



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 1ACL / pdb_00001acl
Title : QUATERNARY LIGAND BINDING TO AROMATIC RESIDUES IN THE
ACTIVE-SITE GORGE OF ACETYLCHOLINESTERASE
Authors : Sussman, J.L.; Harel, M.; Silman, I.
Deposited on : 1993-08-18
Resolution : 2.80 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

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>.

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

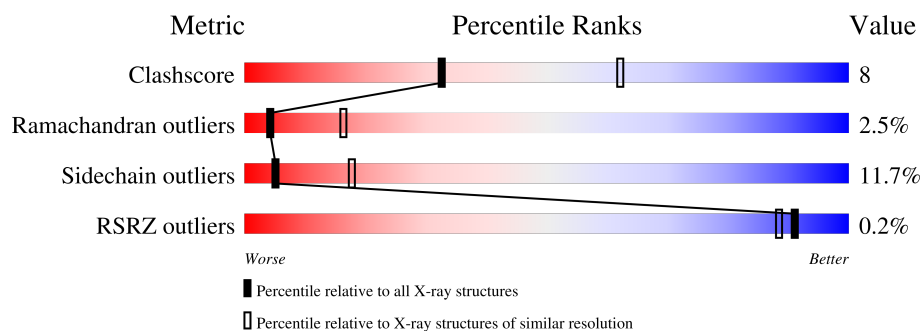
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 ≥ 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	

2 Entry composition [i](#)

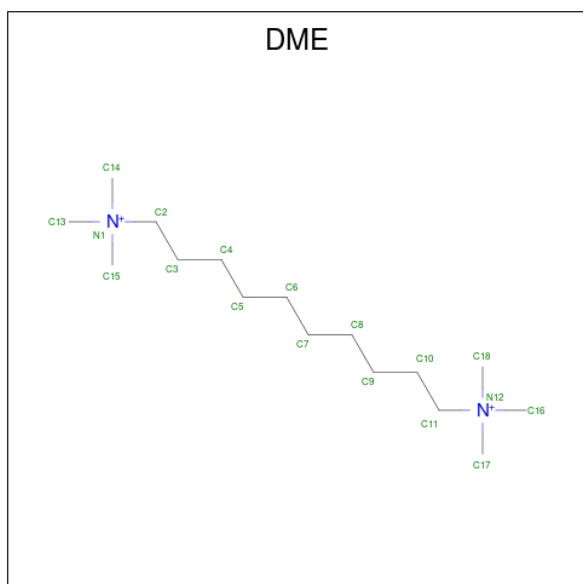
There are 3 unique types of molecules in this entry. The entry contains 4194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	4110	2659	692	738	21	0	0	0

- Molecule 2 is DECAMETHONIUM ION (CCD ID: DME) (formula: $C_{16}H_{38}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	18	16	2	0	0

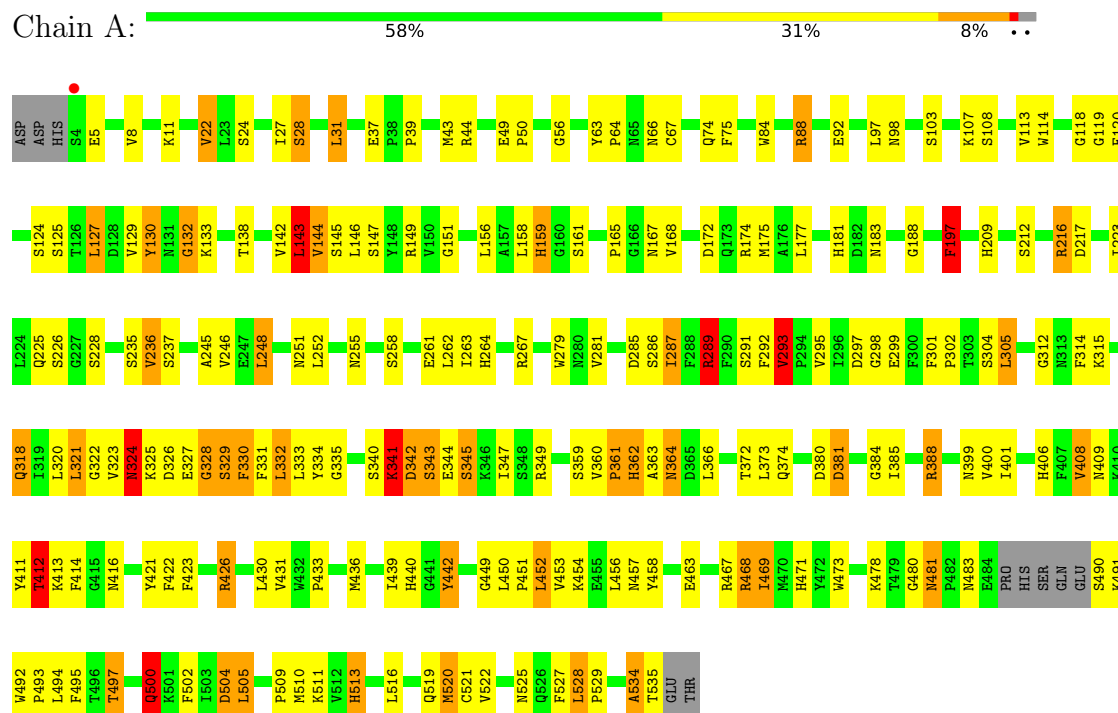
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		

