



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2HA5  
Title : Crystal structure of mutant S203A of acetylcholinesterase complexed with acetylthiocholine  
Authors : Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.  
Deposited on : 2006-06-12  
Resolution : 2.15 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

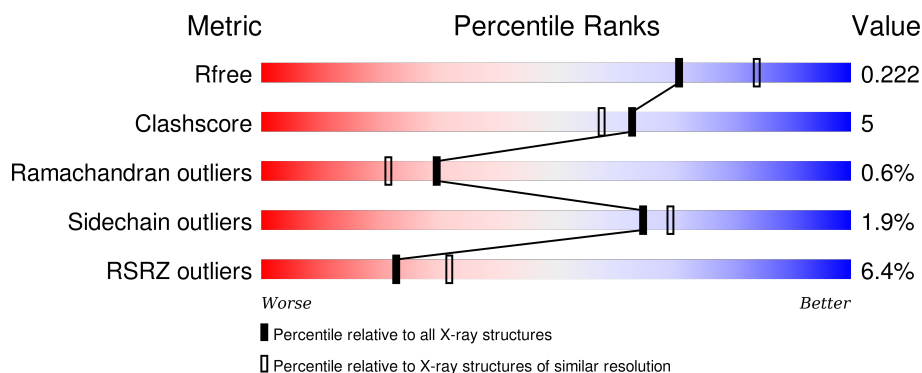
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	543	<div> <div>4%</div> <div>88%</div> <div>10% ..</div> </div>
1	B	543	<div> <div>9%</div> <div>88%</div> <div>9% ..</div> </div>

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
4	ACT	A	1903	-	-	X	X
4	ACT	B	1953	-	-	-	X
5	AT3	A	1901[A]	-	-	-	X
5	AT3	A	1902	-	-	-	X
5	AT3	B	1951[A]	-	-	-	X
5	AT3	B	1952	-	-	-	X
6	ETM	A	1909[B]	-	-	-	X
6	ETM	B	1955	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9414 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	1	7	0
			4211	2702	734	761	14			
1	B	533	Total	C	N	O	S	0	3	0
			4174	2681	722	757	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	SER	ENGINEERED	UNP P21836
B	203	ALA	SER	ENGINEERED	UNP P21836

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

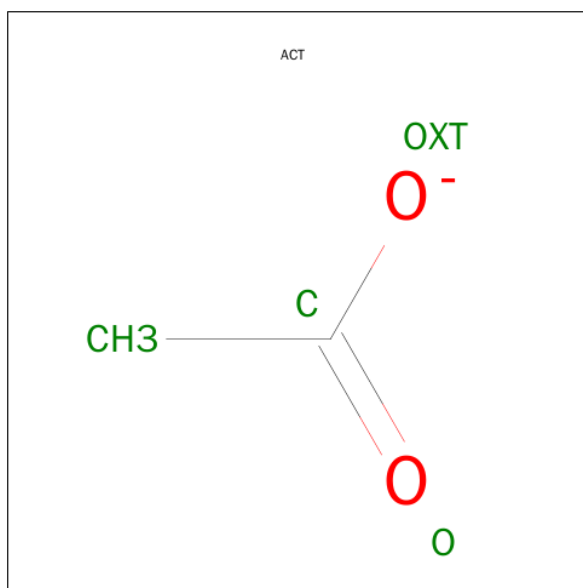
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



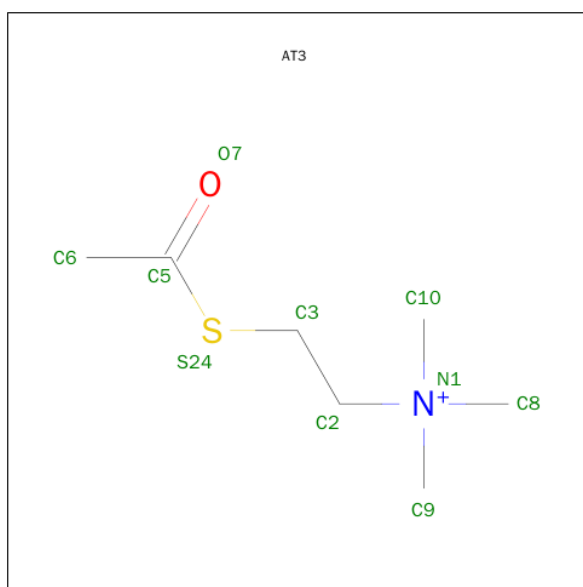
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



