



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:17 AM GMT

PDB ID : 2C4H  
Title : TORPEDO CALIFORNICA ACETYLCHOLINESTERASE IN COMPLEX  
WITH 500MM ACETYLTHIOCHOLINE  
Authors : Colletier, J.P.; Fournier, D.; Greenblatt, H.M.; Sussman, J.L.; Zaccai, G.;  
Silman, I.; Weik, M.  
Deposited on : 2005-10-19  
Resolution : 2.15 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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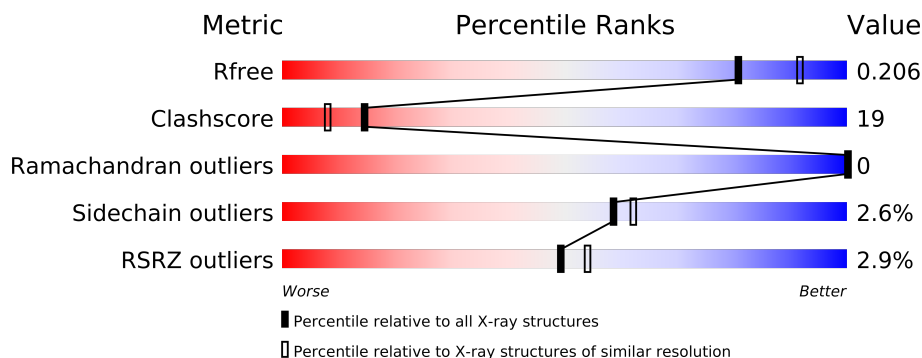
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance


The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	537	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	1536	-	X
3	NDG	A	1537	-	X
4	PGE	A	1539	-	X
5	AT3	A	1540	-	X
5	AT3	A	1541	-	X
6	ACE	A	1543[A]	-	X
7	CL	A	1551	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	CL	A	1552	-	X
8	ACT	A	1555[B]	-	X

## 2 Entry composition i

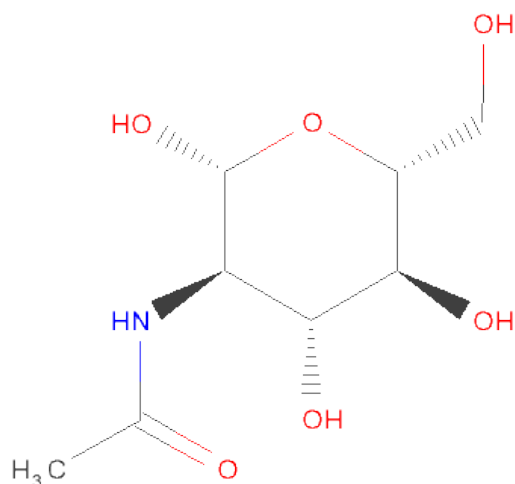
There are 9 unique types of molecules in this entry. The entry contains 5535 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ACETYLCHOLINESTERASE.

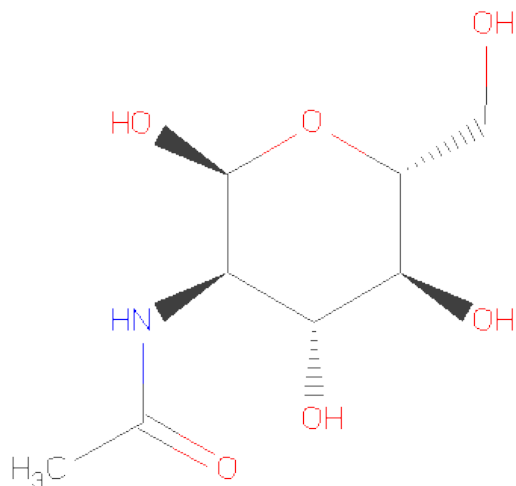
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	533	4501	2874	770	830	27	0	29	1

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



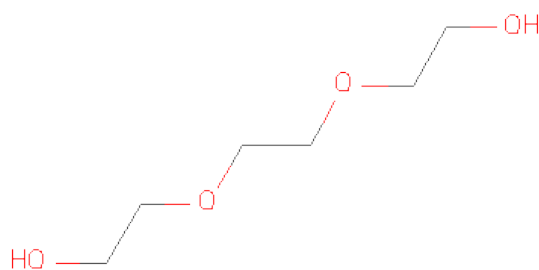
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