3 Residue-property plots

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, α , β , γ	113.05Å 113.05Å 137.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 85.8 (8.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DME

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	1.34	25/4228 (0.6%)	1.99	120/5745 (2.1%)

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
1	A	0	7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CA-C	-6.77	1.43	1.52
1	A	181	HIS	CG-CD2	6.41	1.42	1.35
1	A	471	HIS	CG-CD2	6.24	1.42	1.35
1	A	97	LEU	CA-C	-6.09	1.45	1.52
1	A	209	HIS	CG-CD2	6.07	1.42	1.35
1	A	264	HIS	CG-CD2	6.00	1.42	1.35
1	A	151	GLY	CA-C	-5.99	1.45	1.52
1	A	228	SER	CA-C	-5.98	1.45	1.52
1	A	513	HIS	CG-CD2	5.92	1.42	1.35
1	A	331	PHE	CA-C	-5.84	1.45	1.52
1	A	108	SER	CA-C	-5.77	1.46	1.52
1	A	333	LEU	CA-C	-5.74	1.45	1.52
1	A	362	HIS	CG-CD2	5.73	1.42	1.35
1	A	478	LYS	CA-C	-5.69	1.47	1.52
1	A	286	SER	CA-C	-5.68	1.45	1.52
1	A	159	HIS	CG-CD2	5.68	1.42	1.35
1	A	161	SER	CA-C	-5.61	1.46	1.52
1	A	440	HIS	CG-CD2	5.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	VAL	CA-C	-5.22	1.46	1.52
1	A	344	GLU	CA-CB	5.20	1.60	1.53
1	A	297	ASP	CA-C	-5.17	1.45	1.52
1	A	401	ILE	CA-C	-5.12	1.46	1.52
1	A	406	HIS	CG-CD2	5.08	1.41	1.35
1	A	143	LEU	CA-C	-5.08	1.46	1.52
1	A	39	PRO	CA-C	-5.00	1.48	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASN	CA-CB-CG	-10.11	102.49	112.60
1	A	293	VAL	N-CA-CB	-9.70	97.64	111.21
1	A	165	PRO	CA-C-N	-9.54	108.02	121.67
1	A	165	PRO	C-N-CA	-9.54	108.02	121.67
1	A	255	ASN	CA-CB-CG	-9.28	103.32	112.60
1	A	49	GLU	N-CA-C	-8.67	99.04	110.40
1	A	341	LYS	N-CA-C	-8.54	98.74	110.35
1	A	299	GLU	N-CA-C	-8.41	98.07	110.52
1	A	323	VAL	N-CA-CB	-7.66	99.57	112.44
1	A	328	GLY	N-CA-C	7.49	121.70	112.64
1	A	217	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	165	PRO	CB-CA-C	-7.35	99.87	110.75
1	A	504	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	28	SER	N-CA-C	-7.13	98.11	109.59
1	A	442	TYR	CB-CA-C	7.08	122.75	110.01
1	A	504	ASP	N-CA-CB	7.08	121.95	110.41
1	A	416	ASN	CA-CB-CG	7.08	119.68	112.60
1	A	37	GLU	CA-C-O	-7.04	114.28	120.19