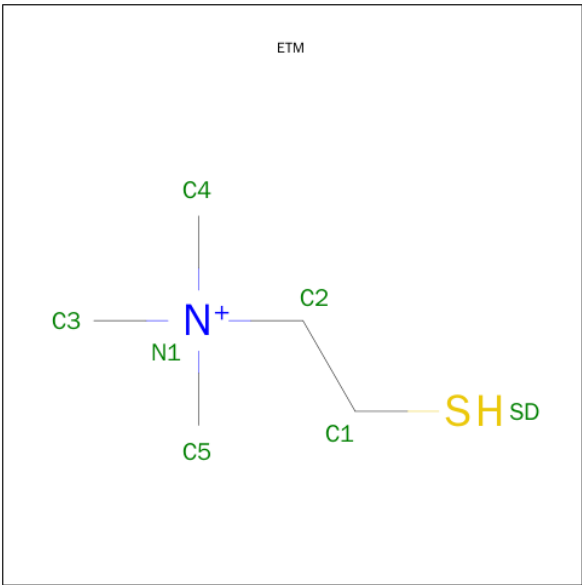
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETYLTHIOCHOLINE (three-letter code: AT3) (formula:  $C_7H_{16}NOS$ ).



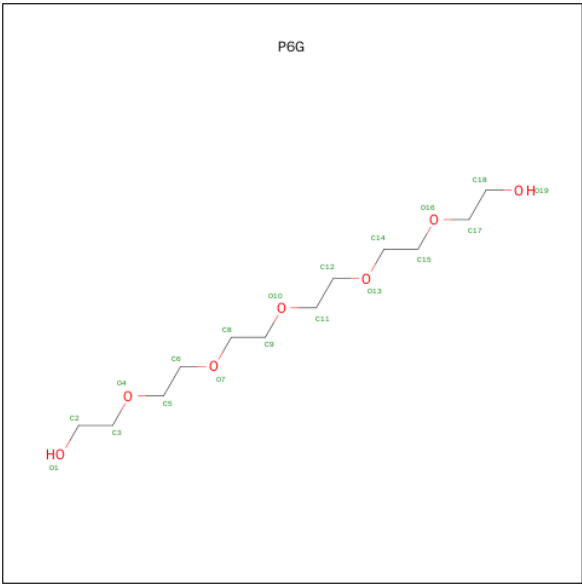
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			10	7	1	1	1		
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	1
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 6 is 2-(TRIMETHYLAMMONIUM)ETHYL THIOL (three-letter code: ETM) (formula: C<sub>5</sub>H<sub>14</sub>NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	1
			7	5	1	1		
6	A	1	Total	C	N	S	0	0
			7	5	1	1		
6	B	1	Total	C	N	S	0	1
			7	5	1	1		
6	B	1	Total	C	N	S	0	0
			7	5	1	1		

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is water.