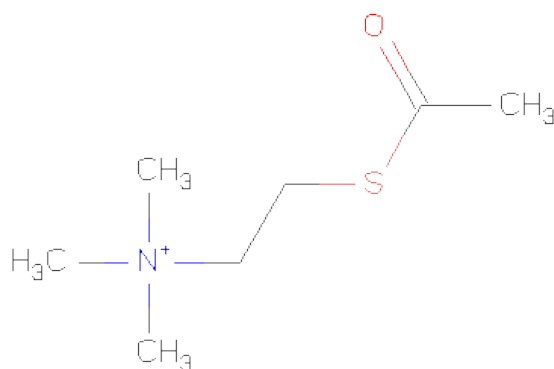
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



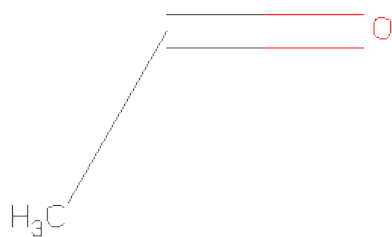
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
4	A	1	10	6	4	0	0

- Molecule 5 is ACETYLTHIOCHOLINE (three-letter code: AT3) (formula: C<sub>7</sub>H<sub>16</sub>NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 6 is ACETYL GROUP (three-letter code: ACE) (formula:  $C_2H_4O$ ).

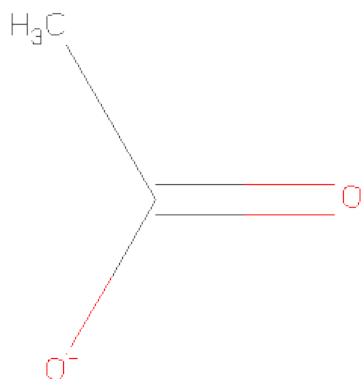


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			3	2	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	1
			4	2	2		

- Molecule 9 is water.

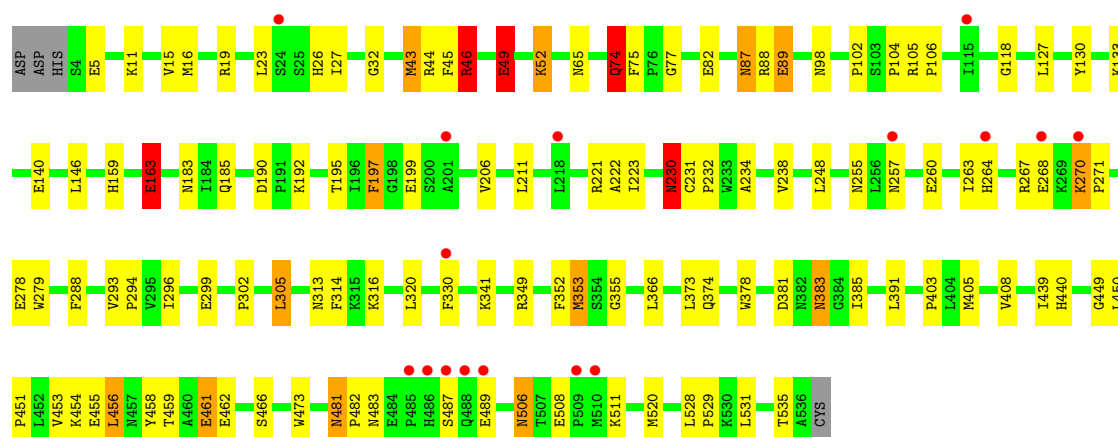
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	948	Total	O	0	0
			948	948		

### 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: ACETYLCHOLINESTERASE

Chain A: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.99Å 111.99Å 137.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.15 48.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.80-2.15) 99.6 (48.49-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.169 , 0.209 0.167 , 0.206	Depositor DCC
$R_{free}$ test set	2770 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 95.6	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54312 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: PGE, NAG, ACE, CL, NDG, AT3, ACT

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	6.39	20/4627 (0.4%)	2.63	36/6277 (0.6%)