1	A	480	GLY	N-CA-C	-7.02	105.64	115.32
1	A	291	SER	N-CA-C	6.98	118.78	111.03
1	A	147	SER	CB-CA-C	-6.92	98.37	109.80
1	A	88	ARG	N-CA-C	-6.77	99.03	109.52
1	A	142	VAL	N-CA-C	-6.77	98.43	109.12
1	A	343	SER	N-CA-C	-6.75	100.47	110.46
1	A	286	SER	CB-CA-C	-6.63	98.02	110.16
1	A	228	SER	CA-C-O	-6.62	114.25	120.34
1	A	324	ASN	CB-CA-C	6.61	122.47	109.66
1	A	426	ARG	CA-C-N	-6.59	110.79	120.75
1	A	426	ARG	C-N-CA	-6.59	110.79	120.75
1	A	344	GLU	N-CA-C	-6.47	101.84	111.81
1	A	364	ASN	N-CA-C	-6.46	100.35	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	CA-C-N	-6.42	114.64	122.15
1	A	188	GLY	C-N-CA	-6.42	114.64	122.15
1	A	197	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	183	ASN	CB-CA-C	-6.32	99.00	109.99
1	A	412	THR	CA-CB-OG1	6.27	119.01	109.60
1	A	159	HIS	N-CA-C	6.27	124.15	110.80
1	A	325	LYS	N-CA-C	6.22	121.57	111.37
1	A	458	TYR	N-CA-C	-6.20	101.03	109.95
1	A	401	ILE	CA-C-N	-6.20	112.10	119.78
1	A	401	ILE	C-N-CA	-6.20	112.10	119.78
1	A	92	GLU	N-CA-C	-6.17	104.64	111.36
1	A	287	ILE	N-CA-C	-6.16	99.68	109.17
1	A	511	LYS	N-CA-CB	-6.09	100.45	110.68
1	A	56	GLY	CA-C-N	-6.09	115.26	122.93
1	A	56	GLY	C-N-CA	-6.09	115.26	122.93
1	A	412	THR	N-CA-CB	6.07	120.60	110.41
1	A	251	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	252	LEU	CA-C-O	6.02	126.48	119.32
1	A	504	ASP	N-CA-C	-6.00	100.79	110.32
1	A	84	TRP	CB-CA-C	-5.93	100.53	110.56
1	A	344	GLU	CA-CB-CG	5.93	125.96	114.10
1	A	439	ILE	CA-C-O	5.91	127.68	121.59
1	A	414	PHE	CA-C-N	-5.88	116.24	122.30
1	A	414	PHE	C-N-CA	-5.88	116.24	122.30
1	A	127	LEU	CB-CA-C	-5.84	97.56	109.65
1	A	457	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	145	SER	CB-CA-C	-5.77	98.36	109.37
1	A	183	ASN	N-CA-C	5.76	122.25	113.61
1	A	341	LYS	CA-C-O	-5.75	115.45	121.55
1	A	522	VAL	N-CA-C	-5.75	105.13	110.53
1	A	304	SER	CB-CA-C	5.74	119.25	109.72
1	A	285	ASP	N-CA-C	-5.74	99.84	108.96
1	A	490	SER	CA-CB-OG	-5.73	99.63	111.10
1	A	285	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	494	LEU	CB-CA-C	-5.71	99.74	109.51
1	A	513	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	A	248	LEU	N-CA-C	-5.63	105.28	111.82
