



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:37 AM GMT

PDB ID : 2XQF  
Title : X-RAY STRUCTURE OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY RACEMIC VX  
Authors : Wandhammer, M.; Carletti, E.; Gillon, E.; Masson, P.; Goeldner, M.; Noort, D.; Nachon, F.  
Deposited on : 2010-09-02  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

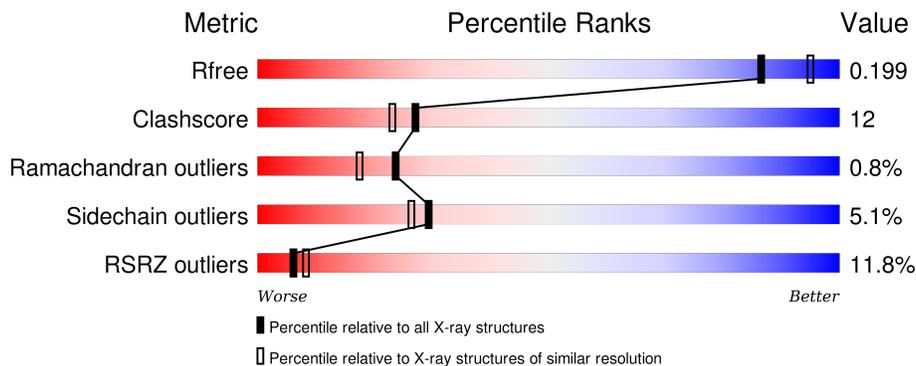
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	527	

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	1543	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	1554	-	-	X	-
3	UNX	A	1562	-	-	-	X
3	UNX	A	1565	-	-	-	X
3	UNX	A	1567	-	-	-	X
3	UNX	A	1583	-	-	-	X
8	SO4	A	1537	-	-	-	X
9	NAG	A	1545	X	-	-	-
9	FUL	A	1547	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4894 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.

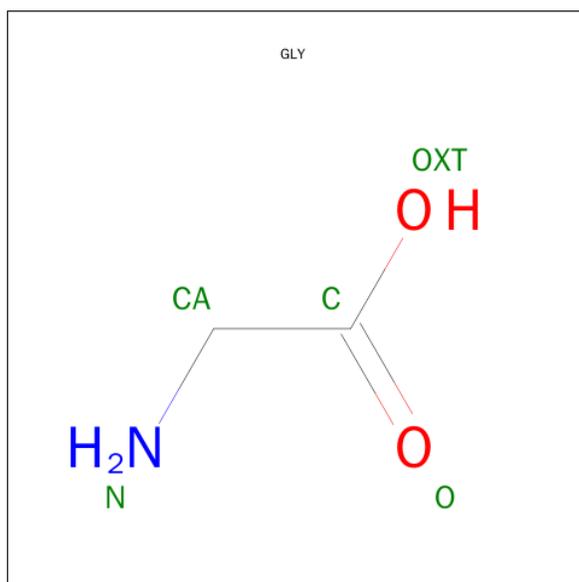
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4269	2759	712	782	16	0	11	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: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).

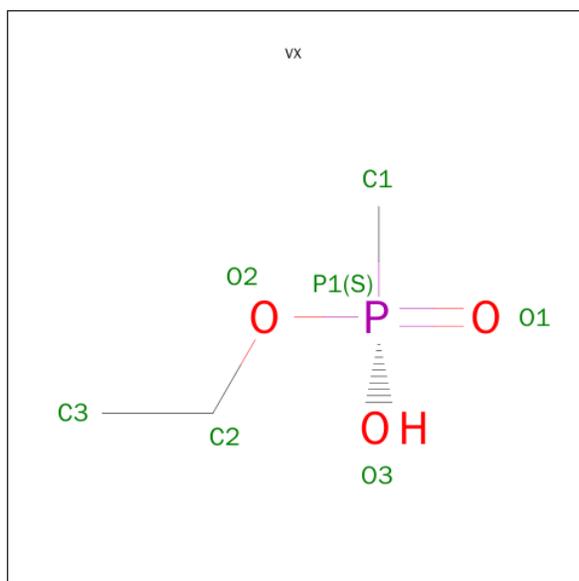


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	5	2	1	2	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total X 36 36	0	0

