



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:27 PM GMT

PDB ID : 4AXB
Title : Crystal structure of soman-aged human butyrylcholinesterase in complex with 2-PAM
Authors : Wandhammer, M.; de Koning, M.; Noort, D.; Goeldner, M.; Nachon, F.
Deposited on : 2012-06-12
Resolution : 2.40 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

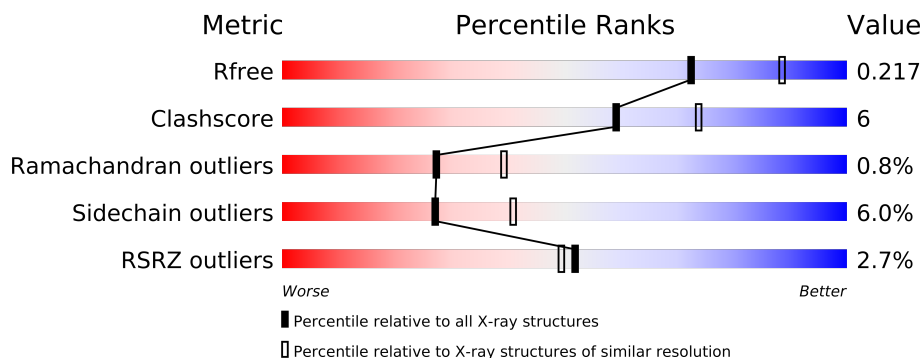
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	527	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	K	A	1538	-	X
3	SO4	A	1531	-	X
4	GOL	A	1532	-	X
4	GOL	A	1533	-	X
4	GOL	A	1540	-	X
5	CL	A	1534	-	X
5	CL	A	1537	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	FP1	A	1535	-	X
8	NAG	A	1544	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 4792 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

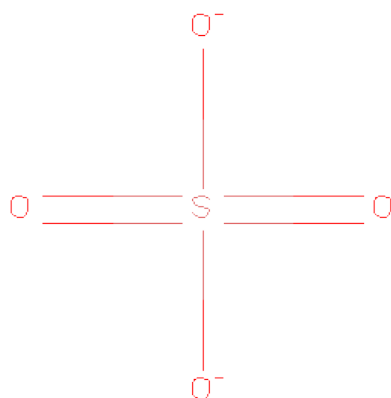
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	P	S	0	10	0
			4261	2751	713	780	1	16			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

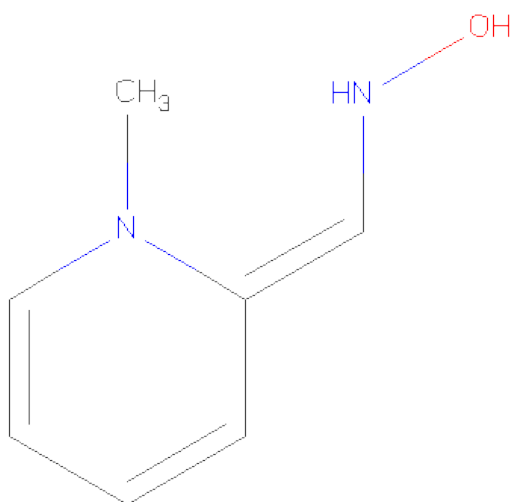


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		

- Molecule 6 is N-HYDROXY-1-(1-METHYLPYRIDIN-2(1H)-YLIDENE)METHANAMINE (three-letter code: FP1) (formula: $C_7H_{10}N_2O$).

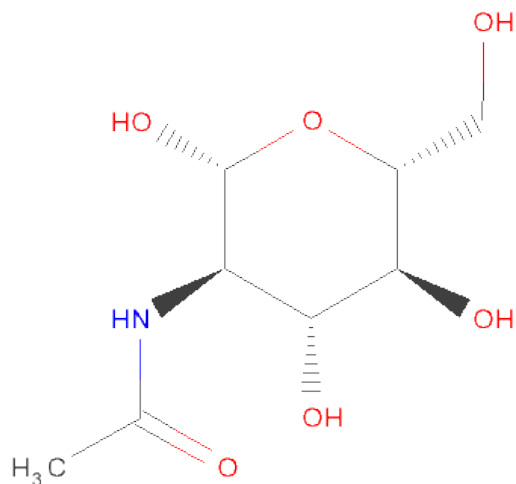


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

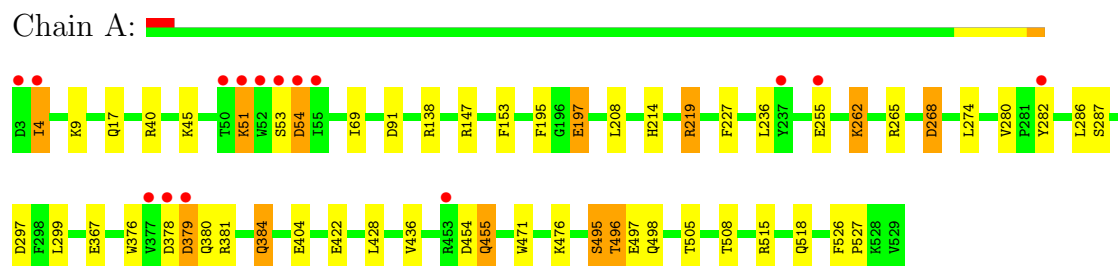
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	356	Total	O	0	0
			356	356		