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	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49[A]	GLU	CD-OE1	229.03	3.77	1.25
1	A	49[B]	GLU	CD-OE1	229.03	3.77	1.25
1	A	46[A]	ARG	CZ-NH1	170.88	3.55	1.33
1	A	46[B]	ARG	CZ-NH1	170.88	3.55	1.33
1	A	461[A]	GLU	CG-CD	66.43	2.51	1.51
1	A	461[B]	GLU	CG-CD	66.43	2.51	1.51
1	A	163[A]	GLU	CD-OE1	63.51	1.95	1.25
1	A	163[B]	GLU	CD-OE1	63.51	1.95	1.25
1	A	270[A]	LYS	CD-CE	55.23	2.89	1.51
1	A	270[B]	LYS	CD-CE	55.23	2.89	1.51
1	A	43[A]	MET	SD-CE	18.91	2.83	1.77
1	A	43[B]	MET	SD-CE	18.91	2.83	1.77
1	A	74[A]	GLN	CG-CD	18.57	1.93	1.51
1	A	74[B]	GLN	CG-CD	18.57	1.93	1.51
1	A	89[A]	GLU	CB-CG	-10.21	1.32	1.52
1	A	89[B]	GLU	CB-CG	-10.21	1.32	1.52
1	A	52[A]	LYS	CB-CG	8.89	1.76	1.52
1	A	52[B]	LYS	CB-CG	8.89	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353[A]	MET	CG-SD	-6.24	1.65	1.81
1	A	353[B]	MET	CG-SD	-6.24	1.65	1.81

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46[A]	ARG	NH1-CZ-NH2	-81.70	29.52	119.40
1	A	46[B]	ARG	NH1-CZ-NH2	-81.70	29.52	119.40
1	A	15[A]	VAL	CG1-CB-CG2	-67.28	3.26	110.90
1	A	15[B]	VAL	CG1-CB-CG2	-67.28	3.26	110.90
1	A	46[A]	ARG	NE-CZ-NH1	-56.93	91.84	120.30
1	A	46[B]	ARG	NE-CZ-NH1	-56.93	91.84	120.30
1	A	49[A]	GLU	CG-CD-OE1	-42.52	33.26	118.30
1	A	49[B]	GLU	CG-CD-OE1	-42.52	33.26	118.30
1	A	163[A]	GLU	OE1-CD-OE2	-32.70	84.06	123.30
1	A	163[B]	GLU	OE1-CD-OE2	-32.70	84.06	123.30
1	A	49[A]	GLU	OE1-CD-OE2	-29.51	87.89	123.30
1	A	49[B]	GLU	OE1-CD-OE2	-29.51	87.89	123.30
1	A	163[A]	GLU	CG-CD-OE2	25.77	169.83	118.30
1	A	163[B]	GLU	CG-CD-OE2	25.77	169.83	118.30
1	A	43[A]	MET	CG-SD-CE	-19.11	69.62	100.20
1	A	43[B]	MET	CG-SD-CE	-19.11	69.62	100.20
1	A	270[A]	LYS	CG-CD-CE	-17.20	60.29	111.90
1	A	270[B]	LYS	CG-CD-CE	-17.20	60.29	111.90
1	A	461[A]	GLU	CB-CG-CD	-13.07	78.91	114.20
1	A	461[B]	GLU	CB-CG-CD	-13.07	78.91	114.20
1	A	270[A]	LYS	CD-CE-NZ	12.60	140.67	111.70
1	A	270[B]	LYS	CD-CE-NZ	12.60	140.67	111.70
1	A	74[A]	GLN	CG-CD-OE1	-11.87	97.86	121.60
1	A	74[B]	GLN	CG-CD-OE1	-11.87	97.86	121.60
1	A	74[A]	GLN	OE1-CD-NE2	10.01	144.92	121.90
1	A	74[B]	GLN	OE1-CD-NE2	10.01	144.92	121.90
1	A	163[A]	GLU	CG-CD-OE1	-7.81	102.67	118.30
1	A	163[B]	GLU	CG-CD-OE1	-7.81	102.67	118.30
1	A	230[A]	ASN	OD1-CG-ND2	-7.80	103.95	121.90
1	A	230[B]	ASN	OD1-CG-ND2	-7.80	103.95	121.90
1	A	52[A]	LYS	CA-CB-CG	-7.33	97.27	113.40
1	A	52[B]	LYS	CA-CB-CG	-7.33	97.27	113.40
1	A	74[A]	GLN	CB-CG-CD	-6.94	93.56	111.60
1	A	74[B]	GLN	CB-CG-CD	-6.94	93.56	111.60
1	A	230[A]	ASN	O-C-N	-5.89	113.27	122.70
1	A	230[B]	ASN	O-C-N	-5.89	113.27	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163[A]	GLU	Sidechain
1	A	230[A]	ASN	Sidechain,Mainchain
1	A	230[B]	ASN	Mainchain
1	A	46[A]	ARG	Sidechain
1	A	49[A]	GLU	Sidechain
1	A	74[A]	GLN	Sidechain