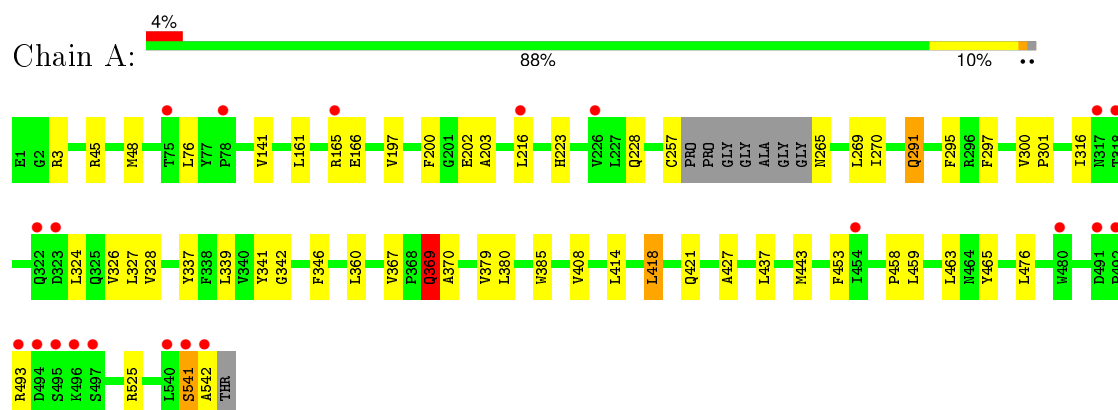
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	485	Total	O	0	0
			485	485		
8	B	401	Total	O	0	0
			401	401		



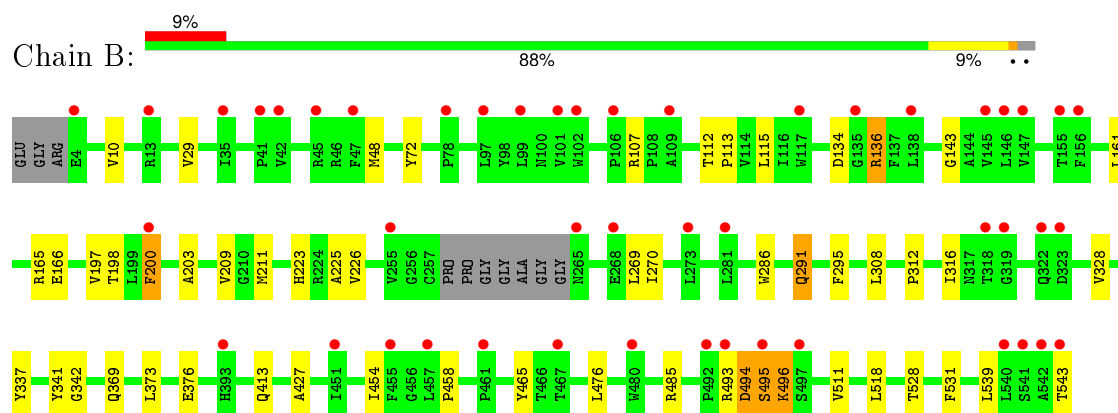
### 3 Residue-property plots

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



#### • Molecule 1: Acetylcholinesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.48Å 109.84Å 227.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.15) 86.6 (29.02-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.177 , 0.210 0.187 , 0.222	Depositor DCC
$R_{free}$ test set	2062 reflections (2.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 103355 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, AT3, FUC, P6G, ACT, ETM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	4/4365 (0.1%)	0.72	6/5961 (0.1%)
1	B	0.45	0/4309	0.62	0/5888
All	All	0.52	4/8674 (0.0%)	0.67	6/11849 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369[A]	GLN	CB-CG	-13.22	1.16	1.52
1	A	369[B]	GLN	CB-CG	-13.22	1.16	1.52
1	A	369[A]	GLN	CA-CB	5.39	1.65	1.53
1	A	369[B]	GLN	CA-CB	5.39	1.65	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369[A]	GLN	CA-CB-CG	15.94	148.47	113.40
1	A	369[B]	GLN	CA-CB-CG	15.94	148.47	113.40
1	A	369[A]	GLN	N-CA-CB	-5.50	100.69	110.60
1	A	369[B]	GLN	N-CA-CB	-5.50	100.69	110.60
1	A	369[A]	GLN	CB-CA-C	-5.04	100.32	110.40
1	A	369[B]	GLN	CB-CA-C	-5.04	100.32	110.40

There are no chirality outliers.

