/1/1/1
4	NAG	A	590	1	-	0/6/23/26	0/1/1/1
6	SO4	A	700	-	-	0/0/0/0	0/0/0/0
6	SO4	A	701	-	-	0/0/0/0	0/0/0/0
6	SO4	A	702	-	-	0/0/0/0	0/0/0/0
6	SO4	A	703	-	-	0/0/0/0	0/0/0/0
6	SO4	A	704	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	580	NAG	O5-C1-C2	-2.08	108.58	111.47
4	A	550	NAG	C1-O5-C5	4.60	118.51	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	550	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1530	4OJ	2	0
6	A	703	SO4	0	1

## 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	527/529 (99%)	0.03	27 (5%)	29 27	16, 35, 74, 125	5 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	7.0
1	A	258	THR	3.9
1	A	255	GLU	3.7
1	A	237	TYR	3.3
1	A	261	ILE	3.2
1	A	259	GLU	2.9
1	A	156	LEU	2.8
1	A	51	LYS	2.8
1	A	53	SER	2.7
1	A	54	ASP	2.6
1	A	4	ILE	2.6
1	A	282	TYR	2.5
1	A	378	ASP	2.5
1	A	257	GLU	2.5
1	A	15	GLY	2.5
1	A	453	ARG	2.4
1	A	52	TRP	2.4
1	A	40	ARG	2.3
1	A	260	ILE	2.3
1	A	5	ILE	2.2
1	A	13	VAL	2.2
1	A	6	ILE	2.2
1	A	376	TRP	2.2
1	A	281	PRO	2.1
1	A	265	ARG	2.1
1	A	14	ARG	2.1
1	A	161	GLU	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
5	FUL	A	562	10/11	0.90	0.47	4.02	87,94,99,101	0
5	NAG	A	570	14/15	0.96	0.16	-0.12	24,42,55,59	0
3	NAG	A	540	14/15	0.91	0.32	-	76,87,89,92	0
5	FUL	A	572	10/11	0.85	0.28	-	34,48,54,59	10
5	NAG	A	571	14/15	0.85	0.18	-	66,75,80,81	0
3	FUL	A	541	10/11	0.73	0.30	-	95,103,112,113	0
5	NAG	A	561	14/15	0.73	0.57	-	94,107,118,118	0
5	NAG	A	560	14/15	0.81	0.35	-	79,90,96,104	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
2	UNX	A	712	1/1	0.91	0.93	25.32	30,30,30,30	0
2	UNX	A	705	1/1	0.95	0.39	13.31	44,44,44,44	0
2	UNX	A	706	1/1	0.94	0.41	12.43	41,41,41,41	0
6	SO4	A	703	5/5	0.86	0.28	5.64	75,79,84,86	5
4	NAG	A	580	14/15	0.82	0.22	2.36	45,65,77,78	0
8	4OJ	A	1530	11/12	0.98	0.20	1.51	21,39,46,53	0
6	SO4	A	704	5/5	0.96	0.16	-0.29	54,64,65,74	5
4	NAG	A	590	14/15	0.88	0.36	-	78,87,91,91	0
2	UNX	A	711	1/1	0.92	0.87	-	32,32,32,32	0
2	UNX	A	709	1/1	0.97	0.32	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	550	14/15	0.83	0.19	-	56,67,70,70	0
6	SO4	A	702	5/5	0.89	0.16	-	93,94,101,101	0
2	UNX	A	710	1/1	0.99	0.30	-	45,45,45,45	0
2	UNX	A	707	1/1	0.84	0.40	-	53,53,53,53	0
6	SO4	A	701	5/5	0.98	0.09	-	88,91,93,94	0
7	CL	A	713	1/1	0.77	0.14	-	77,77,77,77	0
6	SO4	A	700	5/5	0.98	0.12	-	22,24,29,33	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.