W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:36 AM GMT

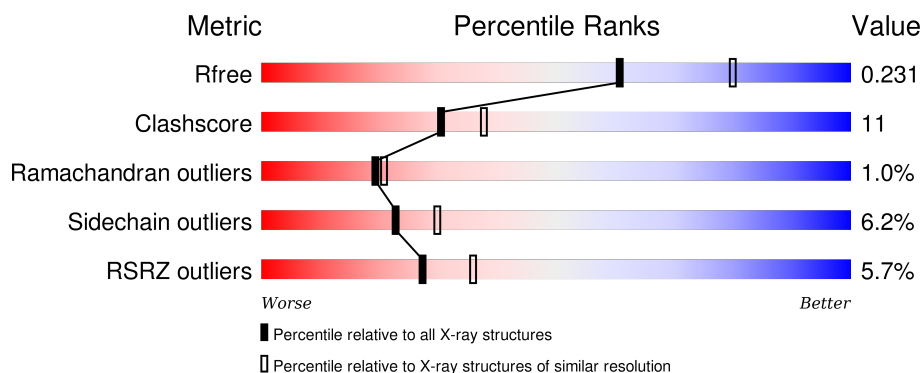|		
PDB ID	:	2XQG
Title	:	X-ray Structure of human butyrylcholinesterase inhibited by racemic VR
Authors	:	Wandhammer, M.; Carletti, E.; Gillon, E.; Masson, P.; Goeldner, M.; Noort, D.; Nachon, F.
Deposited on	:	2010-09-02
Resolution	:	2.30 Å(reported)

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 2.30 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		11
Ramachandran outliers		1.0%
Sidechain outliers		6.2%
RSRZ outliers		5.7%

Worse .... *Better*

▋ Percentile relative to all X-ray structures
❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	527	6% ... 81% ... 14% · ·

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
10	NAG	A	1561	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	1508	-	-	-	X
2	UNX	A	1510	-	-	-	X
2	UNX	A	1523	-	-	-	X
9	NAG	A	1563	X	-	-	-
9	FUL	A	1565	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 4862 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 4258	C 2750	N 712	O 780	S 16	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 UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	X 23	0	0

- Molecule 3 is 2-METHYLPROPYL HYDROGEN (R)-METHYLPHOSPHONATE (three-letter code: VR) (formula: $C_5H_{13}O_3P$).
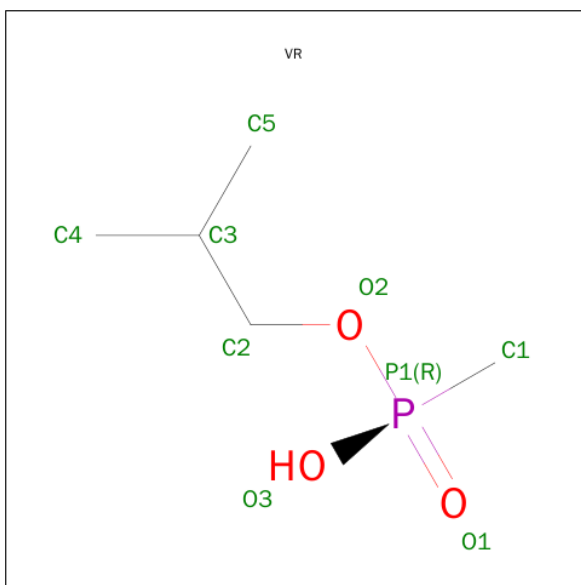
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	5	2	1		

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).
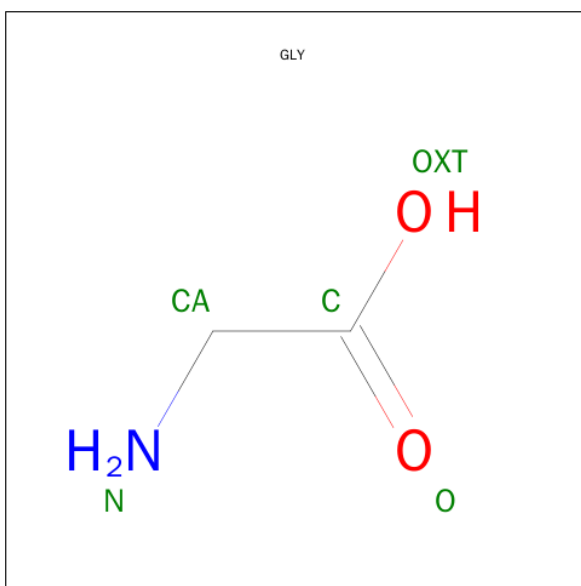
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Ca 3	0	0