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	4211	0	4102	40	0
1	B	4174	0	4067	45	0
2	A	24	0	22	0	0
3	A	14	0	13	1	0
4	A	4	0	3	2	0
4	B	4	0	3	1	0
5	A	20	0	32	1	0
5	B	30	0	48	6	0
6	A	14	0	28	3	0
6	B	14	0	28	8	0
7	B	19	0	26	0	0
8	A	485	0	0	3	0
8	B	401	0	0	2	0
All	All	9414	0	8372	90	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 5.

All (90) 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:B:161:LEU:HD11	1:B:269:LEU:HD22	1.59	0.85
1:B:543:THR:HG23	8:B:3179:HOH:O	1.78	0.83
1:B:286:TRP:CZ2	6:B:1955:ETM:H53	2.15	0.81
1:A:337:TYR:OH	6:A:1909[B]:ETM:SD	2.43	0.76
1:B:341:TYR:CE2	6:B:1955:ETM:H42	2.24	0.72
1:B:286:TRP:CZ2	6:B:1955:ETM:C5	2.73	0.72
1:B:72:TYR:CE1	6:B:1955:ETM:H52	2.25	0.72
1:A:48:MET:HE1	1:A:165:ARG:O	1.90	0.71
1:A:380:LEU:HD23	1:A:385:TRP:HZ2	1.57	0.69
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:C9	2.81	0.69
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:H9C2	2.33	0.68
1:B:203:ALA:HB1	4:B:1953:ACT:C	2.25	0.67
1:A:337:TYR:HA	1:A:443[A]:MET:HE1	1.80	0.64
1:B:48:MET:HE3	1:B:48:MET:HA	1.80	0.63
1:A:203:ALA:HB1	4:A:1903:ACT:C	2.29	0.63
1:B:286:TRP:CE2	6:B:1955:ETM:H53	2.33	0.62
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.81	0.62
1:A:380:LEU:HD23	1:A:385:TRP:CZ2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:MET:HA	1:B:48:MET:CE	2.31	0.61
1:B:495:SER:OG	1:B:496:LYS:N	2.33	0.60
1:B:465:TYR:OH	5:B:1952:AT3:H9C1	2.02	0.60
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.84	0.59
1:B:341:TYR:CD2	6:B:1955:ETM:H42	2.37	0.59
1:B:48:MET:HE1	1:B:165:ARG:O	2.03	0.58
1:B:291:GLN:HE22	1:B:369:GLN:NE2	2.01	0.58
1:A:541:SER:O	1:A:542:ALA:HB3	2.05	0.57
1:A:316:ILE:O	1:A:421:GLN:NE2	2.25	0.56
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.52	0.56
1:B:134:ASP:OD1	1:B:136:ARG:HD2	2.06	0.55
1:A:48:MET:HE1	1:A:166:GLU:HA	1.88	0.55
1:B:197:VAL:H	1:B:223:HIS:CD2	2.25	0.54
1:A:291:GLN:NE2	1:A:369[B]:GLN:HE21	2.05	0.54
1:B:493:ARG:O	1:B:494:ASP:HB3	2.09	0.53
1:A:337:TYR:HA	1:A:443[A]:MET:CE	2.39	0.52
1:A:541:SER:O	1:A:542:ALA:CB	2.57	0.52
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.91	0.52
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.39	0.52
1:B:493:ARG:O	1:B:494:ASP:CB	2.59	0.51
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.26	0.50
1:A:76:LEU:HD22	1:A:341:TYR:CE2	2.46	0.50
