



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:15 PM GMT

PDB ID : 2XQI
Title : X-ray Structure of human butyrylcholinesteraseinhibited by racemic CVX
Authors : Wandhammer, M.; Carletti, E.; Gillon, E.; Masson, P.; Goeldner, M.; Noort, D.; Nachon, F.
Deposited on : 2010-09-02
Resolution : 2.60 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>

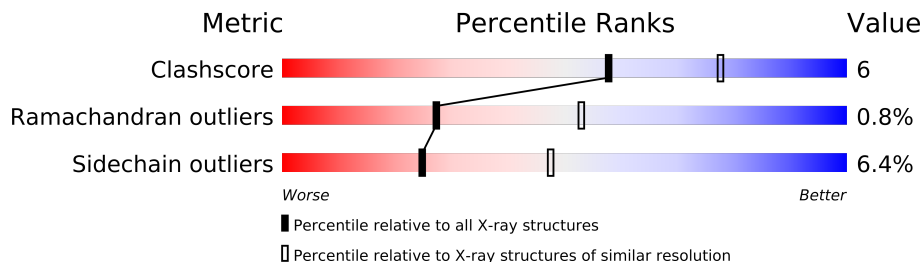
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
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 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	527	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 4691 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.

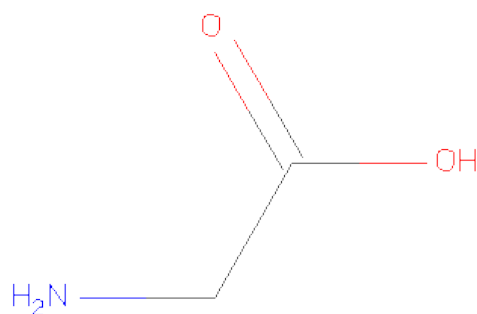
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4258	2749	712	782	15	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

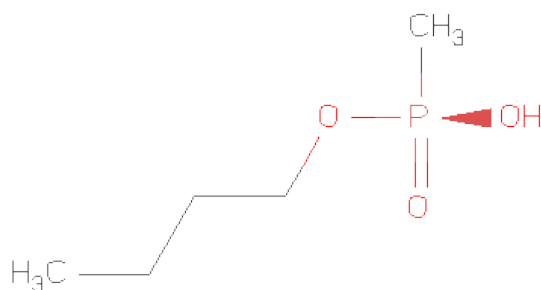
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	5	2	1	2	0	0

- Molecule 3 is O-BUTYLMETHYLPHOSPHONICACID ESTER GROUP (three-letter code: CVX) (formula: $C_5H_{13}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	5	2	1		

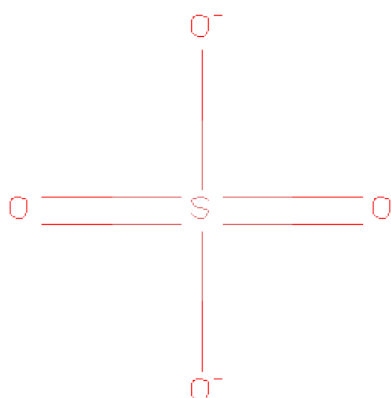
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		

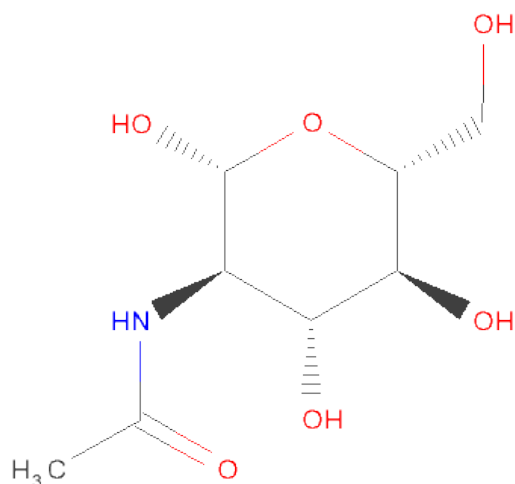
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

There are 4 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
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

There are 4 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
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 10 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	25	Total 25	X 25	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	247	Total 247	O 247	0	0

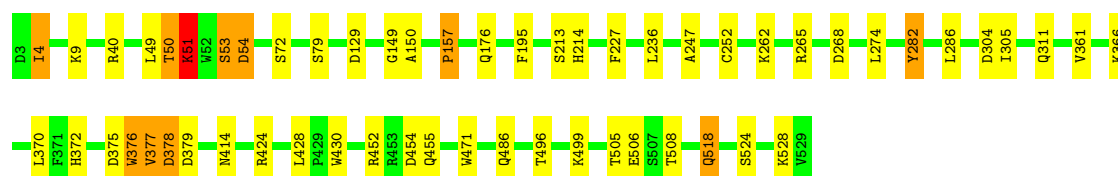
3 Residue-property plots

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.

Note EDS failed to run properly.