## 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	4501	0	4318	166	0
2	A	14	0	13	0	0
3	A	14	0	13	0	0
4	A	20	0	28	2	0
5	A	20	0	32	32	0
6	A	3	0	3	0	0
7	A	11	0	0	1	0
8	A	4	0	3	1	0
9	A	948	0	0	16	2
All	All	5535	0	4410	174	2

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 19.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52[A]:LYS:CB	1:A:52[A]:LYS:CG	1.76	1.61
1:A:461[B]:GLU:CG	1:A:461[B]:GLU:CD	1.82	1.47
1:A:74[A]:GLN:CD	1:A:74[A]:GLN:CG	1.93	1.35
1:A:74[B]:GLN:CD	1:A:74[B]:GLN:OE1	1.75	1.23
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:CD	1.95	1.04
1:A:270[A]:LYS:HG3	1:A:270[A]:LYS:CE	1.87	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:461[B]:GLU:CG	1:A:461[B]:GLU:OE1	2.08	1.00
1:A:270[B]:LYS:HG2	1:A:270[B]:LYS:CE	1.91	0.99
1:A:330[B]:PHE:CG	5:A:1540:AT3:H6C2	1.99	0.98
1:A:270[B]:LYS:HG2	1:A:270[B]:LYS:HE2	1.46	0.95
1:A:46[A]:ARG:NH1	1:A:46[A]:ARG:HH21	1.71	0.88
1:A:270[A]:LYS:CG	1:A:270[A]:LYS:CE	2.51	0.87
1:A:52[A]:LYS:CA	1:A:52[A]:LYS:CG	2.53	0.87
1:A:49[A]:GLU:HG2	1:A:49[A]:GLU:OE1	1.77	0.85
1:A:330[A]:PHE:HE2	5:A:1541:AT3:C6	1.92	0.81
1:A:270[B]:LYS:CG	1:A:270[B]:LYS:CE	2.58	0.80
1:A:270[B]:LYS:CD	1:A:270[B]:LYS:CE	2.60	0.80
1:A:461[A]:GLU:CG	1:A:461[A]:GLU:CD	2.51	0.78
1:A:330[A]:PHE:CE2	5:A:1541:AT3:C6	2.67	0.78
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.82	0.78
1:A:74[A]:GLN:CD	1:A:74[A]:GLN:CB	2.52	0.78
5:A:1540:AT3:H2C1	9:A:2122:HOH:O	1.83	0.78
1:A:270[A]:LYS:HE3	1:A:270[A]:LYS:HG3	1.66	0.77
1:A:49[B]:GLU:HG3	1:A:49[B]:GLU:OE1	1.87	0.75
1:A:330[A]:PHE:HB2	5:A:1540:AT3:H6C2	1.69	0.75
1:A:330[B]:PHE:CB	5:A:1540:AT3:H6C2	2.17	0.74
1:A:330[A]:PHE:CE2	5:A:1541:AT3:H6C2	2.22	0.74
1:A:43[B]:MET:SD	1:A:43[B]:MET:CE	2.76	0.74
1:A:43[A]:MET:HG3	1:A:43[A]:MET:CE	2.18	0.73
1:A:52[A]:LYS:CB	1:A:52[A]:LYS:CD	2.65	0.72
1:A:11:LYS:H	1:A:183:ASN:ND2	1.86	0.72
1:A:199:GLU:OE1	5:A:1540:AT3:H103	1.88	0.72
1:A:238[B]:VAL:HG21	4:A:1539:PGE:H1	1.72	0.72
1:A:74[A]:GLN:CG	1:A:74[A]:GLN:OE1	2.39	0.70
1:A:279:TRP:CD2	5:A:1541:AT3:H101	2.26	0.70
1:A:74[B]:GLN:CG	1:A:74[B]:GLN:OE1	2.40	0.69