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total 2	Na 2	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
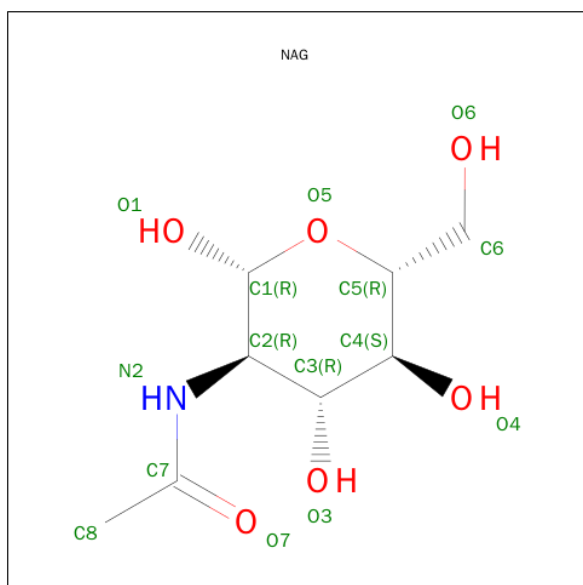
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total 14	C 8	N 1	O 5	0	0
10	A	1	Total 14	C 8	N 1	O 5	0	0
10	A	1	Total 14	C 8	N 1	O 5	0	0
10	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	419	Total 419	O 419	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.

• Molecule 1: CHOLINESTERASE
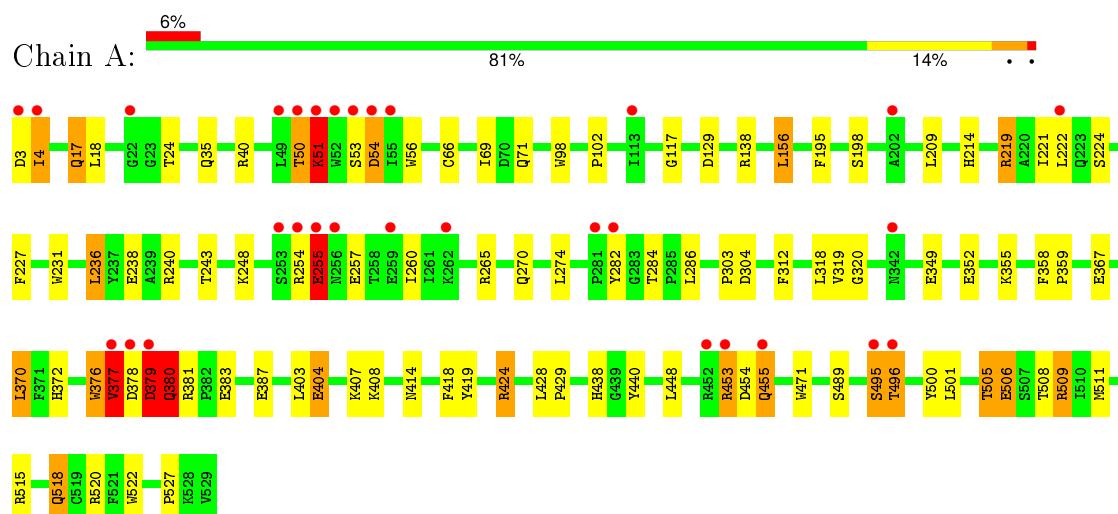
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.60Å 154.60Å 127.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.51 – 2.30 41.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.51-2.30) 99.8 (41.51-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.162 , 0.215 0.178 , 0.231	Depositor DCC
R_{free} test set	1036 reflections (3.10%)	DCC
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 34419 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4862	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 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, UNX, NA, CA, VR, SO4, BR, 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	1.35	6/4402 (0.1%)	0.97	12/5974 (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
1	A	0	2
9	A	1	0
All	All	1	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	35.94	2.22	1.32
1	A	455[B]	GLN	CD-NE2	35.94	2.22	1.32
1	A	231	TRP	CE3-CZ3	6.00	1.48	1.38
1	A	255	GLU	CB-CG	5.42	1.62	1.52
1	A	404	GLU	CG-CD	5.35	1.59	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455[A]	GLN	CG-CD-NE2	-10.66	91.11	116.70
1	A	455[B]	GLN	CG-CD-NE2	-10.66	91.11	116.70
1	A	219	ARG	NE-CZ-NH1	-10.03	115.29	120.30
1	A	455[A]	GLN	OE1-CD-NE2	9.12	142.87	121.90
1	A	455[B]	GLN	OE1-CD-NE2	9.12	142.87	121.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1563	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	VAL	Peptide
1	A	380	GLN	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	4258	0	4166	93	0
2	A	23	0	0	1	0
3	A	8	0	12	3	0
4	A	5	0	2	2	0
5	A	10	0	0	0	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
9	A	76	0	68	2	0
10	A	56	0	52	1	0
11	A	1	0	0	0	0
12	A	419	0	0	22	0
All	All	4862	0	4300	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 96 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:4:ILE:HD12	1:A:4:ILE:H	1.01	1.11
1:A:4:ILE:N	1:A:4:ILE:HD12	1.66	1.10
1:A:453:ARG:HG2	1:A:453:ARG:NH1	1.49	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HH11	1:A:453:ARG:CG	1.69	1.05
1:A:4:ILE:CD1	1:A:4:ILE:H	1.75	0.98