• Molecule 1: CHOLINESTERASE

Chain A: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.15Å 155.15Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.60	Depositor
% Data completeness (in resolution range)	96.0 (49.06-2.60)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.247	Depositor
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.138	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 23433 reflections	Xtriage
Total number of atoms	4691	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: NAG, CVX, CL, UNX, NA, 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	0.97	1/4402 (0.0%)	0.84	1/5975 (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
9	A	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	ASP	C-N	5.01	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	LEU	CA-CB-CG	5.19	127.23	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1564	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	455	GLN	Peptide

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	4258	0	0	27	0
2	A	5	0	2	1	0
3	A	8	0	12	0	0
4	A	3	0	0	0	0
5	A	3	0	0	0	0
6	A	10	0	0	2	0
7	A	38	0	33	0	0
8	A	56	0	52	1	0
9	A	38	0	34	0	0
10	A	25	0	0	1	0
11	A	247	0	0	9	1
All	All	4691	0	133	29	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 (29) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:376:TRP:O	11:A:2155:HOH:O	1.94	0.85
1:A:414[A]:ASN:ND2	6:A:1555:SO4:O1	2.21	0.74
1:A:361:VAL:O	1:A:366:LYS:NZ	2.27	0.67
1:A:129:ASP:OD1	2:A:1554:GLY:N	2.28	0.66
1:A:265:ARG:NE	11:A:2108:HOH:O	2.35	0.60
1:A:4:ILE:N	1:A:4:ILE:CD1	2.64	0.60
10:A:1647:UNX:UNK	10:A:1655:UNX:UNK	1.44	0.60
1:A:311:GLN:NE2	11:A:2124:HOH:O	2.34	0.59
8:A:1563:NAG:H82	11:A:2245:HOH:O	2.03	0.59
1:A:508:THR:N	11:A:2223:HOH:O	2.38	0.57
1:A:282:TYR:O	1:A:282:TYR:CD2	2.58	0.56
1:A:176[A]:GLN:NE2	11:A:2080:HOH:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:PHE:CD1	1:A:227:PHE:C	2.81	0.54
1:A:149:GLY:O	1:A:150:ALA:C	2.46	0.52
1:A:372[B]:HIS:NE2	6:A:1556:SO4:O3	2.45	0.48
1:A:377:VAL:N	1:A:378:ASP:CA	2.77	0.48
1:A:50:THR:O	1:A:51:LYS:CB	2.62	0.47
1:A:40:ARG:NH2	11:A:2014:HOH:O	2.49	0.46
1:A:53:SER:O	1:A:54:ASP:CG	2.54	0.46
1:A:518:GLN:N	1:A:518:GLN:NE2	2.63	0.45
1:A:213:SER:O	1:A:214:HIS:C	2.55	0.45
1:A:268:ASP:OD1	1:A:268:ASP:N	2.49	0.44
1:A:377:VAL:N	1:A:378:ASP:CB	2.81	0.44
1:A:524:SER:O	1:A:528:LYS:NZ	2.51	0.43
1:A:51:LYS:N	11:A:2022:HOH:O	2.52	0.41
1:A:282:TYR:N	1:A:282:TYR:CD2	2.85	0.41
1:A:424:ARG:NH2	1:A:430:TRP:O	2.53	0.41
1:A:499:LYS:NZ	11:A:2217:HOH:O	2.52	0.41
1:A:247:ALA:O	1:A:252:CYS:N	2.54	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	Distance(Å)	Clash(Å)
11:A:2074:HOH:O	11:A:2225:HOH:O[7_555]	2.10	0.10

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%)	497 (93%)	33 (6%)	4 (1%)	30 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	157	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	ASP
1	A	496	THR

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	461/452 (102%)	430 (93%)	31 (7%)	23	44

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	49	LEU
1	A	50	THR
1	A	51	LYS
1	A	53	SER
1	A	54	ASP
1	A	72	SER
1	A	79	SER
1	A	157	PRO
1	A	195	PHE
1	A	236	LEU
1	A	262	LYS
1	A	274	LEU
1	A	282	TYR
1	A	286	LEU
1	A	304[A]	ASP
1	A	304[B]	ASP
1	A	305	ILE
1	A	375	ASP
1	A	376	TRP
1	A	377	VAL
1	A	379	ASP
1	A	428	LEU
1	A	452	ARG
1	A	471	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	GLN
1	A	505	THR
1	A	506[A]	GLU
1	A	506[B]	GLU
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 ⓘ

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

5.5 Carbohydrates ⓘ

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	FUL	A	1559	7	9,10,11	1.12	0	10,14,16	2.02	2 (20%)
9	NAG	A	1564	1,9	12,14,15	0.64	0	15,19,21	1.65	3 (20%)
9	NAG	A	1565	9	12,14,15	0.87	1 (8%)	15,19,21	1.81	4 (26%)
9	FUL	A	1566	9	9,10,11	0.96	0	10,14,16	1.66	2 (20%)
7	NAG	A	1567	1,7	12,14,15	1.01	1 (8%)	15,19,21	2.23	7 (46%)
7	NAG	A	1568	7	12,14,15	0.75	0	15,19,21	2.48	5 (33%)