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: CHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.95Å 155.95Å 127.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.27 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (110.27-2.40) 99.6 (49.32-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.221 0.166 , 0.217	Depositor DCC
R_{free} test set	1563 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30991 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4792	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL, K, FP1, SO4, FUL, SBG

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	3.50	7/4406 (0.2%)	1.07	10/5978 (0.2%)

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
7	A	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	155.49	5.21	1.32
1	A	455[B]	GLN	CD-NE2	155.49	5.21	1.32
1	A	436	VAL	CB-CG2	6.42	1.66	1.52
1	A	153	PHE	CE1-CZ	5.99	1.48	1.37
1	A	404	GLU	CG-CD	5.88	1.60	1.51
1	A	497	GLU	CD-OE1	5.80	1.32	1.25
1	A	197	GLU	CB-CG	5.25	1.62	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455[A]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[B]	GLN	CG-CD-NE2	-27.78	50.02	116.70
1	A	455[A]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	455[B]	GLN	OE1-CD-NE2	10.69	146.48	121.90
1	A	219	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	236	LEU	CA-CB-CG	-6.10	101.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	147	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	138	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	265	ARG	NE-CZ-NH1	-5.01	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1548	NAG	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4261	0	0	24	0
2	A	2	0	0	0	1
3	A	10	0	0	2	0
4	A	18	0	24	1	0
5	A	3	0	0	1	0
6	A	10	0	10	1	0
7	A	76	0	68	1	0
8	A	56	0	52	1	0
9	A	356	0	0	10	0
All	All	4792	0	154	28	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1536:CL:CL	9:A:2230:HOH:O	2.20	0.95
1:A:496:THR:N	9:A:2317:HOH:O	2.03	0.90
3:A:1531:SO4:O2	9:A:2269:HOH:O	1.93	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:376:TRP:O	9:A:2241:HOH:O	2.05	0.73
1:A:4:ILE:N	1:A:4:ILE:CD1	2.54	0.71
7:A:1549:NAG:H2	7:A:1550:FUL:O2	1.98	0.63
1:A:495:SER:CA	9:A:2317:HOH:O	2.48	0.61
1:A:262:LYS:NZ	9:A:2179:HOH:O	2.35	0.59
1:A:53:SER:O	1:A:54:ASP:CG	2.43	0.57
1:A:378:ASP:O	1:A:379:ASP:C	2.42	0.56
1:A:40:ARG:NE	9:A:2029:HOH:O	2.37	0.56
8:A:1545:NAG:C6	9:A:2348:HOH:O	2.54	0.55
1:A:381:ARG:NH1	1:A:384:GLN:NE2	2.56	0.54
1:A:268:ASP:OD1	1:A:268:ASP:N	2.40	0.54
1:A:495:SER:O	1:A:496:THR:OG1	2.27	0.53
1:A:227:PHE:CD1	1:A:227:PHE:C	2.82	0.52
1:A:45:LYS:NZ	1:A:297:ASP:OD2	2.43	0.52
1:A:378:ASP:O	1:A:379:ASP:O	2.28	0.51
1:A:378:ASP:O	1:A:380:GLN:NE2	2.45	0.49
1:A:45:LYS:NZ	4:A:1532:GOL:H12	2.27	0.49
1:A:476:LYS:NZ	9:A:2122:HOH:O	2.48	0.47
1:A:54:ASP:C	1:A:54:ASP:OD1	2.53	0.47
1:A:378:ASP:C	1:A:379:ASP:O	2.53	0.44
1:A:498:GLN:NE2	9:A:2322:HOH:O	2.51	0.43
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.72	0.42
1:A:197:GLU:OE1	6:A:1535:FP1:H3	2.19	0.42
1:A:526:PHE:N	1:A:527:PRO:CD	2.83	0.42
1:A:515:ARG:N	3:A:1531:SO4:O1	2.53	0.42

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	Distance(Å)	Clash(Å)
2:A:1538:K:K	2:A:1538:K:K[5_555]	1.93	0.27

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	534/527 (101%)	508 (95%)	22 (4%)	4 (1%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	379	ASP
1	A	496	THR
1	A	54	ASP

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	461/451 (102%)	432 (94%)	29 (6%)	25	38