1:A:461[B]:GLU:CB	1:A:461[B]:GLU:CD	2.60	0.69
1:A:330[B]:PHE:CD1	5:A:1540:AT3:H6C2	2.27	0.68
1:A:279:TRP:CG	5:A:1541:AT3:H101	2.28	0.68
1:A:87:ASN:HD22	1:A:87:ASN:H	1.40	0.67
1:A:330[A]:PHE:CB	5:A:1540:AT3:H6C2	2.21	0.67
1:A:43[B]:MET:HG2	1:A:43[B]:MET:CE	2.25	0.67
1:A:43[A]:MET:SD	1:A:43[A]:MET:CE	2.83	0.67
5:A:1540:AT3:H101	8:A:1555[B]:ACT:O	1.95	0.66
1:A:102:PRO:HB3	1:A:140:GLU:OE1	1.95	0.66
1:A:461[A]:GLU:HB2	1:A:461[A]:GLU:CD	2.18	0.64
1:A:481:ASN:ND2	1:A:483:ASN:H	1.94	0.64
1:A:43[A]:MET:CG	1:A:43[A]:MET:CE	2.76	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1541:AT3:H9C3	9:A:2631:HOH:O	1.98	0.64
1:A:330[B]:PHE:CG	5:A:1540:AT3:C6	2.80	0.64
1:A:302:PRO:HB2	9:A:2610:HOH:O	1.97	0.63
1:A:11:LYS:HB2	1:A:183:ASN:HD21	1.63	0.63
1:A:330[A]:PHE:CG	5:A:1540:AT3:H6C2	2.34	0.62
1:A:461[A]:GLU:CD	1:A:461[A]:GLU:CB	2.67	0.62
1:A:508:GLU:HG3	9:A:2865:HOH:O	1.99	0.62
1:A:383:ASN:HD22	1:A:383:ASN:C	2.03	0.61
1:A:43[B]:MET:CG	1:A:43[B]:MET:CE	2.78	0.61
1:A:330[A]:PHE:CD1	5:A:1540:AT3:H6C2	2.34	0.61
1:A:230[B]:ASN:CG	1:A:230[B]:ASN:O	2.39	0.60
1:A:238[A]:VAL:HG21	4:A:1539:PGE:H1	1.83	0.60
1:A:487:SER:OG	1:A:489:GLU:HG2	2.02	0.60
1:A:313:ASN:ND2	9:A:2610:HOH:O	2.34	0.60
5:A:1541:AT3:H3C1	9:A:2631:HOH:O	2.00	0.59
1:A:453:VAL:HB	1:A:456:LEU:HD22	1.83	0.59
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:OE2	2.19	0.59
1:A:46[A]:ARG:NH1	1:A:46[A]:ARG:NH2	2.48	0.58
1:A:163[A]:GLU:HG3	9:A:2154:HOH:O	2.05	0.57
1:A:440:HIS:HB3	5:A:1540:AT3:H6C3	1.86	0.57
1:A:481:ASN:HD22	1:A:482:PRO:N	2.02	0.57
1:A:481:ASN:HD22	1:A:482:PRO:CD	2.18	0.57
1:A:159:HIS:HB3	1:A:238[B]:VAL:HG13	1.87	0.56
1:A:330[B]:PHE:HB2	5:A:1540:AT3:H6C2	1.85	0.56
1:A:279:TRP:CE2	5:A:1541:AT3:H101	2.40	0.56
1:A:264[B]:HIS:O	1:A:268[B]:GLU:HG3	2.06	0.56
1:A:279:TRP:CD1	5:A:1541:AT3:H101	2.41	0.55
1:A:506:ASN:HD22	1:A:506:ASN:C	2.10	0.55
1:A:231[B]:CYS:HB2	1:A:232:PRO:HD2	1.89	0.55
1:A:373:LEU:HD12	1:A:378:TRP:HE1	1.72	0.54
1:A:87:ASN:ND2	1:A:87:ASN:H	2.05	0.54
1:A:531:LEU:HD23	1:A:531:LEU:C	2.28	0.54
1:A:87:ASN:HD22	1:A:87:ASN:N	2.01	0.54
1:A:366:LEU:HD23	1:A:535:THR:HG21	1.89	0.54
