



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 PM UTC

PDB ID : 2ACE / pdb\_00002ace  
Title : NATIVE ACETYLCHOLINESTERASE (E.C. 3.1.1.7) FROM TORPEDO CALIFORNICA  
Authors : Harel, M.; Raves, M.L.; Silman, I.; Sussman, J.L.  
Deposited on : 1996-06-23  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

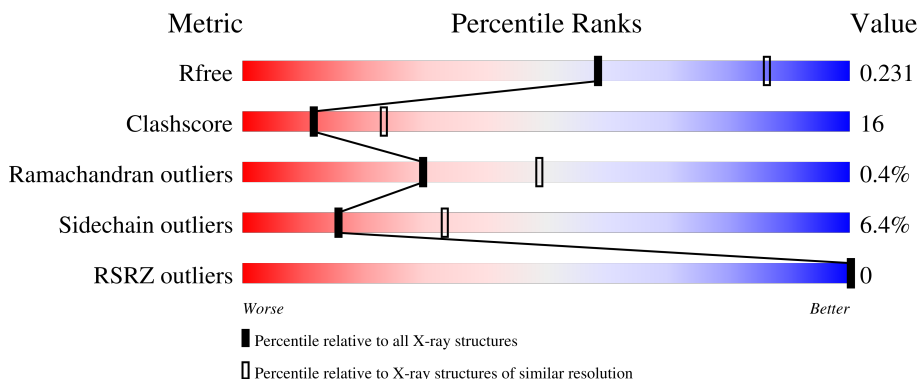
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	537	 64% 28% 6%

## 2 Entry composition [i](#)

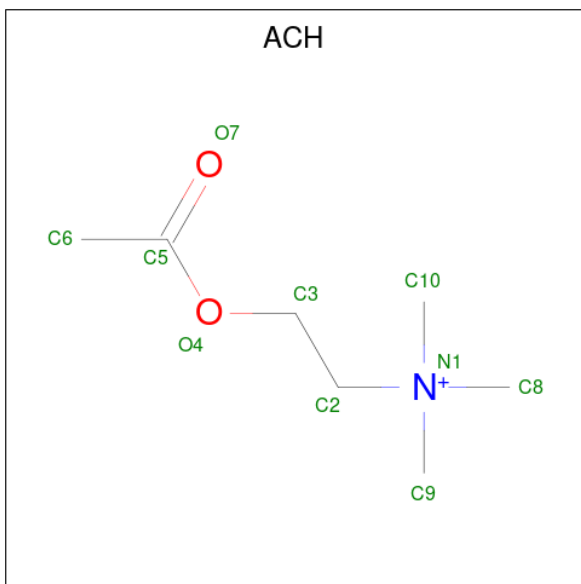
There are 3 unique types of molecules in this entry. The entry contains 4357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	527	4143	2677	693	751	22	0	0	0

- Molecule 2 is ACETYLCHOLINE (CCD ID: ACH) (formula: C<sub>7</sub>H<sub>16</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	7	1	2	10	0