- Molecule 4 is O-ETHYLMETHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VX) (formula: C<sub>3</sub>H<sub>9</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 6 3 2 1	0	0

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

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

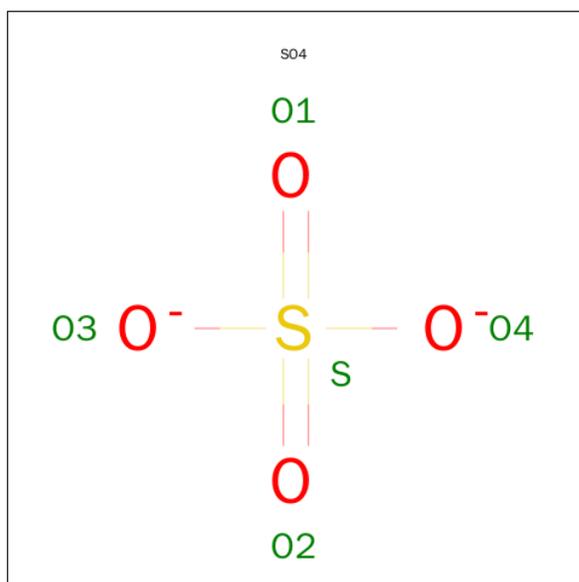
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

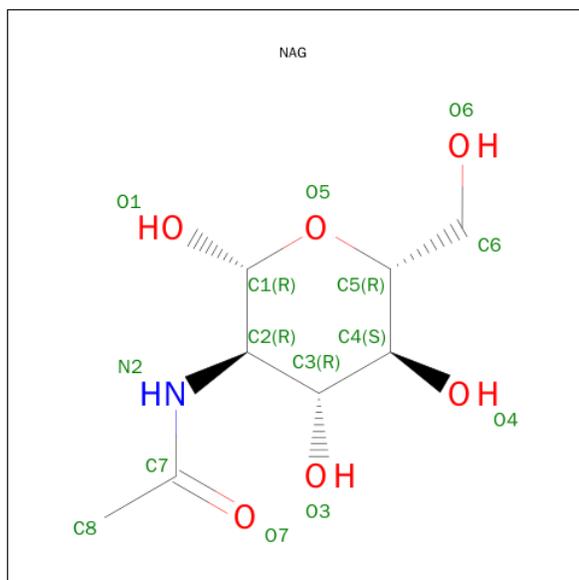


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0

- 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 38 22 2 14	0	0
9	A	3	Total C N O 38 22 2 14	0	0

- Molecule 10 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
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

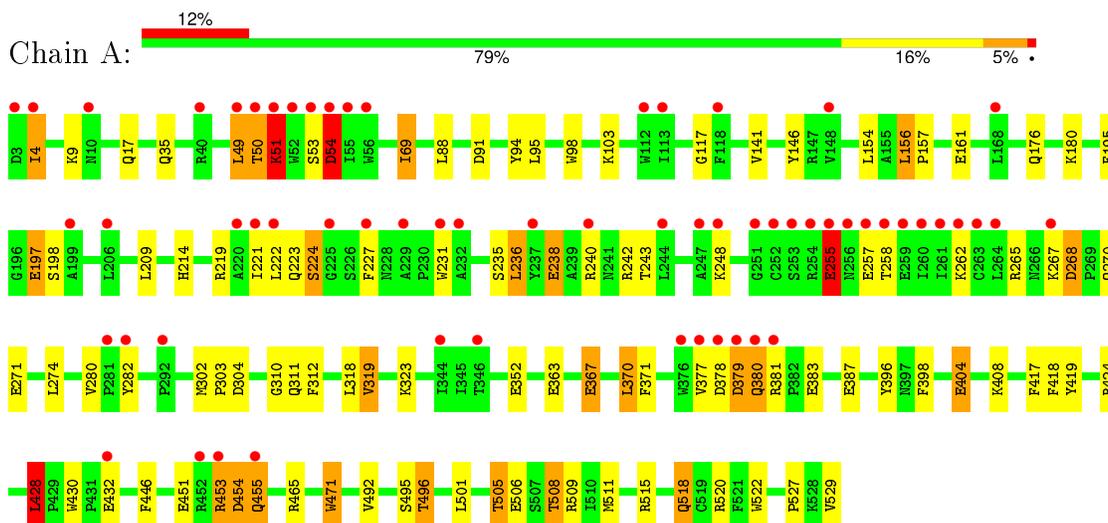
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	432	Total	O	0	0
			432	432		