1	A	344	GLU	N-CA-CB	5.62	119.46	111.25
1	A	493	PRO	CB-CA-C	-5.62	103.87	111.12
1	A	452	LEU	N-CA-C	-5.61	106.57	113.41
1	A	463	GLU	N-CA-C	-5.61	105.07	111.07
1	A	492	TRP	CB-CA-C	5.59	116.51	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	PHE	N-CA-C	5.59	118.09	111.33
1	A	156	LEU	O-C-N	-5.58	116.09	122.68
1	A	252	LEU	CB-CA-C	5.58	119.60	110.17
1	A	297	ASP	N-CA-C	5.54	120.03	113.16
1	A	326	ASP	CA-C-N	-5.52	112.45	120.29
1	A	326	ASP	C-N-CA	-5.52	112.45	120.29
1	A	236	VAL	CB-CA-C	-5.51	103.64	111.19
1	A	245	ALA	CB-CA-C	5.51	121.51	109.99
1	A	422	PHE	CA-C-O	-5.51	114.38	120.33
1	A	5	GLU	N-CA-C	5.51	117.99	111.33
1	A	156	LEU	CA-C-N	-5.51	111.02	121.54
1	A	156	LEU	C-N-CA	-5.51	111.02	121.54
1	A	449	GLY	N-CA-C	5.47	123.56	114.48
1	A	361	PRO	CB-CA-C	-5.45	103.67	111.62
1	A	138	THR	N-CA-C	5.44	116.89	111.07
1	A	409	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	24	SER	N-CA-CB	-5.43	103.06	110.56
1	A	67	CYS	CA-C-O	-5.39	115.36	121.72
1	A	494	LEU	N-CA-C	-5.36	101.81	110.32
1	A	492	TRP	N-CA-CB	-5.35	103.38	110.17
1	A	301	PHE	CB-CA-C	-5.34	103.40	110.34
1	A	145	SER	CA-C-N	-5.33	113.86	122.81
1	A	145	SER	C-N-CA	-5.33	113.86	122.81
1	A	22	VAL	N-CA-C	-5.31	98.29	109.34
1	A	228	SER	N-CA-C	-5.31	102.09	108.25
1	A	468	ARG	CB-CA-C	-5.30	101.99	110.79
1	A	315	LYS	CA-C-O	-5.30	115.72	121.44
1	A	388	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	527	PHE	N-CA-C	5.27	116.72	110.97
1	A	343	SER	CB-CA-C	-5.26	101.34	110.45
1	A	431	VAL	CA-C-O	5.25	124.23	119.20
1	A	481	ASN	CB-CA-C	5.24	117.78	109.55
1	A	327	GLU	O-C-N	5.24	128.12	122.15
1	A	453	VAL	N-CA-CB	-5.20	105.05	110.82
1	A	454	LYS	CA-C-O	5.19	125.94	119.97
1	A	292	PHE	CA-C-O	5.15	125.87	120.36
1	A	457	ASN	N-CA-C	5.12	121.70	110.80
1	A	409	ASN	N-CA-C	5.12	116.86	111.28
1	A	305	LEU	CA-C-N	-5.10	113.05	120.29
1	A	305	LEU	C-N-CA	-5.10	113.05	120.29
1	A	108	SER	CB-CA-C	-5.10	104.42	110.94
1	A	505	LEU	N-CA-CB	-5.07	101.89	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	A	332	LEU	N-CA-C	-5.05	105.46	110.97
1	A	133	LYS	N-CA-C	5.04	117.51	111.71
1	A	103	SER	N-CA-C	-5.01	97.64	107.91
1	A	132	GLY	N-CA-C	5.01	120.18	114.67