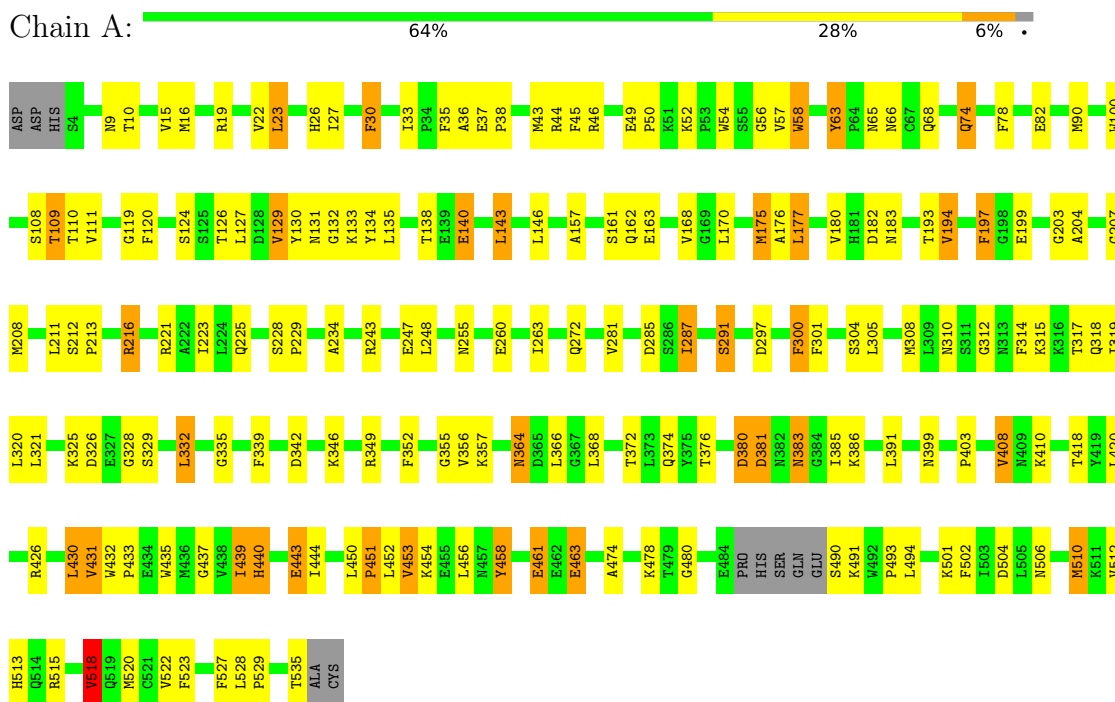
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	204	Total	O	0	0
			204	204		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.41Å 112.41Å 136.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (8.00-2.50) 85.7 (8.00-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.26Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.199 , 0.258 0.181 , 0.231	Depositor DCC
$R_{free}$ test set	2302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.406	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ACH

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	0.92	2/4262 (0.0%)	1.24	41/5788 (0.7%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	MET	SD-CE	5.14	1.92	1.79
1	A	474	ALA	CA-CB	-5.09	1.45	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	N-CA-C	-9.13	93.71	108.41
1	A	443	GLU	N-CA-C	-7.91	103.76	113.41
1	A	56	GLY	N-CA-C	-7.83	102.85	112.33
1	A	255	ASN	N-CA-C	-7.42	99.04	110.10
1	A	291	SER	N-CA-C	7.32	119.16	111.03
1	A	332	LEU	N-CA-C	-7.30	103.25	111.14
1	A	463	GLU	N-CA-C	-6.98	103.75	111.36
1	A	342	ASP	N-CA-C	6.95	121.47	112.92
1	A	297	ASP	N-CA-C	6.95	121.50	112.89
1	A	439	ILE	N-CA-C	6.92	119.01	109.80
1	A	52	LYS	N-CA-C	-6.90	101.66	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	N-CA-C	-6.64	96.40	108.02
1	A	364	ASN	N-CA-C	-6.54	101.32	110.35
1	A	522	VAL	N-CA-C	-6.53	104.13	110.72
1	A	182	ASP	N-CA-C	6.41	118.34	111.36
1	A	458	TYR	N-CA-C	-6.40	101.31	110.59
1	A	58	TRP	N-CA-C	-6.38	100.11	110.20
1	A	518	VAL	CB-CA-C	-6.31	103.75	112.02
1	A	161	SER	N-CA-C	-6.05	101.05	110.42
1	A	399	ASN	N-CA-C	5.97	120.63	113.23
1	A	494	LEU	N-CA-C	-5.84	100.14	109.96
1	A	157	ALA	N-CA-C	5.82	119.38	107.69
1	A	527	PHE	N-CA-C	5.81	117.48	111.03
1	A	162	GLN	N-CA-C	-5.76	106.23	113.72
1	A	248	LEU	N-CA-C	-5.73	105.03	111.28
1	A	38	PRO	CA-C-N	5.73	127.00	119.84
1	A	38	PRO	C-N-CA	5.73	127.00	119.84
1	A	431	VAL	CB-CA-C	-5.69	105.64	112.19
1	A	403	PRO	N-CA-C	-5.55	106.30	113.57
1	A	300	PHE	N-CA-C	-5.50	105.28	111.28
1	A	100	TRP	N-CA-C	-5.36	100.44	109.07
1	A	504	ASP	N-CA-C	-5.24	102.73	110.48
1	A	381	ASP	N-CA-C	5.22	119.28	113.01
1	A	346	LYS	N-CA-C	-5.22	102.66	110.23
1	A	203	GLY	N-CA-C	-5.16	106.46	113.37
1	A	440	HIS	N-CA-C	-5.10	102.74	110.24
1	A	177	LEU	N-CA-C	-5.07	105.83	111.36
1	A	90	MET	N-CA-C	-5.03	102.32	110.32
1	A	234	ALA	N-CA-C	5.01	119.10	112.89
1	A	212	SER	CA-C-N	5.00	124.44	119.24
1	A	212	SER	C-N-CA	5.00	124.44	119.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	4143	0	3975	129	0
2	A	10	0	16	0	0
3	A	204	0	0	3	0
All	All	4357	0	3991	129	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 16.