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	FUL	A	1559	7	-	0/0/17/20	0/1/1/1
9	NAG	A	1564	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	A	1565	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1566	9	-	0/0/17/20	0/1/1/1
7	NAG	A	1567	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1568	7	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1567	NAG	C2-N2	-2.61	1.43	1.46
9	A	1565	NAG	C2-N2	2.24	1.49	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1568	NAG	O5-C5-C6	6.02	113.30	106.98
7	A	1568	NAG	C3-C2-N2	-5.80	102.94	111.76
7	A	1567	NAG	C2-N2-C7	5.14	131.72	123.09
9	A	1565	NAG	C2-N2-C7	4.42	130.51	123.09
7	A	1559	FUL	C4-C3-C2	4.21	116.15	110.50
9	A	1564	NAG	O5-C5-C4	3.47	115.06	110.65
9	A	1566	FUL	O2-C2-C3	-3.36	102.93	110.18
7	A	1559	FUL	C3-C4-C5	3.33	115.38	109.84
7	A	1567	NAG	O5-C5-C6	3.04	110.17	106.98
9	A	1565	NAG	O5-C5-C4	2.80	114.20	110.65
9	A	1564	NAG	C2-N2-C7	2.79	127.78	123.09
7	A	1567	NAG	C3-C4-C5	-2.77	105.25	110.20
7	A	1567	NAG	C6-C5-C4	2.72	119.58	113.00
7	A	1567	NAG	O6-C6-C5	2.68	120.58	111.36
9	A	1565	NAG	O5-C5-C6	2.62	109.73	106.98
9	A	1566	FUL	C3-C4-C5	2.61	114.19	109.84
9	A	1564	NAG	O5-C5-C6	2.48	109.58	106.98
7	A	1568	NAG	O5-C5-C4	-2.25	107.79	110.65
9	A	1565	NAG	O7-C7-N2	2.16	126.42	121.90
7	A	1567	NAG	C8-C7-N2	2.14	120.29	116.11
7	A	1568	NAG	C2-N2-C7	2.12	126.64	123.09
7	A	1567	NAG	C3-C2-N2	-2.01	108.70	111.76
7	A	1568	NAG	C4-C3-C2	2.00	116.22	111.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1564	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 25 are unknown and 6 are monoatomic - leaving 8 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	CVX	A	1530	1	5,7,8	1.50	1 (20%)	4,7,10	1.00	0
2	GLY	A	1554	-	4,4,4	0.79	0	4,4,4	1.17	0
6	SO4	A	1555	-	4,4,4	0.27	0	6,6,6	0.27	0
6	SO4	A	1556	-	4,4,4	0.10	0	6,6,6	0.24	0
8	NAG	A	1560	1	12,14,15	0.68	0	15,19,21	1.44	3 (20%)
8	NAG	A	1561	1	12,14,15	0.76	0	15,19,21	1.41	5 (33%)
8	NAG	A	1562	1	12,14,15	0.66	0	15,19,21	1.22	2 (13%)
8	NAG	A	1563	1	12,14,15	0.93	0	15,19,21	2.74	5 (33%)

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	CVX	A	1530	1	-	0/3/5/6	0/0/0/0
2	GLY	A	1554	-	-	0/2/2/2	0/0/0/0
6	SO4	A	1555	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1556	-	-	0/0/0/0	0/0/0/0
8	NAG	A	1560	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1561	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1562	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1563	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)
3	A	1530	CVX	P-O3	-3.11	1.54	1.60

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1563	NAG	O5-C5-C6	7.00	114.32	106.98
8	A	1563	NAG	O5-C5-C4	-5.37	103.84	110.65
8	A	1560	NAG	O5-C5-C6	3.22	110.36	106.98
8	A	1563	NAG	C2-N2-C7	2.85	127.87	123.09
8	A	1562	NAG	O5-C5-C6	2.63	109.74	106.98
8	A	1563	NAG	C3-C4-C5	-2.60	105.55	110.20
8	A	1560	NAG	O4-C4-C5	2.49	115.85	109.28
8	A	1561	NAG	O5-C5-C6	2.46	109.56	106.98
8	A	1563	NAG	O4-C4-C3	2.43	115.80	110.35
8	A	1562	NAG	C2-N2-C7	-2.21	119.37	123.09
8	A	1561	NAG	C8-C7-N2	2.17	120.34	116.11
8	A	1560	NAG	C8-C7-N2	2.16	120.32	116.11
8	A	1561	NAG	C3-C4-C5	2.13	114.00	110.20
8	A	1561	NAG	O7-C7-C8	-2.09	117.96	122.04
8	A	1561	NAG	C3-C2-N2	2.06	114.91	111.76

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.