There are no symmetry-related clashes.

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	534/527 (101%)	515 (96%)	14 (3%)	5 (1%)	21 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	377	VAL
1	A	51	LYS
1	A	496	THR
1	A	379	ASP

5.3.2 Protein sidechains (i)

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%)	431 (94%)	30 (6%)	21 27

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LEU
1	A	376	TRP
1	A	506[B]	GLU
1	A	370	LEU
1	A	377	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	518	GLN
1	A	275	ASN
1	A	172	GLN
1	A	517	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#|Z| > 2$
9	NAG	A	1556	1,9	14,14,15	0.66	0	15,19,21	2.35	7 (46%)
9	NAG	A	1557	9	14,14,15	0.75	0	15,19,21	2.61	3 (20%)
9	FUL	A	1558	9	10,10,11	1.05	0	14,14,16	3.21	6 (42%)
9	NAG	A	1563	1,9	14,14,15	0.54	0	15,19,21	2.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	NAG	A	1564	9	14,14,15	1.35	2 (14%)	15,19,21	2.59	4 (26%)
9	FUL	A	1565	9	10,10,11	0.91	1 (10%)	14,14,16	2.65	8 (57%)

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
9	NAG	A	1556	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1557	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1558	9	-	0/0/17/20	0/1/1/1
9	NAG	A	1563	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	A	1564	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1565	9	-	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)
9	A	1565	FUL	C4-C5	2.03	1.57	1.52
9	A	1564	NAG	C2-N2	2.27	1.50	1.46
9	A	1564	NAG	C1-C2	3.84	1.57	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1558	FUL	C1-C2-C3	-8.59	99.38	109.54
9	A	1565	FUL	C1-O5-C5	-5.30	104.20	112.38
9	A	1556	NAG	C3-C4-C5	-5.29	100.98	110.20
9	A	1558	FUL	C1-O5-C5	-4.77	105.01	112.38
9	A	1565	FUL	C1-C2-C3	-4.52	104.19	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1563	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1564	NAG	1	0
9	A	1565	FUL	1	0

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 23 are unknown and 7 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	VR	A	1530	1	3,7,8	0.42	0	4,8,11	0.68	0
4	GLY	A	1548	-	1,4,4	0.66	0	0,4,4	0.00	-
5	SO4	A	1549	-	4,4,4	0.50	0	6,6,6	0.34	0
5	SO4	A	1550	-	4,4,4	0.41	0	6,6,6	0.44	0
10	NAG	A	1559	1	14,14,15	1.15	1 (7%)	15,19,21	2.10	3 (20%)
10	NAG	A	1560	1	14,14,15	0.58	0	15,19,21	2.29	5 (33%)
10	NAG	A	1561	1	14,14,15	0.87	0	15,19,21	1.75	2 (13%)
10	NAG	A	1562	1	14,14,15	0.96	1 (7%)	15,19,21	1.67	3 (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
3	VR	A	1530	1	-	0/3/5/6	0/0/0/0
4	GLY	A	1548	-	-	0/0/2/2	0/0/0/0
5	SO4	A	1549	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1550	-	-	0/0/0/0	0/0/0/0
10	NAG	A	1559	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1560	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1561	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1562	1	-	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)
10	A	1562	NAG	C1-C2	2.40	1.55	1.52
10	A	1559	NAG	C1-C2	2.91	1.56	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1559	NAG	O7-C7-C8	-3.14	116.30	122.06
10	A	1560	NAG	O7-C7-C8	-2.09	118.23	122.06
10	A	1562	NAG	O3-C3-C2	2.09	113.25	109.11
10	A	1560	NAG	C3-C2-N2	2.48	116.49	110.56
10	A	1560	NAG	C8-C7-N2	2.48	120.86	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1530	VR	3	0
4	A	1548	GLY	2	0
10	A	1559	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.27	30 (5%)	27	36	19, 34, 62, 95	14 (2%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLU	5.8
1	A	378	ASP	5.3
1	A	455[A]	GLN	5.0
1	A	379	ASP	4.8
1	A	50	THR	4.7