All (129) 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:VAL:HG22	1:A:456:LEU:HG	1.54	0.88
1:A:374:GLN:NE2	3:A:732:HOH:O	2.04	0.87
1:A:287:ILE:HD11	1:A:335:GLY:HA3	1.59	0.84
1:A:349:ARG:HH12	1:A:376:THR:HG23	1.41	0.84
1:A:515:ARG:HB3	1:A:518:VAL:HG22	1.62	0.81
1:A:349:ARG:HD3	1:A:381:ASP:O	1.81	0.80
1:A:515:ARG:HB3	1:A:518:VAL:CG2	2.11	0.80
1:A:366:LEU:HD23	1:A:535:THR:HG21	1.66	0.78
1:A:49:GLU:C	1:A:175:MET:HE1	2.11	0.76
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.67	0.76
1:A:221:ARG:HD3	1:A:480:GLY:HA2	1.68	0.75
1:A:78:PHE:HZ	1:A:431:VAL:O	1.73	0.71
1:A:110:THR:HG23	1:A:193:THR:HG22	1.72	0.69
1:A:491:LYS:O	1:A:493:PRO:HD3	1.94	0.67
1:A:16:MET:HB2	1:A:57:VAL:CG1	2.24	0.67
1:A:247:GLU:HG3	3:A:762:HOH:O	1.95	0.67
1:A:211:LEU:HD13	1:A:305:LEU:HD22	1.76	0.66
1:A:37:GLU:CG	1:A:49:GLU:HG2	2.26	0.65
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.33	0.64
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.81	0.62
1:A:349:ARG:NH1	1:A:376:THR:HG23	2.13	0.62
1:A:110:THR:OG1	1:A:478:LYS:HG2	1.99	0.62
1:A:37:GLU:HG3	1:A:49:GLU:HG2	1.81	0.61
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.84	0.60
1:A:380:ASP:OD1	1:A:383:ASN:HB2	2.02	0.59
1:A:520:MET:O	1:A:523:PHE:HB3	2.03	0.58
1:A:131:ASN:HD22	1:A:134:TYR:HE1	1.50	0.57
1:A:176:ALA:O	1:A:180:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:NH2	1:A:26:HIS:HB2	2.20	0.56
1:A:454:LYS:C	1:A:456:LEU:H	2.12	0.56
1:A:30:PHE:HB3	1:A:33:ILE:HD11	1.86	0.56
1:A:197:PHE:CB	1:A:223:ILE:HB	2.36	0.55
1:A:211:LEU:CD1	1:A:305:LEU:HD22	2.36	0.55
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.87	0.55
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.89	0.55
1:A:408:VAL:HG22	1:A:418:THR:HG21	1.89	0.55
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.89	0.55
1:A:515:ARG:HB3	1:A:518:VAL:HG21	1.88	0.54
1:A:216:ARG:HB3	1:A:315:LYS:HB2	1.87	0.54
1:A:204:ALA:O	1:A:208:MET:HG3	2.07	0.54
1:A:349:ARG:HH12	1:A:376:THR:CG2	2.16	0.54
1:A:320:LEU:C	1:A:320:LEU:HD23	2.33	0.54
1:A:501:LYS:HD3	1:A:512:VAL:HG11	1.88	0.54
1:A:65:ASN:C	1:A:66:ASN:HD22	2.16	0.53
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.43	0.53
1:A:364:ASN:ND2	1:A:535:THR:OG1	2.42	0.53
1:A:78:PHE:CZ	1:A:431:VAL:O	2.60	0.51
1:A:131:ASN:ND2	1:A:134:TYR:CE1	2.79	0.51
1:A:36:ALA:HB2	1:A:175:MET:HE2	1.93	0.50
1:A:49:GLU:O	1:A:175:MET:HE1	2.11	0.50
1:A:43:MET:O	1:A:46:ARG:HB2	2.11	0.50
1:A:124:SER:HB2	1:A:127:LEU:CD2	2.42	0.50
1:A:170:LEU:HB3	1:A:300:PHE:CZ	2.47	0.49
1:A:281:VAL:CG2	1:A:291:SER:HB3	2.42	0.49
1:A:383:ASN:HD21	1:A:385:ILE:HB	1.77	0.49
1:A:163:GLU:HB2	1:A:263:ILE:HD13	1.94	0.49
1:A:221:ARG:CD	1:A:480:GLY:HA2	2.40	0.49
1:A:321:LEU:O	1:A:420:LEU:HD12	2.12	0.49
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.93	0.49
1:A:326:ASP:OD2	1:A:437:GLY:HA3	2.13	0.48
1:A:131:ASN:ND2	1:A:133:LYS:HG2	2.29	0.48
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.95	0.48
1:A:433:PRO:HB2	1:A:435:TRP:CD1	2.48	0.48
1:A:310:ASN:OD1	1:A:410:LYS:NZ	2.37	0.48
1:A:216:ARG:HD2	1:A:315:LYS:HB2	1.95	0.48