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	17	GLN
1	A	51	LYS
1	A	69	ILE
1	A	195	PHE
1	A	219	ARG
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	280	VAL
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	299	LEU
1	A	367[A]	GLU
1	A	367[B]	GLU
1	A	384	GLN

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Mol	Chain	Res	Type
1	A	422	GLU
1	A	428	LEU
1	A	454	ASP
1	A	455[A]	GLN
1	A	455[B]	GLN
1	A	471	TRP
1	A	495	SER
1	A	505	THR
1	A	508	THR
1	A	518	GLN

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 chains 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	SBG	A	198	1	9,9,10	6.02	3 (33%)	10,12,14	2.75	5 (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	SBG	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SBG	O-C	16.53	1.22	1.11
1	A	198	SBG	P1-OG	6.19	1.67	1.58
1	A	198	SBG	CA-C	3.03	1.54	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SBG	OG-P1-O2	-5.80	93.99	111.99
1	A	198	SBG	C-CA-N	-4.21	109.62	113.83
1	A	198	SBG	OG-CB-CA	2.68	112.48	108.69
1	A	198	SBG	O1-P1-OG	2.66	114.33	105.82
1	A	198	SBG	O1-P1-C1	2.38	116.81	108.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

6 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	$\# Z > 2$
7	NAG	A	1541	1,7	12,14,15	1.09	2 (16%)	15,19,21	2.25	6 (40%)
7	NAG	A	1542	7	12,14,15	0.76	0	15,19,21	2.07	5 (33%)
7	FUL	A	1543	7	9,10,11	1.21	0	10,14,16	2.19	4 (40%)
7	NAG	A	1548	1,7	12,14,15	0.61	0	15,19,21	1.77	5 (33%)
7	NAG	A	1549	7	12,14,15	0.94	0	15,19,21	1.64	3 (20%)
7	FUL	A	1550	7	9,10,11	1.03	0	10,14,16	1.69	2 (20%)

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
7	NAG	A	1541	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1542	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1543	7	-	0/0/17/20	0/1/1/1
7	NAG	A	1548	1,7	1/1/5/7	0/6/23/26	1/1/1/1
7	NAG	A	1549	7	-	0/6/23/26	0/1/1/1
7	FUL	A	1550	7	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1541	NAG	C2-N2	-2.63	1.43	1.46
7	A	1541	NAG	O5-C5	-2.02	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1541	NAG	O5-C5-C6	4.67	111.88	106.98
7	A	1542	NAG	O5-C5-C6	4.45	111.65	106.98
7	A	1543	FUL	C6-C5-C4	4.40	120.21	113.06
7	A	1549	NAG	C2-N2-C7	3.97	129.75	123.09
7	A	1541	NAG	C8-C7-N2	3.83	123.59	116.11
7	A	1541	NAG	C2-N2-C7	3.78	129.43	123.09
7	A	1543	FUL	C3-C4-C5	3.77	116.12	109.84
7	A	1550	FUL	C3-C4-C5	3.42	115.53	109.84
7	A	1542	NAG	C3-C4-C5	3.35	116.18	110.20
7	A	1548	NAG	C8-C7-N2	3.17	122.30	116.11
7	A	1548	NAG	O7-C7-C8	-3.16	115.88	122.04
7	A	1542	NAG	O7-C7-C8	-3.07	116.05	122.04
7	A	1543	FUL	C4-C3-C2	2.83	114.30	110.50
7	A	1550	FUL	O5-C5-C6	2.80	112.54	108.03
7	A	1549	NAG	O5-C5-C6	2.78	109.89	106.98
7	A	1541	NAG	O7-C7-C8	-2.61	116.94	122.04
7	A	1542	NAG	C4-C3-C2	2.44	117.30	111.32
7	A	1548	NAG	C3-C4-C5	-2.40	105.92	110.20
7	A	1549	NAG	C3-C4-C5	2.29	114.30	110.20
7	A	1548	NAG	C2-N2-C7	2.27	126.90	123.09
7	A	1543	FUL	O5-C5-C6	2.23	111.62	108.03
7	A	1541	NAG	O6-C6-C5	2.19	118.91	111.36
7	A	1548	NAG	C3-C2-N2	2.17	115.06	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1541	NAG	O4-C4-C5	-2.03	103.93	109.28
7	A	1542	NAG	C3-C2-N2	-2.01	108.70	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1548	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1548	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\# Z > 2$
3	SO4	A	1531	-	4,4,4	0.77	0	6,6,6	0.57	0
4	GOL	A	1532	-	5,5,5	0.32	0	5,5,5	0.83	0
4	GOL	A	1533	-	5,5,5	0.31	0	5,5,5	1.42	1 (20%)
6	FP1	A	1535	-	10,10,10	1.72	1 (10%)	10,12,12	2.88	4 (40%)
3	SO4	A	1539	-	4,4,4	0.21	0	6,6,6	0.43	0
4	GOL	A	1540	-	5,5,5	0.59	0	5,5,5	0.31	0
8	NAG	A	1544	1	12,14,15	0.76	0	15,19,21	1.90	4 (26%)
8	NAG	A	1545	1	12,14,15	0.59	0	15,19,21	2.63	4 (26%)
8	NAG	A	1546	1	12,14,15	0.63	0	15,19,21	2.04	3 (20%)
8	NAG	A	1547	1	12,14,15	0.80	0	15,19,21	2.38	2 (13%)