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	TYR	Sidechain
1	A	149	ARG	Sidechain
1	A	174	ARG	Sidechain
1	A	334	TYR	Sidechain
1	A	442	TYR	Sidechain
1	A	467	ARG	Sidechain
1	A	63	TYR	Sidechain

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	4110	0	3944	64	0
2	A	18	0	38	2	0
3	A	66	0	0	0	0
All	All	4194	0	3982	64	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 8.

All (64) 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:324:ASN:HB3	1:A:423:PHE:HB3	1.76	0.66
1:A:341:LYS:O	1:A:342:ASP:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:O	1:A:412:THR:HG23	2.04	0.57
1:A:279:TRP:CZ2	2:A:999:DME:H143	2.41	0.54
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.90	0.53
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.43	0.53
1:A:347:ILE:O	1:A:384:GLY:HA2	2.11	0.50
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.46	0.50
1:A:31:LEU:HD12	1:A:98:ASN:HD22	1.76	0.49
1:A:374:GLN:HE21	1:A:520:MET:HE1	1.77	0.49
1:A:341:LYS:O	1:A:342:ASP:CB	2.58	0.49
1:A:236:VAL:HG13	1:A:293:VAL:HG12	1.94	0.48
1:A:113:VAL:HG13	1:A:144:VAL:HG22	1.96	0.48
1:A:225:GLN:NE2	1:A:473:TRP:HE1	2.12	0.47
1:A:66:ASN:OD1	1:A:124:SER:HB3	2.14	0.47
1:A:495:PHE:CZ	1:A:500:GLN:HB3	2.50	0.47
1:A:495:PHE:CE2	1:A:500:GLN:HB3	2.49	0.47
1:A:279:TRP:CE2	2:A:999:DME:H143	2.50	0.47
1:A:305:LEU:HD12	1:A:305:LEU:N	2.30	0.47
1:A:314:PHE:CE1	1:A:411:TYR:CD2	3.03	0.47
1:A:66:ASN:ND2	1:A:88:ARG:HB2	2.31	0.46
1:A:520:MET:HE2	1:A:520:MET:HA	1.97	0.46
1:A:146:LEU:C	1:A:146:LEU:HD12	2.41	0.46
1:A:534:ALA:O	1:A:535:THR:HB	2.16	0.46
1:A:132:GLY:HA3	1:A:143:LEU:HD22	1.98	0.45
1:A:289:ARG:NH2	1:A:399:ASN:OD1	2.49	0.45
1:A:318:GLN:H	1:A:318:GLN:CD	2.24	0.45
1:A:168:VAL:O	1:A:172:ASP:OD1	2.33	0.45
1:A:349:ARG:HD3	1:A:381:ASP:O	2.17	0.45
1:A:345:SER:O	1:A:388:ARG:HG3	2.16	0.44
1:A:50:PRO:HA	1:A:175:MET:SD	2.57	0.44
1:A:258:SER:O	1:A:261:GLU:HB2	2.18	0.44
1:A:433:PRO:HD2	1:A:436:MET:SD	2.57	0.44
1:A:158:LEU:HD12	1:A:263:ILE:CD1	2.48	0.44
1:A:43:MET:O	1:A:44:ARG:C	2.61	0.44
1:A:364:ASN:OD1	1:A:364:ASN:C	2.61	0.44
1:A:236:VAL:HG23	1:A:237:SER:O	2.17	0.43
1:A:469:ILE:HD13	1:A:505:LEU:HD21	2.00	0.43
1:A:98:ASN:O	1:A:144:VAL:HA	2.19	0.43
1:A:114:TRP:HB2	1:A:197:PHE:CE1	2.54	0.43
1:A:225:GLN:HE21	1:A:473:TRP:HE1	1.68	0.42
1:A:287:ILE:HD11	1:A:332:LEU:HA	2.01	0.42
1:A:321:LEU:N	1:A:321:LEU:CD2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:O	1:A:302:PRO:HA	2.19	0.42
1:A:223:ILE:HA	1:A:320:LEU:O	2.19	0.42
1:A:328:GLY:O	1:A:329:SER:C	2.62	0.42
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.55	0.42
1:A:528:LEU:O	1:A:529:PRO:C	2.63	0.42
1:A:119:GLY:O	1:A:120:PHE:HB2	2.20	0.41
1:A:64:PRO:HD3	1:A:98:ASN:HD21	1.85	0.41
1:A:31:LEU:HA	1:A:98:ASN:HD22	1.86	0.41
1:A:212:SER:O	1:A:216:ARG:HD2	2.20	0.41
1:A:521:CYS:O	1:A:525:ASN:HB2	2.21	0.41
1:A:107:LYS:HA	1:A:107:LYS:HE2	2.02	0.41
1:A:359:SER:C	1:A:361:PRO:HD3	2.45	0.41
1:A:262:LEU:C	1:A:262:LEU:HD23	2.46	0.41
1:A:322:GLY:HA3	1:A:421:TYR:CE1	2.56	0.41
1:A:362:HIS:CD2	1:A:362:HIS:H	2.38	0.41
1:A:360:VAL:HG12	1:A:363:ALA:HB2	2.04	0.40
1:A:468:ARG:HH22	1:A:510:MET:HB3	1.86	0.40
1:A:127:LEU:CD1	1:A:130:TYR:CE2	3.04	0.40
1:A:167:ASN:O	1:A:168:VAL:C	2.61	0.40
1:A:372:THR:O	1:A:373:LEU:C	2.64	0.40
1:A:74:GLN:HG2	1:A:75:PHE:CE1	2.57	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%)	462 (88%)	48 (9%)	13 (2%)	4 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	A	500	GLN
1	A	380	ASP
1	A	534	ALA
1	A	118	GLY
1	A	159	HIS
1	A	335	GLY
1	A	342	ASP
1	A	497	THR
1	A	329	SER
1	A	381	ASP
1	A	451	PRO
1	A	509	PRO