1:A:481:ASN:HD22	1:A:482:PRO:HD2	1.73	0.54
1:A:255:ASN:HD21	1:A:257:ASN:HD22	1.54	0.54
1:A:481:ASN:C	1:A:481:ASN:HD22	2.11	0.54
1:A:5:GLU:OE2	1:A:104:PRO:HA	2.07	0.54
1:A:159:HIS:CB	1:A:238[B]:VAL:HG13	2.38	0.54
1:A:330[A]:PHE:C	1:A:330[A]:PHE:CD2	2.81	0.53
1:A:330[A]:PHE:CZ	5:A:1541:AT3:H6C2	2.43	0.53
1:A:77:GLY:N	1:A:82[A]:GLU:OE1	2.36	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.91	0.52
5:A:1541:AT3:O7	9:A:2947:HOH:O	2.18	0.51
1:A:278:GLU:HB2	9:A:2558:HOH:O	2.11	0.51
1:A:197:PHE:CB	1:A:223:ILE:HB	2.40	0.51
1:A:481:ASN:HD21	1:A:483:ASN:HD22	1.57	0.51
1:A:506:ASN:ND2	1:A:508:GLU:H	2.08	0.51
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.92	0.51
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.46	0.51
1:A:195:THR:OG1	1:A:221:ARG:HG3	2.11	0.50
1:A:260:GLU:HG3	1:A:264[A]:HIS:CE1	2.46	0.50
1:A:270[A]:LYS:CD	1:A:270[A]:LYS:CE	2.89	0.50
1:A:255:ASN:HD21	1:A:257:ASN:ND2	2.07	0.50
1:A:506:ASN:HD22	1:A:508:GLU:H	1.58	0.50
1:A:461[B]:GLU:HG3	1:A:461[B]:GLU:OE1	2.07	0.50
1:A:330[A]:PHE:CD1	5:A:1540:AT3:C6	2.95	0.50
1:A:185:GLN:NE2	9:A:2464:HOH:O	2.44	0.49
1:A:264[B]:HIS:HE1	1:A:268[B]:GLU:OE2	1.96	0.49
1:A:449:GLY:HA2	1:A:466:SER:OG	2.12	0.49
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.12	0.49
1:A:163[A]:GLU:HB2	1:A:263:ILE:HD13	1.94	0.49
1:A:223:ILE:HA	1:A:320:LEU:O	2.13	0.48
1:A:163[B]:GLU:HB3	1:A:267:ARG:NH2	2.27	0.48
1:A:374:GLN:HE21	1:A:520:MET:CE	2.26	0.48
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.48	0.48
1:A:296:ILE:HD12	1:A:305:LEU:HD13	1.96	0.47
1:A:11:LYS:H	1:A:183:ASN:HD21	1.62	0.47
1:A:314:PHE:O	1:A:316:LYS:HD2	2.14	0.47
1:A:32:GLY:H	1:A:98:ASN:HD22	1.61	0.47
1:A:511:LYS:HE2	9:A:2867:HOH:O	2.14	0.47
1:A:481:ASN:ND2	1:A:482:PRO:HD2	2.30	0.47
1:A:352:PHE:HD2	1:A:353[A]:MET:HE2	1.80	0.46
1:A:16[B]:MET:HE3	9:A:2065:HOH:O	2.15	0.46
1:A:163[B]:GLU:HB3	1:A:267:ARG:HH22	1.80	0.46
1:A:271:PRO:HD2	7:A:1550:CL:CL	2.52	0.46
1:A:270[A]:LYS:CG	1:A:270[A]:LYS:HE3	2.36	0.46
1:A:450:LEU:N	1:A:451:PRO:CD	2.78	0.46
1:A:231[B]:CYS:SG	1:A:234:ALA:HB2	2.56	0.46
5:A:1541:AT3:H3C1	5:A:1541:AT3:H8C2	1.72	0.46