### 3 Residue-property plots [i](#)

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

- Molecule 1: CHOLINESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.11Å 155.11Å 128.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.10 47.95 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.10) 99.6 (47.95-2.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.12 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.149 , 0.189 0.199 , 0.199	Depositor DCC
$R_{free}$ test set	1242 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.762	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Outliers	0 of 31041 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 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, K, SO4, VX, 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	1.54	24/4419 (0.5%)	1.08	21/5997 (0.4%)

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
9	A	1	0

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	29.84	2.07	1.32
1	A	455[B]	GLN	CD-NE2	29.84	2.07	1.32
1	A	471	TRP	CB-CG	8.46	1.65	1.50
1	A	219	ARG	CG-CD	7.64	1.71	1.51
1	A	396	TYR	CD1-CE1	6.89	1.49	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NE-CZ-NH1	-10.75	114.92	120.30
1	A	515	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	515	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	370	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	465	ARG	NE-CZ-NH2	-6.88	116.86	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1545	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	4269	0	4183	99	0
2	A	5	0	2	1	0
3	A	36	0	0	4	0
4	A	6	0	8	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	10	0	0	0	0
9	A	76	0	67	2	0
10	A	56	0	52	1	0
11	A	432	0	0	28	4
All	All	4894	0	4312	105	4

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 12.

The worst 5 of 105 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:453:ARG:HH11	1:A:453:ARG:CG	1.47	1.27
1:A:495:SER:HA	11:A:2385:HOH:O	1.51	1.10
1:A:453:ARG:HG2	1:A:453:ARG:NH1	1.33	1.09
1:A:455[A]:GLN:NE2	1:A:455[A]:GLN:CD	2.07	1.08
1:A:4:ILE:H	1:A:4:ILE:HD12	1.23	1.01

All (4) 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)
11:A:2240:HOH:O	11:A:2365:HOH:O[3_555]	1.86	0.34
11:A:2239:HOH:O	11:A:2365:HOH:O[3_555]	2.05	0.15
11:A:2179:HOH:O	11:A:2239:HOH:O[4_555]	2.14	0.06
11:A:2233:HOH:O	11:A:2368:HOH:O[3_555]	2.19	0.01

### 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	536/527 (102%)	516 (96%)	16 (3%)	4 (1%)	26 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	A	496	THR
1	A	51	LYS
1	A	54	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	463/452 (102%)	438 (95%)	25 (5%)	27 24

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	280	VAL
1	A	518	GLN
1	A	268	ASP
1	A	367[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	518	GLN
1	A	311	GLN
1	A	214	HIS
1	A	380	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	1538	1,9	14,14,15	1.66	3 (21%)	15,19,21	1.92	4 (26%)
9	NAG	A	1539	9	14,14,15	0.58	0	15,19,21	2.38	5 (33%)
9	FUL	A	1540	9	10,10,11	1.14	1 (10%)	14,14,16	3.96	5 (35%)
9	NAG	A	1545	1,9	14,14,15	0.78	0	15,19,21	2.13	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	1546	9	14,14,15	1.50	2 (14%)	15,19,21	2.59	5 (33%)
9	FUL	A	1547	9	10,10,11	0.78	0	14,14,16	3.00	5 (35%)