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	429/470 (91%)	379 (88%)	50 (12%)	5 18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	LYS
1	A	22	VAL
1	A	27	ILE
1	A	28	SER
1	A	31	LEU
1	A	125	SER
1	A	129	VAL
1	A	143	LEU
1	A	144	VAL
1	A	177	LEU
1	A	197	PHE
1	A	216	ARG
1	A	226	SER

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Mol	Chain	Res	Type
1	A	235	SER
1	A	246	VAL
1	A	248	LEU
1	A	267	ARG
1	A	289	ARG
1	A	293	VAL
1	A	295	VAL
1	A	318	GLN
1	A	321	LEU
1	A	324	ASN
1	A	330	PHE
1	A	340	SER
1	A	341	LYS
1	A	343	SER
1	A	366	LEU
1	A	385	ILE
1	A	400	VAL
1	A	408	VAL
1	A	412	THR
1	A	413	LYS
1	A	426	ARG
1	A	430	LEU
1	A	450	LEU
1	A	452	LEU
1	A	456	LEU
1	A	469	ILE
1	A	481	ASN
1	A	483	ASN
1	A	491	LYS
1	A	497	THR
1	A	500	GLN
1	A	504	ASP
1	A	516	LEU
1	A	519	GLN
1	A	520	MET
1	A	528	LEU

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	59	ASN
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	324	ASN
1	A	362	HIS
1	A	374	GLN
1	A	409	ASN
1	A	500	GLN
1	A	513	HIS

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	DME	A	999	-	17,17,17	0.63	0	22,22,22	0.93	0

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	DME	A	999	-	-	2/15/15/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

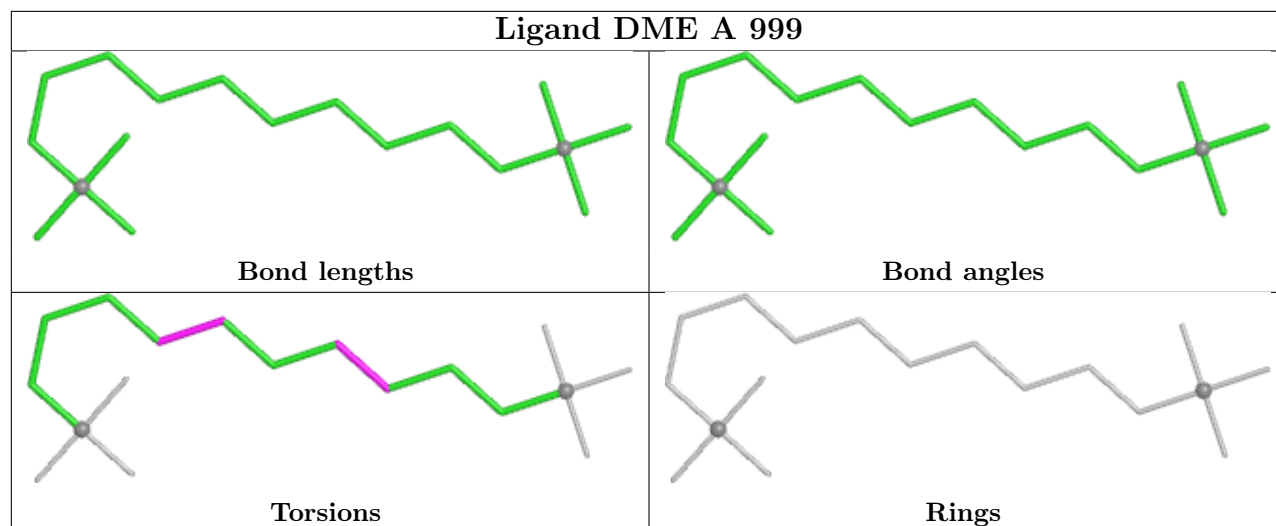
Mol	Chain	Res	Type	Atoms
2	A	999	DME	C7-C8-C9-C10
2	A	999	DME	C4-C5-C6-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	DME	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	A	527/537 (98%)	-0.84	1 (0%) 91 88	4, 19, 46, 83	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	SER	3.1

