



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:37 AM GMT

PDB ID : 2XQJ  
Title : X-RAY STRUCTURE OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY PURE ENANTIOMER VX-(R)  
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Deposited on : 2010-09-02  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

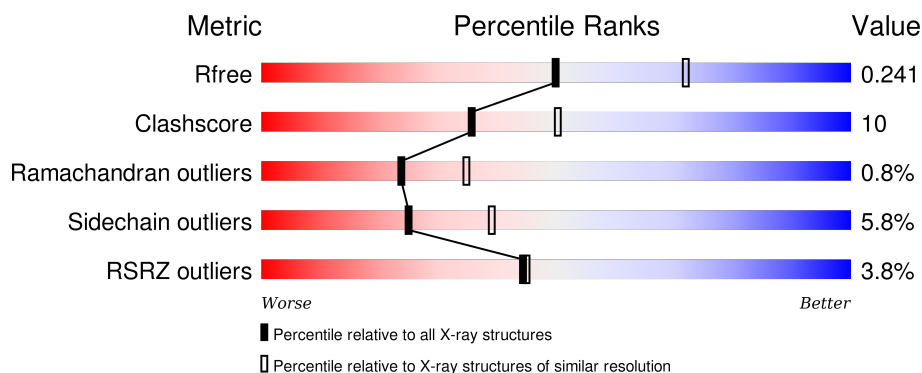
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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  $\geq 3$ , 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
10	NAG	A	1544	X	-	-	-
3	VX	A	1530	-	-	-	X
9	NAG	A	1545	X	-	-	X
9	FUL	A	1547	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4753 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

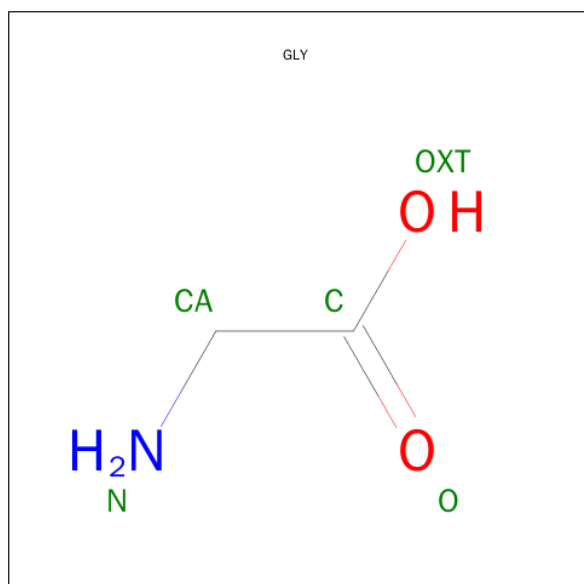
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	7	0
			4246	2743	712	775	16			

There are 4 discrepancies between the modelled and reference sequences:

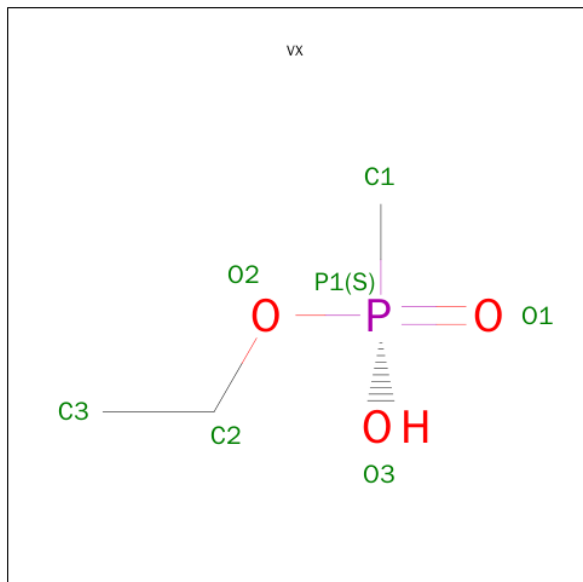
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