1:A:19[A]:ARG:NH1	1:A:26:HIS:HB2	2.31	0.46
1:A:341:LYS:HE3	9:A:2645:HOH:O	2.16	0.45
1:A:383:ASN:HD21	1:A:385:ILE:HB	1.81	0.45
1:A:278:GLU:HB3	9:A:2566:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405:MET:O	1:A:408:VAL:HG12	2.17	0.45
1:A:330[A]:PHE:CG	5:A:1540:AT3:C6	3.00	0.44
1:A:32:GLY:H	1:A:98:ASN:ND2	2.14	0.44
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.98	0.44
1:A:43[A]:MET:HG3	1:A:43[A]:MET:HE3	2.00	0.44
1:A:268[A]:GLU:HA	1:A:268[A]:GLU:OE2	2.18	0.44
1:A:453:VAL:HG12	1:A:455:GLU:HG2	1.99	0.43
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.48	0.43
1:A:230[B]:ASN:O	1:A:230[B]:ASN:ND2	2.51	0.43
1:A:231[B]:CYS:SG	1:A:234:ALA:CB	3.07	0.43
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.99	0.43
1:A:349:ARG:HD3	1:A:381:ASP:O	2.19	0.43
1:A:461[B]:GLU:HB3	1:A:461[B]:GLU:CD	2.37	0.43
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:HA	2.19	0.43
1:A:44:ARG:O	1:A:45:PHE:HB2	2.18	0.43
1:A:439:ILE:HG22	1:A:440:HIS:N	2.34	0.43
1:A:279:TRP:CD1	5:A:1541:AT3:C10	3.03	0.42
1:A:260:GLU:O	1:A:264[A]:HIS:ND1	2.52	0.42
1:A:355:GLY:HA3	1:A:391:LEU:HD11	2.01	0.42
1:A:481:ASN:HD22	1:A:483:ASN:H	1.65	0.42
1:A:19[A]:ARG:NH1	1:A:26:HIS:CB	2.82	0.42
1:A:293:VAL:HB	1:A:294:PRO:HD2	2.01	0.42
1:A:146:LEU:HD12	1:A:146:LEU:C	2.39	0.42
1:A:43[B]:MET:HG2	1:A:43[B]:MET:HE2	1.99	0.42
1:A:118:GLY:N	5:A:1540:AT3:C9	2.83	0.42
1:A:299:GLU:HG3	9:A:2586:HOH:O	2.20	0.42
1:A:230[B]:ASN:O	1:A:403:PRO:HB3	2.20	0.42
5:A:1540:AT3:H3C2	5:A:1540:AT3:H102	1.77	0.41
5:A:1540:AT3:H8C1	9:A:2373:HOH:O	2.20	0.41
1:A:65:ASN:OD1	1:A:89[B]:GLU:HG2	2.21	0.41
1:A:330[A]:PHE:CZ	5:A:1541:AT3:C6	3.01	0.41
1:A:87:ASN:ND2	1:A:87:ASN:N	2.66	0.41
1:A:461[A]:GLU:OE1	1:A:461[A]:GLU:N	2.46	0.41
1:A:197:PHE:HB2	1:A:223:ILE:HB	2.03	0.41
1:A:349:ARG:O	1:A:353[B]:MET:HG3	2.21	0.41
1:A:105:ARG:HA	1:A:106:PRO:HD3	1.97	0.41
1:A:74[A]:GLN:OE1	1:A:74[A]:GLN:CB	2.68	0.40
1:A:43[A]:MET:HE1	1:A:49[A]:GLU:HG3	2.03	0.40
1:A:349:ARG:HA	1:A:349:ARG:HD2	1.79	0.40
1:A:74[A]:GLN:HG3	1:A:75:PHE:CE2	2.56	0.40
1:A:87:ASN:ND2	1:A:88[A]:ARG:HG2	2.36	0.40
1:A:456:LEU:HA	1:A:456:LEU:HD12	1.84	0.40