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.96	0.47
1:A:44:ARG:O	1:A:45:PHE:HB2	2.15	0.47
1:A:439:ILE:HG22	1:A:440:HIS:N	2.28	0.47
1:A:454:LYS:C	1:A:456:LEU:N	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:HG23	1:A:193:THR:CG2	2.41	0.47
1:A:199:GLU:HA	1:A:225:GLN:O	2.15	0.47
1:A:506:ASN:OD1	1:A:506:ASN:C	2.57	0.47
1:A:66:ASN:HD22	1:A:66:ASN:N	2.10	0.46
1:A:130:TYR:HE1	1:A:444:ILE:HD13	1.80	0.46
1:A:317:THR:OG1	1:A:318:GLN:N	2.49	0.46
1:A:426:ARG:NH2	1:A:433:PRO:O	2.49	0.46
1:A:175:MET:O	1:A:175:MET:HG3	2.15	0.46
1:A:450:LEU:O	1:A:453:VAL:HG13	2.16	0.46
1:A:328:GLY:O	1:A:329:SER:C	2.58	0.46
1:A:430:LEU:CD2	1:A:432:TRP:HD1	2.28	0.46
1:A:383:ASN:HD22	1:A:385:ILE:N	2.14	0.45
1:A:129:VAL:HG22	3:A:706:HOH:O	2.16	0.45
1:A:22:VAL:O	1:A:23:LEU:C	2.59	0.45
1:A:124:SER:HB2	1:A:127:LEU:HD21	1.97	0.45
1:A:10:THR:HB	1:A:183:ASN:OD1	2.17	0.45
1:A:301:PHE:CD1	1:A:305:LEU:HD21	2.51	0.45
1:A:319:ILE:O	1:A:319:ILE:HG13	2.17	0.45
1:A:119:GLY:O	1:A:120:PHE:HB2	2.17	0.45
1:A:272:GLN:O	1:A:272:GLN:HG3	2.15	0.45
1:A:304:SER:O	1:A:305:LEU:C	2.59	0.45
1:A:26:HIS:O	1:A:27:ILE:HG23	2.17	0.45
1:A:199:GLU:HG3	1:A:443:GLU:OE2	2.16	0.45
1:A:45:PHE:O	1:A:168:VAL:HG11	2.17	0.44
1:A:287:ILE:HD12	1:A:287:ILE:HA	1.60	0.44
1:A:332:LEU:HD13	1:A:339:PHE:CZ	2.53	0.44
1:A:74:GLN:HE21	1:A:74:GLN:HA	1.82	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.87	0.43
1:A:450:LEU:C	1:A:452:LEU:H	2.26	0.43
1:A:109:THR:HG21	1:A:140:GLU:O	2.19	0.43
1:A:339:PHE:CZ	1:A:391:LEU:HD23	2.53	0.43
1:A:408:VAL:CG2	1:A:418:THR:HG21	2.48	0.43
1:A:461:GLU:H	1:A:461:GLU:CD	2.25	0.43
1:A:260:GLU:H	1:A:260:GLU:CD	2.27	0.43
1:A:223:ILE:HA	1:A:320:LEU:O	2.18	0.42
1:A:450:LEU:O	1:A:452:LEU:N	2.52	0.42
1:A:35:PHE:O	1:A:175:MET:HE3	2.18	0.42
1:A:383:ASN:ND2	1:A:386:LYS:H	2.17	0.42
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.54	0.42
1:A:35:PHE:CD1	1:A:35:PHE:C	2.97	0.42
1:A:111:VAL:O	1:A:194:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:HIS:O	1:A:27:ILE:CG2	2.68	0.41
1:A:135:LEU:HD23	1:A:143:LEU:HD11	2.01	0.41
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.41
1:A:50:PRO:HA	1:A:175:MET:CE	2.51	0.41
1:A:357:LYS:HD2	1:A:368:LEU:HD11	2.03	0.41
1:A:502:PHE:CE2	1:A:513:HIS:HB2	2.56	0.41
1:A:131:ASN:HD21	1:A:133:LYS:HG2	1.85	0.41
1:A:170:LEU:HD13	1:A:300:PHE:CE1	2.56	0.41
1:A:312:GLY:O	1:A:314:PHE:N	2.52	0.41
1:A:383:ASN:ND2	1:A:385:ILE:H	2.19	0.41
1:A:352:PHE:HE2	1:A:372:THR:HG23	1.86	0.41
1:A:454:LYS:HE2	1:A:463:GLU:OE1	2.20	0.41
1:A:44:ARG:O	1:A:45:PHE:CB	2.69	0.40
1:A:211:LEU:O	1:A:308:MET:HE1	2.21	0.40
1:A:450:LEU:C	1:A:452:LEU:N	2.79	0.40
1:A:54:TRP:NE1	1:A:58:TRP:HB2	2.36	0.40
1:A:134:TYR:O	1:A:138:THR:HB	2.21	0.40
1:A:146:LEU:C	1:A:146:LEU:HD12	2.46	0.40
1:A:321:LEU:HD23	1:A:321:LEU:H	1.86	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	523/537 (97%)	479 (92%)	42 (8%)	2 (0%)	<span style="border: 1px solid red; padding: 2px;">30</span> 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASP
1	A	23	LEU