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	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1532	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1533	-	-	0/4/4/4	0/0/0/0
6	FP1	A	1535	-	-	0/0/3/3	0/1/1/1
3	SO4	A	1539	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1540	-	-	0/4/4/4	0/0/0/0
8	NAG	A	1544	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1545	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1546	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1547	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1535	FP1	O1-N2	4.27	1.47	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1547	NAG	O5-C5-C6	7.77	115.14	106.98
8	A	1545	NAG	O5-C5-C6	7.50	114.86	106.98
6	A	1535	FP1	C4-C5-N1	5.49	121.47	117.41
8	A	1546	NAG	O5-C5-C6	5.39	112.64	106.98
6	A	1535	FP1	C5-C6-N2	-4.90	112.48	125.33
6	A	1535	FP1	C1-N1-C5	-4.57	117.17	121.76
8	A	1545	NAG	O5-C5-C4	3.77	115.44	110.65
8	A	1545	NAG	C6-C5-C4	-3.73	103.98	113.00
8	A	1547	NAG	O5-C5-C4	-3.58	106.11	110.65
8	A	1544	NAG	C2-N2-C7	3.48	128.94	123.09
8	A	1544	NAG	C8-C7-N2	3.23	122.43	116.11
8	A	1546	NAG	C3-C4-C5	3.04	115.63	110.20
8	A	1546	NAG	O5-C5-C4	2.99	114.44	110.65
8	A	1544	NAG	O4-C4-C5	2.97	117.12	109.28
8	A	1545	NAG	C8-C7-N2	2.28	120.56	116.11
8	A	1544	NAG	O5-C5-C6	2.19	109.28	106.98
6	A	1535	FP1	C7-N1-C5	2.07	122.34	120.74
4	A	1533	GOL	C3-C2-C1	-2.06	102.15	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	527/527 (100%)	-0.37	15 (2%)	50 48	18, 33, 62, 80	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	3.9
1	A	55	ILE	3.4
1	A	54	ASP	3.3
1	A	53	SER	3.1
1	A	237	TYR	3.1
1	A	378	ASP	3.0
1	A	255	GLU	2.7
1	A	379	ASP	2.6
1	A	453	ARG	2.6
1	A	377	VAL	2.5
1	A	51	LYS	2.4
1	A	282	TYR	2.4
1	A	50	THR	2.4
1	A	4	ILE	2.1
1	A	52	TRP	2.1

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SBG	A	198	10/11	0.12	-0.55	11,18,22,22	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	FUL	A	1543	10/11	0.26	29.87	71,76,77,77	0
7	NAG	A	1542	14/15	0.17	4.03	69,73,77,79	0
7	FUL	A	1550	10/11	0.31	1.95	77,79,80,80	0
7	NAG	A	1548	14/15	0.23	0.06	70,80,85,90	0
7	NAG	A	1541	14/15	0.14	-0.15	42,53,63,68	0
7	NAG	A	1549	14/15	0.42	-	98,104,107,108	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	1532	6/6	0.23	7.68	74,75,76,76	0
6	FP1	A	1535	10/10	0.27	6.05	50,56,57,59	0
4	GOL	A	1533	6/6	0.20	4.38	47,54,55,56	0
2	K	A	1538	1/1	0.26	4.00	112,112,112,112	0
5	CL	A	1537	1/1	0.14	3.60	73,73,73,73	0
8	NAG	A	1544	14/15	0.20	3.16	59,65,68,69	0
3	SO4	A	1531	5/5	0.22	3.05	76,77,79,80	0
5	CL	A	1534	1/1	0.20	2.71	52,52,52,52	0
4	GOL	A	1540	6/6	0.21	2.18	44,52,56,58	0
8	NAG	A	1547	14/15	0.35	1.69	77,84,87,87	0
8	NAG	A	1546	14/15	0.20	1.56	60,73,80,81	0
2	K	A	1530	1/1	0.15	0.87	63,63,63,63	0
3	SO4	A	1539	5/5	0.13	-0.60	94,94,94,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	A	1536	1/1	0.06	-3.64	80,80,80,80	0
8	NAG	A	1545	14/15	0.29	-	66,72,77,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.