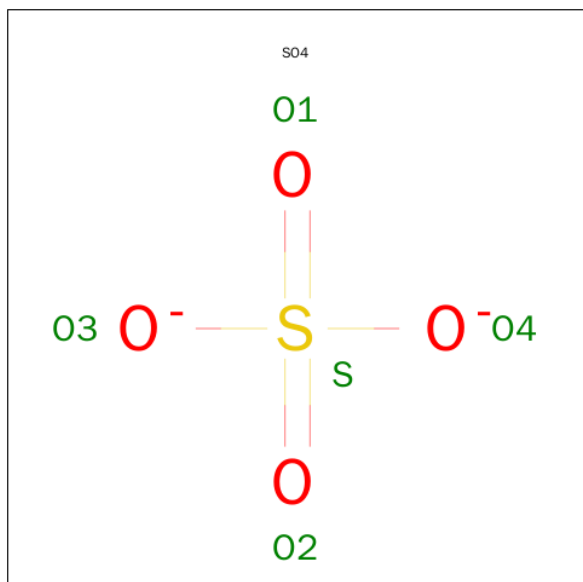
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is O-ETHYLMETHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VX) (formula:  $C_3H_9O_3P$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

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

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

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

- 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

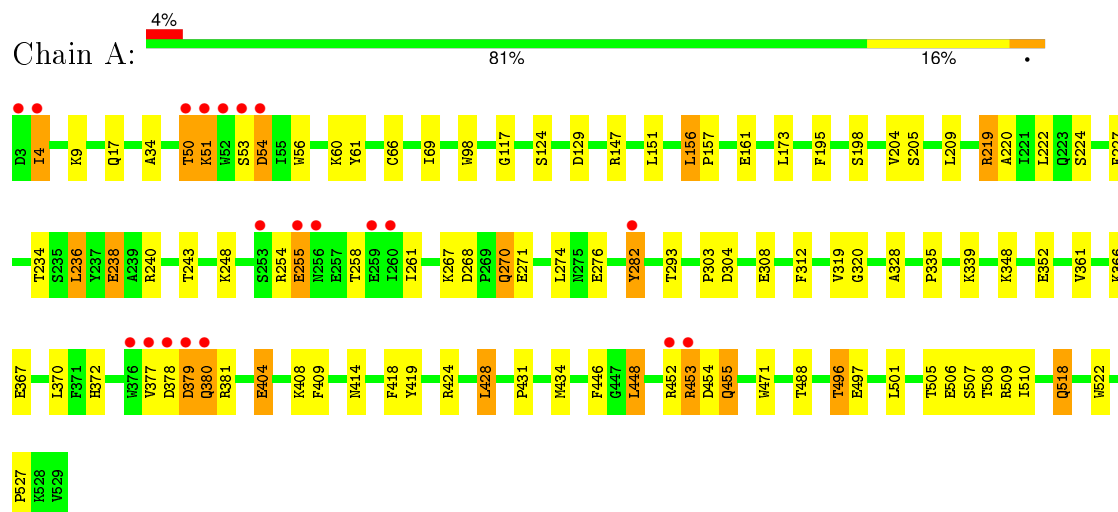
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	346	Total	O	0	0
			346	346		

### 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	155.82Å 155.82Å 128.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.40 48.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.27-2.40) 99.9 (48.14-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.168 , 0.223 0.189 , 0.241	Depositor DCC
$R_{free}$ test set	1242 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31041 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: MG, NAG, CL, NA, K, SO4, VX, FUL, CA

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	1.07	3/4384 (0.1%)	0.88	4/5949 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CG-CD	6.86	1.62	1.51
1	A	446	PHE	CE2-CZ	5.67	1.48	1.37
1	A	276	GLU	CG-CD	5.08	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	A	147	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	370	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	448	LEU	CA-CB-CG	5.36	127.62	115.30