1:A:324:LEU:HG	1:A:326:VAL:HG13	1.94	0.50
1:A:463:LEU:HA	3:A:701:NAG:H82	1.94	0.49
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.48	0.49
1:B:291:GLN:NE2	1:B:369:GLN:HE21	2.11	0.49
1:B:197:VAL:H	1:B:223:HIS:HD2	1.61	0.48
1:A:291:GLN:NE2	1:A:369[B]:GLN:NE2	2.60	0.48
1:B:328:VAL:O	1:B:427:ALA:HA	2.13	0.48
1:B:291:GLN:NE2	1:B:369:GLN:NE2	2.62	0.48
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.95	0.47
1:A:291:GLN:NE2	8:A:2368:HOH:O	2.35	0.47
1:A:76:LEU:HD22	1:A:341:TYR:CD2	2.49	0.47
1:A:465:TYR:OH	5:A:1902:AT3:H9C1	2.15	0.47
1:B:115:LEU:HD23	1:B:198:THR:HB	1.97	0.47
1:B:312:PRO:O	1:B:316:ILE:HG23	2.15	0.46
1:A:197:VAL:H	1:A:223:HIS:HD2	1.63	0.46
1:B:286:TRP:CZ2	6:B:1955:ETM:H51	2.51	0.46
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.98	0.46
1:B:454:ILE:HD13	1:B:476:LEU:HB3	1.98	0.45
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.98	0.45
1:B:200:PHE:CB	1:B:226:VAL:HB	2.47	0.45
1:B:209:VAL:CG1	1:B:225:ALA:HB1	2.47	0.45
1:B:539:LEU:O	1:B:543:THR:N	2.50	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.53	0.44
1:A:367:VAL:HG12	1:A:370:ALA:HB2	1.99	0.44
1:A:300:VAL:HB	1:A:301:PRO:HD2	2.01	0.43
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.99	0.43
6:B:1959[B]:ETM:H33	6:B:1959[B]:ETM:H12	1.86	0.43
1:A:141:VAL:HG21	1:A:459:LEU:HD23	2.01	0.42
1:A:408:VAL:HG11	1:A:525:ARG:HG3	2.01	0.42
1:A:202:GLU:OE1	6:A:1909[B]:ETM:H41	2.20	0.42
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.01	0.42
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.54	0.42
1:B:166:GLU:HB2	1:B:270:ILE:HD13	2.02	0.42
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.00	0.42
1:A:297:PHE:CZ	4:A:1903:ACT:H2	2.55	0.41
1:B:112:THR:HG21	1:B:143:GLY:O	2.20	0.41
5:B:1951[A]:AT3:S24	5:B:1951[A]:AT3:H9C3	2.61	0.41
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.03	0.41
5:B:1952:AT3:H9C2	8:B:3066:HOH:O	2.19	0.41
1:A:337:TYR:CZ	6:A:1909[B]:ETM:SD	3.11	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.41
1:A:265:ASN:ND2	8:A:2302:HOH:O	2.53	0.41
1:B:113:PRO:HG2	1:B:485:ARG:HG2	2.03	0.41
1:B:337:TYR:CE2	5:B:1951[A]:AT3:H6C1	2.56	0.41
1:B:373:LEU:HD23	1:B:539:LEU:HD11	2.03	0.40
1:A:257:CYS:C	8:A:2019:HOH:O	2.60	0.40
1:B:528:THR:O	1:B:531:PHE:HB3	2.21	0.40
1:A:197:VAL:H	1:A:223:HIS:CD2	2.39	0.40
1:A:202:GLU:HA	1:A:228:GLN:O	2.21	0.40