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](#)

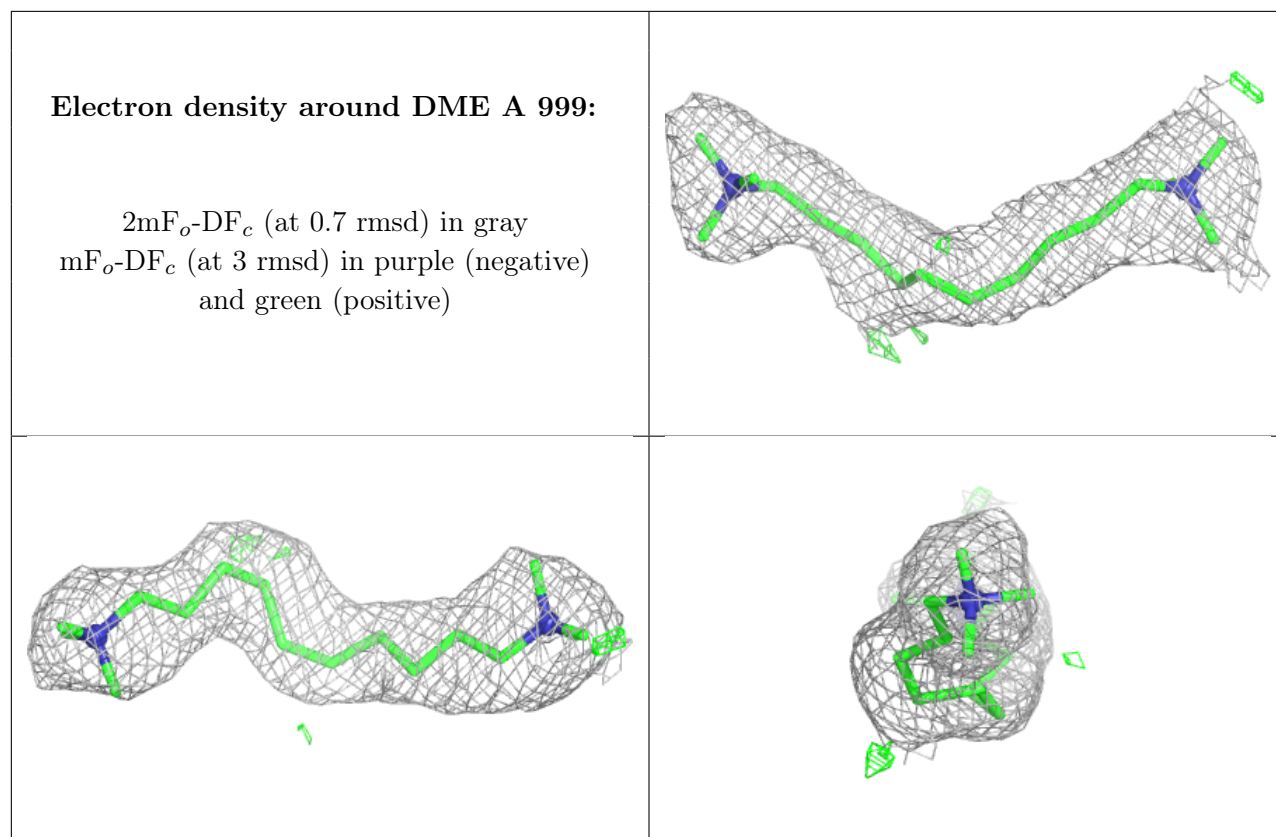
There are no oligosaccharides in this entry.

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, 95th 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 ²)	Q<0.9
2	DME	A	999	18/18	0.96	0.07	12,20,26,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.