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	4246	0	4159	81	0
2	A	5	0	2	2	0
3	A	6	0	8	1	0
4	A	10	0	0	1	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	2	0	0	0	1
9	A	76	0	68	2	0
10	A	56	0	52	1	0
11	A	1	0	0	0	0
12	A	346	0	0	19	1
All	All	4753	0	4289	84	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (84) 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:507:SER:HA	12:A:2318:HOH:O	1.44	1.15
1:A:240:ARG:HG2	12:A:2117:HOH:O	1.49	1.11
1:A:380:GLN:HA	1:A:380:GLN:HE21	1.16	1.09
1:A:380:GLN:HA	1:A:380:GLN:NE2	1.84	0.86
1:A:238[A]:GLU:OE1	1:A:238[A]:GLU:HA	1.75	0.85
1:A:4:ILE:N	1:A:4:ILE:HD12	1.91	0.84
1:A:270:GLN:OE1	1:A:274:LEU:CD1	2.28	0.80
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.16	0.80
1:A:381:ARG:HD2	12:A:2232:HOH:O	1.79	0.80
1:A:454:ASP:O	1:A:455:GLN:HG2	1.84	0.77
1:A:518:GLN:H	1:A:518:GLN:HE21	1.32	0.77
1:A:4:ILE:HD12	1:A:4:ILE:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD12	12:A:2042:HOH:O	1.86	0.76
1:A:367:GLU:HG3	12:A:2226:HOH:O	1.86	0.76
1:A:270:GLN:OE1	1:A:274:LEU:HD13	1.86	0.75
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.22	0.75
1:A:508:THR:OG1	12:A:2317:HOH:O	1.98	0.74
1:A:157:PRO:HD3	12:A:2117:HOH:O	1.89	0.73
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.72	0.72
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.59	0.68
1:A:497:GLU:OE2	12:A:2306:HOH:O	2.13	0.65
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.33	0.63
1:A:209:LEU:HD12	1:A:312:PHE:HB3	1.82	0.61
1:A:377:VAL:O	1:A:377:VAL:HG13	2.02	0.60
1:A:50:THR:O	1:A:51:LYS:CB	2.49	0.60
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.83	0.59
1:A:282:TYR:HD2	1:A:282:TYR:O	1.85	0.59
1:A:522:TRP:O	1:A:527:PRO:HD3	2.03	0.58
1:A:509:ARG:HG2	12:A:2319:HOH:O	2.02	0.58
1:A:50:THR:O	1:A:51:LYS:HB2	2.03	0.58
1:A:270:GLN:OE1	1:A:274:LEU:HD11	2.04	0.57
1:A:227:PHE:CD1	1:A:227:PHE:C	2.78	0.56
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.37	0.55
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.22	0.54
1:A:496:THR:HA	12:A:2303:HOH:O	2.08	0.54
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.90	0.54
1:A:117:GLY:HA2	3:A:1530:VX:H22	1.90	0.53
1:A:304:ASP:HB3	12:A:2062:HOH:O	2.08	0.53