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	1538	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1539	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1540	9	-	0/0/17/20	0/1/1/1
9	NAG	A	1545	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	A	1546	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1547	9	-	0/0/17/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1538	NAG	C2-N2	-3.31	1.40	1.46
9	A	1538	NAG	O5-C1	-3.16	1.38	1.43
9	A	1540	FUL	C4-C5	2.17	1.57	1.52
9	A	1546	NAG	C2-N2	2.69	1.51	1.46
9	A	1538	NAG	C1-C2	3.05	1.56	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1540	FUL	C1-C2-C3	-11.48	95.96	109.54
9	A	1547	FUL	C1-C2-C3	-7.00	101.26	109.54
9	A	1540	FUL	C1-O5-C5	-6.34	102.59	112.38
9	A	1539	NAG	C3-C4-C5	-6.05	99.65	110.20
9	A	1547	FUL	C1-O5-C5	-5.76	103.48	112.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1545	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	1546	NAG	1	0
9	A	1547	FUL	1	0

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 36 are unknown and 4 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$
4	VX	A	1530	1	1,5,6	0.71	0	1,5,8	0.14	0
2	GLY	A	1531	-	1,4,4	0.61	0	0,4,4	0.00	-
8	SO4	A	1536	-	4,4,4	1.37	0	6,6,6	0.52	0
8	SO4	A	1537	-	4,4,4	0.41	0	6,6,6	0.38	0
10	NAG	A	1541	1	14,14,15	1.46	2 (14%)	15,19,21	2.19	5 (33%)
10	NAG	A	1542	1	14,14,15	0.87	0	15,19,21	3.17	5 (33%)
10	NAG	A	1543	1	14,14,15	1.15	1 (7%)	15,19,21	2.20	4 (26%)
10	NAG	A	1544	1	14,14,15	0.83	1 (7%)	15,19,21	1.82	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
4	VX	A	1530	1	-	0/1/3/4	0/0/0/0
2	GLY	A	1531	-	-	0/0/2/2	0/0/0/0
8	SO4	A	1536	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1537	-	-	0/0/0/0	0/0/0/0
10	NAG	A	1541	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1542	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1543	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1544	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1544	NAG	C1-C2	2.16	1.55	1.52
10	A	1541	NAG	C2-N2	2.34	1.50	1.46
10	A	1543	NAG	C1-C2	2.40	1.55	1.52
10	A	1541	NAG	C1-C2	3.40	1.57	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1541	NAG	O7-C7-C8	-4.13	114.49	122.06
10	A	1542	NAG	O7-C7-C8	-2.35	117.75	122.06
10	A	1542	NAG	C3-C4-C5	2.07	113.81	110.20
10	A	1542	NAG	O4-C4-C5	2.08	114.74	109.24
10	A	1544	NAG	O3-C3-C2	2.13	113.33	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1530	VX	2	0
2	A	1531	GLY	1	0
10	A	1542	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, 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	527/527 (100%)	0.86	62 (11%) <b>6</b> <b>8</b>	19, 32, 59, 92	14 (2%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	6.8
1	A	255	GLU	6.3
1	A	50	THR	5.8
1	A	378	ASP	5.7
1	A	54	ASP	5.3