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	538/543 (99%)	519 (96%)	17 (3%)	2 (0%)	39	34
1	B	532/543 (98%)	513 (96%)	15 (3%)	4 (1%)	24	15
All	All	1070/1086 (98%)	1032 (96%)	32 (3%)	6 (1%)	30	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	495	SER
1	A	541	SER
1	B	496	LYS
1	A	342	GLY
1	B	342	GLY

### 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	445/442 (101%)	433 (97%)	12 (3%)	52	53
1	B	440/442 (100%)	434 (99%)	6 (1%)	74	80
All	All	885/884 (100%)	867 (98%)	18 (2%)	65	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	45	ARG
1	A	200	PHE
1	A	216	LEU
1	A	291	GLN
1	A	295	PHE
1	A	327	LEU

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Mol	Chain	Res	Type
1	A	369[A]	GLN
1	A	369[B]	GLN
1	A	418	LEU
1	A	437	LEU
1	A	493	ARG
1	B	136	ARG
1	B	200	PHE
1	B	291	GLN
1	B	295	PHE
1	B	376	GLU
1	B	413	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	291	GLN
1	A	322	GLN
1	A	325	GLN
1	B	223	HIS
1	B	291	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 ⓘ

2 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	$\# Z  > 2$
2	NAG	A	544	1,2	14,14,15	0.63	0	15,19,21	1.19	1 (6%)
2	FUC	A	545	2	10,10,11	0.62	0	14,14,16	1.25	3 (21%)

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	544	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	545	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	545	FUC	O5-C5-C4	2.11	113.19	109.53
2	A	545	FUC	C3-C4-C5	2.15	113.34	109.72
2	A	545	FUC	C1-O5-C5	2.17	115.73	112.38
2	A	544	NAG	C1-O5-C5	3.32	116.46	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

13 ligands 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
5	AT3	A	1901[A]	-	9,9,9	1.12	0	11,12,12	0.63	0
5	AT3	A	1902	-	9,9,9	0.74	0	11,12,12	0.41	0
4	ACT	A	1903	-	1,3,3	0.98	0	0,3,3	0.00	-
6	ETM	A	1905	-	6,6,6	0.63	0	6,8,8	1.40	1 (16%)
6	ETM	A	1909[B]	-	6,6,6	1.02	0	6,8,8	1.11	1 (16%)
3	NAG	A	701	1	14,14,15	0.48	0	15,19,21	0.80	0
5	AT3	B	1951[A]	-	9,9,9	1.14	0	11,12,12	0.44	0
5	AT3	B	1952	-	9,9,9	0.81	0	11,12,12	0.53	0
4	ACT	B	1953	-	1,3,3	1.21	0	0,3,3	0.00	-
6	ETM	B	1955	-	6,6,6	0.71	0	6,8,8	1.05	0
6	ETM	B	1959[B]	-	6,6,6	1.06	0	6,8,8	0.74	0
5	AT3	B	1961	-	9,9,9	0.76	0	11,12,12	0.80	0
7	P6G	B	2901	-	18,18,18	2.21	6 (33%)	17,17,17	1.25	1 (5%)

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
5	AT3	A	1901[A]	-	-	0/7/7/7	0/0/0/0
5	AT3	A	1902	-	-	0/7/7/7	0/0/0/0
4	ACT	A	1903	-	-	0/0/0/0	0/0/0/0
6	ETM	A	1905	-	-	0/4/4/4	0/0/0/0
6	ETM	A	1909[B]	-	-	0/4/4/4	0/0/0/0
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	AT3	B	1951[A]	-	-	2/7/7/7	0/0/0/0
5	AT3	B	1952	-	-	0/7/7/7	0/0/0/0
4	ACT	B	1953	-	-	0/0/0/0	0/0/0/0
6	ETM	B	1955	-	-	0/4/4/4	0/0/0/0
6	ETM	B	1959[B]	-	-	0/4/4/4	0/0/0/0
5	AT3	B	1961	-	-	0/7/7/7	0/0/0/0
7	P6G	B	2901	-	-	0/16/16/16	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2901	P6G	O7-C6	2.89	1.54	1.42
7	B	2901	P6G	O19-C18	3.35	1.60	1.42
7	B	2901	P6G	O4-C3	3.52	1.57	1.42
7	B	2901	P6G	O16-C15	3.62	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2901	P6G	O13-C12	3.83	1.58	1.42
7	B	2901	P6G	O10-C9	4.42	1.60	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1909[B]	ETM	C3-N1-C2	2.09	118.21	109.90
6	A	1905	ETM	C3-N1-C2	2.37	119.34	109.90
7	B	2901	P6G	O1-C2-C3	3.09	131.09	112.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1951[A]	AT3	C6-C5-S24-C3
5	B	1951[A]	AT3	O7-C5-S24-C3

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1902	AT3	1	0
4	A	1903	ACT	2	0
6	A	1909[B]	ETM	3	0
3	A	701	NAG	1	0
5	B	1951[A]	AT3	4	0
5	B	1952	AT3	2	0
4	B	1953	ACT	1	0
6	B	1955	ETM	7	0
6	B	1959[B]	ETM	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 ⓘ