### 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	437/469 (93%)	409 (94%)	28 (6%)	16	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	15	VAL
1	A	68	GLN
1	A	74	GLN
1	A	82	GLU
1	A	108	SER
1	A	109	THR
1	A	129	VAL
1	A	140	GLU
1	A	143	LEU
1	A	175	MET
1	A	194	VAL
1	A	197	PHE
1	A	213	PRO
1	A	216	ARG
1	A	243	ARG
1	A	287	ILE
1	A	325	LYS
1	A	356	VAL
1	A	383	ASN
1	A	408	VAL
1	A	430	LEU
1	A	451	PRO
1	A	453	VAL
1	A	461	GLU
1	A	490	SER
1	A	510	MET
1	A	518	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	68	GLN
1	A	74	GLN
1	A	131	ASN
1	A	159	HIS
1	A	251	ASN
1	A	264	HIS
1	A	280	ASN
1	A	383	ASN

### 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](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	ACH	A	998	1	9,9,9	1.94	2 (22%)	12,12,12	1.78	3 (25%)

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	ACH	A	998	1	-	2/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	ACH	O7-C5	5.09	1.39	1.21
2	A	998	ACH	O4-C5	2.18	1.43	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	ACH	O7-C5-C6	-4.24	109.74	124.77
2	A	998	ACH	C3-O4-C5	2.67	129.04	117.14
2	A	998	ACH	O4-C5-O7	-2.10	111.03	121.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	ACH	O7-C5-O4-C3
2	A	998	ACH	N1-C2-C3-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 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	527/537 (98%)	-0.71	0 <a href="#">100</a> <a href="#">100</a>	11, 22, 35, 46	0

There are no RSRZ outliers to report.

### 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](#)

There are no oligosaccharides in this entry.

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACH	A	998	10/10	-	-	0,0,0,0	10

### 6.5 Other polymers [i](#)

There are no such residues in this entry.