### 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
9	FUL	A	1547	10/11	0.87	0.46	<b>4.38</b>	73,76,77,80	0
9	NAG	A	1538	14/15	0.94	0.16	-0.19	36,49,55,64	0
9	NAG	A	1546	14/15	0.64	0.55	-	91,95,99,100	0
9	NAG	A	1545	14/15	0.84	0.33	-	65,76,85,86	0
9	NAG	A	1539	14/15	0.87	0.30	-	63,71,75,78	0
9	FUL	A	1540	10/11	0.85	0.30	-	67,72,74,74	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
3	UNX	A	1567	1/1	0.88	0.84	16.60	33,33,33,33	0
3	UNX	A	1583	1/1	0.81	0.41	16.38	45,45,45,45	0
3	UNX	A	1565	1/1	0.89	0.78	13.75	30,30,30,30	0
3	UNX	A	1562	1/1	0.93	0.30	3.24	40,40,40,40	0
10	NAG	A	1543	14/15	0.66	0.27	3.16	48,63,72,73	0
8	SO4	A	1537	5/5	0.89	0.27	2.95	67,70,73,73	5
4	VX	A	1530	6/7	0.89	0.23	1.58	24,30,42,43	0
3	UNX	A	1566	1/1	0.89	0.23	1.34	40,40,40,40	0
2	GLY	A	1531	5/5	0.87	0.16	1.03	32,38,43,47	0
8	SO4	A	1536	5/5	0.95	0.18	0.78	25,29,34,37	5
3	UNX	A	1558	1/1	0.78	0.20	-0.00	47,47,47,47	0
3	UNX	A	1568	1/1	0.83	0.36	-	28,28,28,28	0
3	UNX	A	1574	1/1	0.95	0.16	-	53,53,53,53	0
6	CL	A	1534	1/1	0.96	0.10	-	69,69,69,69	0
3	UNX	A	1577	1/1	0.61	0.45	-	53,53,53,53	0
3	UNX	A	1569	1/1	0.52	0.41	-	35,35,35,35	0
6	CL	A	1533	1/1	0.94	0.08	-	72,72,72,72	0
3	UNX	A	1555	1/1	0.97	0.20	-	37,37,37,37	0
10	NAG	A	1542	14/15	0.73	0.41	-	59,69,73,75	0
3	UNX	A	1570	1/1	0.96	0.31	-	37,37,37,37	0
3	UNX	A	1556	1/1	0.86	0.53	-	59,59,59,59	0
3	UNX	A	1586	1/1	0.90	0.30	-	41,41,41,41	0
3	UNX	A	1571	1/1	0.95	0.34	-	39,39,39,39	0
3	UNX	A	1552	1/1	0.60	0.50	-	37,37,37,37	0
3	UNX	A	1572	1/1	0.92	0.29	-	36,36,36,36	0
3	UNX	A	1559	1/1	0.04	0.42	-	27,27,27,27	0
3	UNX	A	1553	1/1	0.82	0.92	-	47,47,47,47	0
3	UNX	A	1584	1/1	0.86	0.17	-	31,31,31,31	0
3	UNX	A	1554	1/1	0.96	0.34	-	41,41,41,41	0
3	UNX	A	1580	1/1	0.89	0.37	-	26,26,26,26	0
3	UNX	A	1573	1/1	0.78	0.84	-	60,60,60,60	0
10	NAG	A	1544	14/15	0.75	0.46	-	78,87,93,94	0
3	UNX	A	1563	1/1	0.75	0.93	-	44,44,44,44	0
3	UNX	A	1561	1/1	0.69	0.47	-	31,31,31,31	0
3	UNX	A	1557	1/1	0.80	0.35	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UNX	A	1582	1/1	0.88	0.44	-	39,39,39,39	0
3	UNX	A	1585	1/1	0.92	0.27	-	43,43,43,43	0
3	UNX	A	1581	1/1	0.85	0.27	-	35,35,35,35	0
3	UNX	A	1560	1/1	0.32	0.74	-	56,56,56,56	0
3	UNX	A	1564	1/1	0.88	1.36	-	54,54,54,54	0
5	NA	A	1532	1/1	0.90	0.29	-	57,57,57,57	1
3	UNX	A	1578	1/1	0.89	0.31	-	46,46,46,46	0
3	UNX	A	1579	1/1	0.80	0.94	-	54,54,54,54	0
3	UNX	A	1551	1/1	0.53	0.74	-	47,47,47,47	0
3	UNX	A	1575	1/1	0.85	0.20	-	46,46,46,46	0
7	K	A	1535	1/1	0.87	0.14	-	89,89,89,89	1
10	NAG	A	1541	14/15	0.84	0.25	-	57,65,69,71	0
3	UNX	A	1576	1/1	0.96	0.23	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.