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, 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
9	FUL	A	1565	10/11	0.86	0.36	2.86	75,78,80,80	0
9	NAG	A	1556	14/15	0.97	0.15	-0.65	35,49,56,65	0
9	FUL	A	1558	10/11	0.83	0.35	-	71,75,76,79	0
9	NAG	A	1563	14/15	0.90	0.28	-	66,77,86,88	0
9	NAG	A	1564	14/15	0.49	0.53	-	93,99,101,101	0
9	NAG	A	1557	14/15	0.85	0.27	-	66,71,75,79	0

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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, 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
2	UNX	A	1523	1/1	0.86	0.40	9.17	43,43,43,43	0
10	NAG	A	1561	14/15	0.80	0.22	3.21	47,66,73,74	0
2	UNX	A	1508	1/1	0.90	0.26	3.09	20,20,20,20	0
2	UNX	A	1510	1/1	0.87	0.24	2.57	32,32,32,32	0
3	VR	A	1530	8/9	0.99	0.23	1.16	16,26,36,38	0
4	GLY	A	1548	5/5	0.94	0.13	1.00	39,41,42,42	0
5	SO4	A	1549	5/5	0.95	0.15	0.25	24,26,27,32	5
2	UNX	A	1509	1/1	0.95	0.12	-0.22	29,29,29,29	0
5	SO4	A	1550	5/5	0.93	0.13	-1.05	61,61,65,65	5
7	BR	A	1554	1/1	0.97	0.16	-	105,105,105,105	0
2	UNX	A	1519	1/1	0.71	0.78	-	51,51,51,51	0
10	NAG	A	1559	14/15	0.82	0.22	-	54,61,64,67	0
10	NAG	A	1562	14/15	0.79	0.41	-	76,84,90,92	0
2	UNX	A	1514	1/1	0.96	0.39	-	36,36,36,36	0
2	UNX	A	1504	1/1	0.89	0.72	-	26,26,26,26	0
10	NAG	A	1560	14/15	0.79	0.38	-	63,71,76,78	0
2	UNX	A	1517	1/1	0.90	0.07	-	40,40,40,40	0
2	UNX	A	1503	1/1	0.52	0.16	-	47,47,47,47	0
2	UNX	A	1513	1/1	0.88	0.25	-	24,24,24,24	0
2	UNX	A	1506	1/1	0.76	0.43	-	23,23,23,23	0
6	CA	A	1553	1/1	0.91	0.22	-	66,66,66,66	0
2	UNX	A	1512	1/1	0.71	0.29	-	33,33,33,33	0
2	UNX	A	1501	1/1	0.69	0.97	-	56,56,56,56	0
2	UNX	A	1515	1/1	0.93	0.46	-	34,34,34,34	0
2	UNX	A	1505	1/1	0.95	0.51	-	37,37,37,37	0
2	UNX	A	1502	1/1	0.31	0.38	-	47,47,47,47	0
6	CA	A	1551	1/1	0.92	0.28	-	73,73,73,73	0
2	UNX	A	1521	1/1	0.82	0.45	-	37,37,37,37	0
8	NA	A	1555	1/1	0.86	0.22	-	60,60,60,60	1
2	UNX	A	1518	1/1	0.92	0.14	-	48,48,48,48	0
2	UNX	A	1522	1/1	0.90	0.38	-	23,23,23,23	0
2	UNX	A	1520	1/1	0.91	0.33	-	45,45,45,45	0
6	CA	A	1552	1/1	0.95	0.25	-	61,61,61,61	0
2	UNX	A	1516	1/1	0.75	0.19	-	34,34,34,34	0
11	CL	A	1566	1/1	0.95	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
8	NA	A	1567	1/1	0.90	0.17	-	63,63,63,63	0
2	UNX	A	1511	1/1	0.87	0.18	-	26,26,26,26	0
2	UNX	A	1507	1/1	0.83	1.29	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.