1:A:452:ARG:NH1	12:A:2274:HOH:O	2.40	0.53
1:A:518:GLN:H	1:A:518:GLN:NE2	2.05	0.53
1:A:98:TRP:HE1	2:A:1551:GLY:N	2.08	0.52
1:A:4:ILE:N	1:A:4:ILE:CD1	2.63	0.51
1:A:404:GLU:OE2	1:A:408[B]:LYS:HE3	2.10	0.51
1:A:453:ARG:NH1	1:A:453:ARG:HG2	2.27	0.49
1:A:378:ASP:O	1:A:379:ASP:C	2.50	0.49
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.48	0.49
1:A:352:GLU:HG3	12:A:2215:HOH:O	2.12	0.49
1:A:308:GLU:OE2	1:A:408[A]:LYS:HE3	2.13	0.48
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.95	0.48
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.50	0.47
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.95	0.47
1:A:404:GLU:HG2	12:A:2148:HOH:O	2.14	0.47
1:A:53:SER:O	1:A:54:ASP:CG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:O	1:A:282:TYR:CD2	2.68	0.47
1:A:319:VAL:O	1:A:418:PHE:HA	2.14	0.46
1:A:234:THR:HB	1:A:293:THR:HG22	1.96	0.46
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.28	0.46
1:A:508:THR:N	12:A:2318:HOH:O	2.48	0.46
10:A:1543:NAG:H3	12:A:2280:HOH:O	2.15	0.46
1:A:501:LEU:HD11	1:A:508:THR:HG23	1.98	0.45
1:A:328:ALA:HA	1:A:434:MET:CE	2.45	0.45
1:A:267:LYS:HE3	1:A:271:GLU:OE2	2.17	0.45
1:A:501:LEU:HD12	1:A:510[A]:ILE:HD13	1.97	0.45
1:A:372[B]:HIS:NE2	4:A:1532:SO4:O3	2.48	0.45
1:A:129:ASP:OD1	2:A:1551:GLY:N	2.50	0.45
9:A:1546:NAG:H5	9:A:1546:NAG:N2	2.31	0.45
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.52	0.44
1:A:409:PHE:O	1:A:414[B]:ASN:ND2	2.50	0.44
1:A:335:PRO:HD2	12:A:2206:HOH:O	2.18	0.44
9:A:1546:NAG:H5	9:A:1546:NAG:HN2	1.82	0.44
1:A:198:SER:HA	1:A:224:SER:O	2.18	0.44
1:A:240:ARG:CB	12:A:2159:HOH:O	2.66	0.43
1:A:66:CYS:HB2	1:A:151:LEU:HD12	2.01	0.43
1:A:339:LYS:O	1:A:431:PRO:HG3	2.19	0.43
1:A:56:TRP:C	1:A:56:TRP:CD1	2.92	0.43
1:A:488:THR:CB	1:A:508:THR:HG22	2.49	0.42
1:A:156:LEU:CD1	1:A:243:THR:HG21	2.46	0.42
1:A:452:ARG:C	1:A:454:ASP:H	2.23	0.41
1:A:34:ALA:HB2	1:A:173:LEU:HD23	2.02	0.41
1:A:361:VAL:O	1:A:366:LYS:HE2	2.21	0.41
1:A:377:VAL:HG12	12:A:2228:HOH:O	2.20	0.41
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.77	0.41
1:A:254:ARG:HB3	1:A:255:GLU:H	1.69	0.40
1:A:454:ASP:O	1:A:455:GLN:CG	2.63	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1537:CL:CL	12:A:2311:HOH:O[7_555]	2.10	0.10