All (2) 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)
9:A:2342:HOH:O	9:A:2342:HOH:O[4_556]	1.71	0.49
9:A:2919:HOH:O	9:A:2919:HOH:O[4_556]	2.05	0.15

## 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	560/537 (104%)	538 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	494/469 (105%)	482 (98%)	12 (2%)	61	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	87	ASN
1	A	197	PHE
1	A	248	LEU
1	A	288	PHE
1	A	305	LEU
1	A	383	ASN
1	A	454	LYS

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Mol	Chain	Res	Type
1	A	456	LEU
1	A	473	TRP
1	A	481	ASN
1	A	506	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	87	ASN
1	A	98	ASN
1	A	183	ASN
1	A	257	ASN
1	A	324	ASN
1	A	362	HIS
1	A	374	GLN
1	A	383	ASN
1	A	387	ASN
1	A	481	ASN
1	A	506	ASN
1	A	519	GLN
1	A	525	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 11 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
2	NAG	A	1536	1	12,14,15	0.43	0	15,19,21	0.71	0
3	NDG	A	1537	1	12,14,15	0.54	0	15,19,21	0.98	0
4	PGE	A	1538	-	9,9,9	0.96	0	8,8,8	0.95	1 (12%)
4	PGE	A	1539	-	9,9,9	0.90	1 (11%)	8,8,8	1.16	1 (12%)
5	AT3	A	1540	-	9,9,9	2.08	1 (11%)	12,12,12	0.65	0
5	AT3	A	1541	-	9,9,9	2.04	1 (11%)	12,12,12	0.55	0
6	ACE	A	1543[A]	1	2,2,2	0.67	0	1,1,1	0.60	0
8	ACT	A	1555[B]	-	1,3,3	1.65	0	0,3,3	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
2	NAG	A	1536	1	-	0/6/23/26	0/1/1/1
3	NDG	A	1537	1	-	2/6/23/26	0/1/1/1
4	PGE	A	1538	-	-	0/7/7/7	0/0/0/0
4	PGE	A	1539	-	-	0/7/7/7	0/0/0/0
5	AT3	A	1540	-	-	0/7/7/7	0/0/0/0
5	AT3	A	1541	-	-	0/7/7/7	0/0/0/0
6	ACE	A	1543[A]	1	-	0/0/0/0	0/0/0/0
8	ACT	A	1555[B]	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1540	AT3	O7-C5	5.87	1.43	1.21
5	A	1541	AT3	O7-C5	5.78	1.43	1.21
4	A	1539	PGE	O3-C5	2.04	1.50	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1539	PGE	O2-C3-C4	-2.04	101.23	110.47
4	A	1538	PGE	O2-C2-C1	2.00	120.23	110.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1537	NDG	C8-C7-N2-C2
3	A	1537	NDG	O7-C7-N2-C2

There are no ring outliers.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	533/537 (99%)	-0.11	16 (3%)	48 53	23, 34, 53, 84	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	6.8
1	A	488	GLN	4.6
1	A	485	PRO	4.2
1	A	487	SER	2.9
1	A	510[A]	MET	2.8
1	A	509	PRO	2.7
1	A	264[A]	HIS	2.7
1	A	201	ALA	2.4
1	A	268[A]	GLU	2.2
1	A	489	GLU	2.2
1	A	115	ILE	2.1
1	A	330[A]	PHE	2.1
1	A	218	LEU	2.1
1	A	270[A]	LYS	2.1
1	A	257	ASN	2.1
1	A	24	SER	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 ⓘ

There are no carbohydrates in this entry.

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	CL	A	1552	1/1	0.27	7.40	82,82,82,82	0
8	ACT	A	1555[B]	4/4	0.34	6.33	19,20,21,23	4
4	PGE	A	1539	10/10	0.33	5.34	67,69,77,79	0
5	AT3	A	1541	10/10	0.39	5.29	81,82,83,84	0
6	ACE	A	1543[A]	3/3	0.32	5.26	32,32,38,39	3
7	CL	A	1551	1/1	0.14	4.47	79,79,79,79	0
2	NAG	A	1536	14/15	0.21	3.41	53,56,59,62	0
5	AT3	A	1540	10/10	0.30	2.68	76,77,78,79	0
3	NDG	A	1537	14/15	0.27	2.67	67,71,72,73	0
4	PGE	A	1538	10/10	0.17	1.48	48,57,60,60	0
7	CL	A	1554	1/1	0.17	0.42	75,75,75,75	0
7	CL	A	1547	1/1	0.11	0.18	82,82,82,82	0
7	CL	A	1550	1/1	0.17	-0.03	80,80,80,80	0
7	CL	A	1548	1/1	0.10	-0.33	69,69,69,69	0
7	CL	A	1549	1/1	0.14	-0.61	88,88,88,88	0
7	CL	A	1546	1/1	0.08	-0.65	58,58,58,58	0
7	CL	A	1553	1/1	0.07	-1.07	69,69,69,69	0
7	CL	A	1544	1/1	0.04	-2.02	49,49,49,49	0
7	CL	A	1545	1/1	0.05	-2.39	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.