### 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	535/543 (98%)	0.17	21 (3%) 43 54	41, 53, 70, 98	0
1	B	533/543 (98%)	0.36	47 (8%) 12 18	43, 59, 78, 99	0
All	All	1068/1086 (98%)	0.26	68 (6%) 23 32	41, 55, 76, 99	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	7.4
1	A	493	ARG	6.3
1	B	492	PRO	6.2
1	B	543	THR	5.9
1	B	495	SER	4.8
1	B	542	ALA	4.7
1	B	106	PRO	4.5
1	B	109	ALA	4.5
1	A	497	SER	4.2
1	B	540	LEU	4.2
1	A	216	LEU	4.1
1	A	492	PRO	4.0
1	A	494	ASP	3.9
1	B	541	SER	3.8
1	A	542	ALA	3.7
1	B	42	VAL	3.7
1	B	138	LEU	3.7
1	B	322	GLN	3.6
1	B	497	SER	3.6
1	A	540	LEU	3.6
1	B	45[A]	ARG	3.4
1	B	101	VAL	3.4
1	B	146	LEU	3.3
1	A	496	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	541	SER	3.2
1	B	493	ARG	3.2
1	B	135	GLY	3.1
1	B	461	PRO	3.0
1	B	323	ASP	3.0
1	B	451	ILE	2.9
1	B	455	PHE	2.9
1	A	165	ARG	2.9
1	A	323[A]	ASP	2.9
1	B	4	GLU	2.8
1	A	317	ASN	2.8
1	B	318	THR	2.8
1	A	75	THR	2.7
1	B	41	PRO	2.7
1	B	47	PHE	2.7
1	A	454	ILE	2.6
1	B	99	LEU	2.6
1	B	281	LEU	2.6
1	B	156	PHE	2.5
1	A	226	VAL	2.5
1	B	147	VAL	2.5
1	B	265	ASN	2.5
1	B	457	LEU	2.4
1	A	322	GLN	2.4
1	B	102	TRP	2.4
1	A	318	THR	2.3
1	B	35	ILE	2.3
1	B	467	THR	2.2
1	A	480	TRP	2.2
1	B	155	THR	2.2
1	B	117	TRP	2.2
1	B	268	GLU	2.2
1	B	319	GLY	2.2
1	B	13	ARG	2.1
1	B	480	TRP	2.1
1	A	491	ASP	2.1
1	B	393	HIS	2.1
1	B	200	PHE	2.1
1	B	273	LEU	2.1
1	B	145	VAL	2.1
1	A	78	PRO	2.0
1	B	78	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	2.0
1	B	255	VAL	2.0

## 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
2	FUC	A	545	10/11	0.46	0.63	-	102,104,105,105	0
2	NAG	A	544	14/15	0.77	0.42	-	83,90,94,98	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
5	AT3	A	1901[A]	10/10	0.80	0.50	15.71	80,81,83,84	10
4	ACT	B	1953	4/4	0.88	0.25	6.80	62,64,64,64	0
5	AT3	A	1902	10/10	0.84	0.30	6.44	78,80,81,81	0
4	ACT	A	1903	4/4	0.91	0.21	5.20	59,60,61,61	0
5	AT3	B	1951[A]	10/10	0.85	0.33	4.98	78,79,83,84	10
6	ETM	A	1909[B]	7/7	0.85	0.28	4.83	58,58,60,62	7
5	AT3	B	1952	10/10	0.84	0.26	2.57	86,90,91,91	0
6	ETM	B	1959[B]	7/7	0.89	0.20	1.54	73,74,75,77	7
5	AT3	B	1961	10/10	0.95	0.18	0.55	68,70,71,73	0
7	P6G	B	2901	19/19	0.89	0.15	0.49	67,72,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ETM	A	1905	7/7	0.72	0.30	-	94,95,96,98	0
6	ETM	B	1955	7/7	0.75	0.34	-	93,93,95,97	7
3	NAG	A	701	14/15	0.74	0.39	-	81,86,89,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.