## 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	532/527 (101%)	503 (94%)	25 (5%)	4 (1%)	24	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	54	ASP
1	A	496	THR
1	A	453	ARG

### 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	459/452 (102%)	432 (94%)	27 (6%)	24	38

All (27) 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	50	THR
1	A	60	LYS
1	A	69	ILE
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	195	PHE
1	A	219	ARG
1	A	236	LEU
1	A	238[A]	GLU
1	A	238[B]	GLU
1	A	248	LYS
1	A	255	GLU
1	A	268	ASP
1	A	270	GLN
1	A	282	TYR
1	A	348	LYS
1	A	379	ASP
1	A	380	GLN
1	A	428	LEU
1	A	448	LEU
1	A	455	GLN
1	A	471	TRP
1	A	505	THR
1	A	506	GLU
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	275	ASN
1	A	380	GLN
1	A	518	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

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	0.74	0	15,19,21	2.52	7 (46%)
9	NAG	A	1539	9	14,14,15	0.57	0	15,19,21	2.03	5 (33%)
9	FUL	A	1540	9	10,10,11	1.14	1 (10%)	14,14,16	3.49	6 (42%)
9	NAG	A	1545	1,9	14,14,15	0.83	0	15,19,21	2.44	4 (26%)
9	NAG	A	1546	9	14,14,15	1.29	1 (7%)	15,19,21	2.12	4 (26%)
9	FUL	A	1547	9	10,10,11	0.78	0	14,14,16	2.25	6 (42%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1540	FUL	C4-C5	2.28	1.57	1.52
9	A	1546	NAG	C1-C2	3.58	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1540	FUL	C1-C2-C3	-9.09	98.79	109.54
9	A	1540	FUL	C1-O5-C5	-5.73	103.53	112.38
9	A	1547	FUL	C1-C2-C3	-4.94	103.70	109.54
9	A	1539	NAG	C3-C4-C5	-4.92	101.61	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1538	NAG	C3-C4-C5	-4.22	102.84	110.20
9	A	1547	FUL	C1-O5-C5	-3.60	106.82	112.38
9	A	1540	FUL	O5-C1-C2	-3.46	105.24	110.86
9	A	1545	NAG	O7-C7-C8	-2.81	116.90	122.06
9	A	1539	NAG	C3-C2-N2	-2.48	104.62	110.56
9	A	1539	NAG	O6-C6-C5	-2.47	103.18	111.33
9	A	1538	NAG	O7-C7-C8	-2.37	117.72	122.06
9	A	1546	NAG	O7-C7-C8	-2.24	117.95	122.06
9	A	1547	FUL	O5-C1-C2	-2.05	107.54	110.86
9	A	1538	NAG	O6-C6-C5	2.17	118.51	111.33
9	A	1546	NAG	O5-C5-C6	2.35	112.44	107.35
9	A	1540	FUL	O2-C2-C1	2.41	114.03	109.21
9	A	1547	FUL	O5-C5-C6	2.45	110.17	106.13
9	A	1547	FUL	O2-C2-C1	2.66	114.54	109.21
9	A	1539	NAG	O3-C3-C2	2.67	114.40	109.11
9	A	1539	NAG	O5-C5-C6	2.68	113.16	107.35
9	A	1538	NAG	C1-O5-C5	2.95	115.99	112.25
9	A	1547	FUL	C3-C4-C5	3.00	114.77	109.72
9	A	1545	NAG	C8-C7-N2	3.05	121.94	116.11
9	A	1538	NAG	C8-C7-N2	3.31	122.44	116.11
9	A	1546	NAG	C1-O5-C5	3.32	116.47	112.25
9	A	1538	NAG	C6-C5-C4	3.39	121.37	113.02
9	A	1540	FUL	C3-C4-C5	3.48	115.58	109.72
9	A	1540	FUL	O5-C5-C6	3.54	111.99	106.13
9	A	1538	NAG	C2-N2-C7	5.46	130.05	123.04
9	A	1545	NAG	C2-N2-C7	5.56	130.19	123.04
9	A	1545	NAG	C1-O5-C5	5.64	119.41	112.25
9	A	1546	NAG	C2-N2-C7	5.91	130.63	123.04

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1546	NAG	2	0

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 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	VX	A	1530	-	1,5,6	0.75	0	1,5,8	0.12	0
4	SO4	A	1531	-	4,4,4	0.38	0	6,6,6	0.65	0
4	SO4	A	1532	-	4,4,4	0.15	0	6,6,6	0.45	0
10	NAG	A	1541	1	14,14,15	1.31	2 (14%)	15,19,21	2.56	6 (40%)
10	NAG	A	1542	1	14,14,15	0.77	0	15,19,21	2.57	2 (13%)
10	NAG	A	1543	1	14,14,15	0.89	1 (7%)	15,19,21	2.21	5 (33%)
10	NAG	A	1544	1	14,14,15	0.84	0	15,19,21	1.57	2 (13%)
2	GLY	A	1551	-	1,4,4	0.87	0	0,4,4	0.00	-

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	VX	A	1530	-	-	0/1/3/4	0/0/0/0
4	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1532	-	-	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	1/1/5/7	0/6/23/26	0/1/1/1
2	GLY	A	1551	-	-	0/0/2/2	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1543	NAG	C3-C2	2.25	1.57	1.52
10	A	1541	NAG	C4-C5	2.33	1.58	1.53
10	A	1541	NAG	C1-C2	2.86	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1542	NAG	C4-C3-C2	-3.46	105.84	111.23
10	A	1543	NAG	O7-C7-C8	-2.79	116.94	122.06
10	A	1541	NAG	O7-C7-C8	-2.60	117.28	122.06
10	A	1543	NAG	C2-N2-C7	-2.53	119.79	123.04
10	A	1543	NAG	O5-C5-C6	2.47	112.69	107.35
10	A	1541	NAG	O4-C4-C5	2.47	115.79	109.24
10	A	1541	NAG	O5-C5-C6	3.04	113.92	107.35
10	A	1544	NAG	O5-C5-C6	3.13	114.13	107.35
10	A	1544	NAG	C2-N2-C7	3.23	127.18	123.04
10	A	1541	NAG	C8-C7-N2	3.45	122.71	116.11
10	A	1541	NAG	O3-C3-C2	3.55	116.14	109.11
10	A	1543	NAG	C4-C3-C2	3.86	117.23	111.23
10	A	1543	NAG	C1-O5-C5	5.09	118.71	112.25
10	A	1541	NAG	C2-N2-C7	6.25	131.07	123.04
10	A	1542	NAG	C1-O5-C5	8.13	122.56	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1544	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1530	VX	1	0
4	A	1532	SO4	1	0
10	A	1543	NAG	1	0
2	A	1551	GLY	2	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	527/527 (100%)	0.07	20 (3%)	44 45	20, 36, 65, 89	15 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	5.1
1	A	3	ASP	5.0
1	A	378	ASP	4.3
1	A	379	ASP	3.9
1	A	255	GLU	3.3
1	A	256	ASN	2.9
1	A	50	THR	2.8
1	A	53	SER	2.8
1	A	54	ASP	2.8
1	A	282	TYR	2.7
1	A	253	SER	2.7
1	A	4	ILE	2.6
1	A	452	ARG	2.6
1	A	453	ARG	2.4
1	A	52	TRP	2.3
1	A	260	ILE	2.3
1	A	380	GLN	2.3
1	A	259	GLU	2.2
1	A	51	LYS	2.2
1	A	376	TRP	2.0

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

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

### 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, 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	0.88	0.41	4.33	82,84,85,86	0
9	NAG	A	1545	14/15	0.87	0.33	2.88	70,82,91,93	0
9	NAG	A	1538	14/15	0.95	0.18	0.04	40,52,62,71	0
9	NAG	A	1539	14/15	0.88	0.23	-	70,75,80,81	0
9	FUL	A	1540	10/11	0.79	0.27	-	75,78,79,80	0
9	NAG	A	1546	14/15	0.62	0.60	-	95,99,100,100	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, 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	VX	A	1530	6/7	0.94	0.28	3.28	25,34,37,38	0
10	NAG	A	1543	14/15	0.71	0.23	2.27	55,68,74,77	0
4	SO4	A	1532	5/5	0.96	0.20	1.03	69,70,70,70	5
4	SO4	A	1531	5/5	0.97	0.14	-0.70	23,23,27,31	5
2	GLY	A	1551	5/5	0.96	0.09	-1.65	46,47,48,49	0
7	CA	A	1535	1/1	0.95	0.34	-	75,75,75,75	0
5	NA	A	1548	1/1	0.74	1.06	-	74,74,74,74	0
8	CL	A	1536	1/1	0.85	0.10	-	75,75,75,75	0
11	MG	A	1550	1/1	0.89	0.50	-	66,66,66,66	0
10	NAG	A	1544	14/15	0.81	0.47	-	71,81,88,88	0
10	NAG	A	1541	14/15	0.73	0.28	-	52,62,64,66	0
10	NAG	A	1542	14/15	0.75	0.38	-	65,74,78,78	0
5	NA	A	1533	1/1	0.88	0.37	-	47,47,47,47	0
7	CA	A	1549	1/1	0.80	0.30	-	93,93,93,93	0
8	CL	A	1537	1/1	0.95	0.05	-	63,63,63,63	0
6	K	A	1534	1/1	0.70	0.13	-	87,87,87,87	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.