



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:55 AM UTC

PDB ID : 1E3Q / pdb_00001e3q
Title : TORPEDO CALIFORNICA ACETYLCHOLINESTERASE COMPLEXED
WITH BW284C51
Authors : Felder, C.E.; Harel, M.; Silman, I.; Sussman, J.L.
Deposited on : 2000-06-21
Resolution : 2.85 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
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

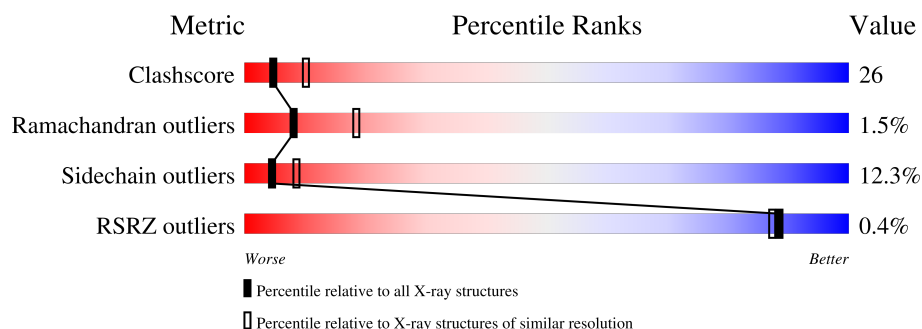
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	543	50% 37% 11% ..

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	NAG	A	603	X	-	-	-

2 Entry composition [i](#)

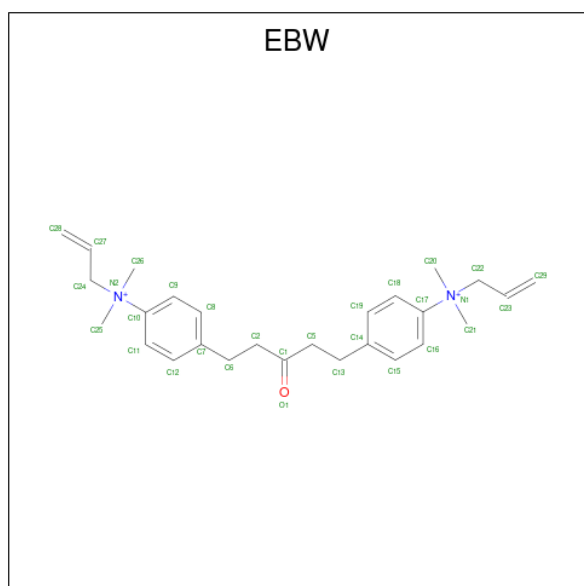
There are 5 unique types of molecules in this entry. The entry contains 4459 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	533	4254	2730	724	778	22	0	1	0

- Molecule 2 is 4-(5-{4-[DIMETHYL(PROP-2-ENYL)AMMONIO]PHENYL}-3-OXOPENTYL)-N,N-DIMETHYL-N-PROP-2-ENYLBENZENAMINIUM (CCD ID: EBW) (formula: C₂₇H₃₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	27	2	1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

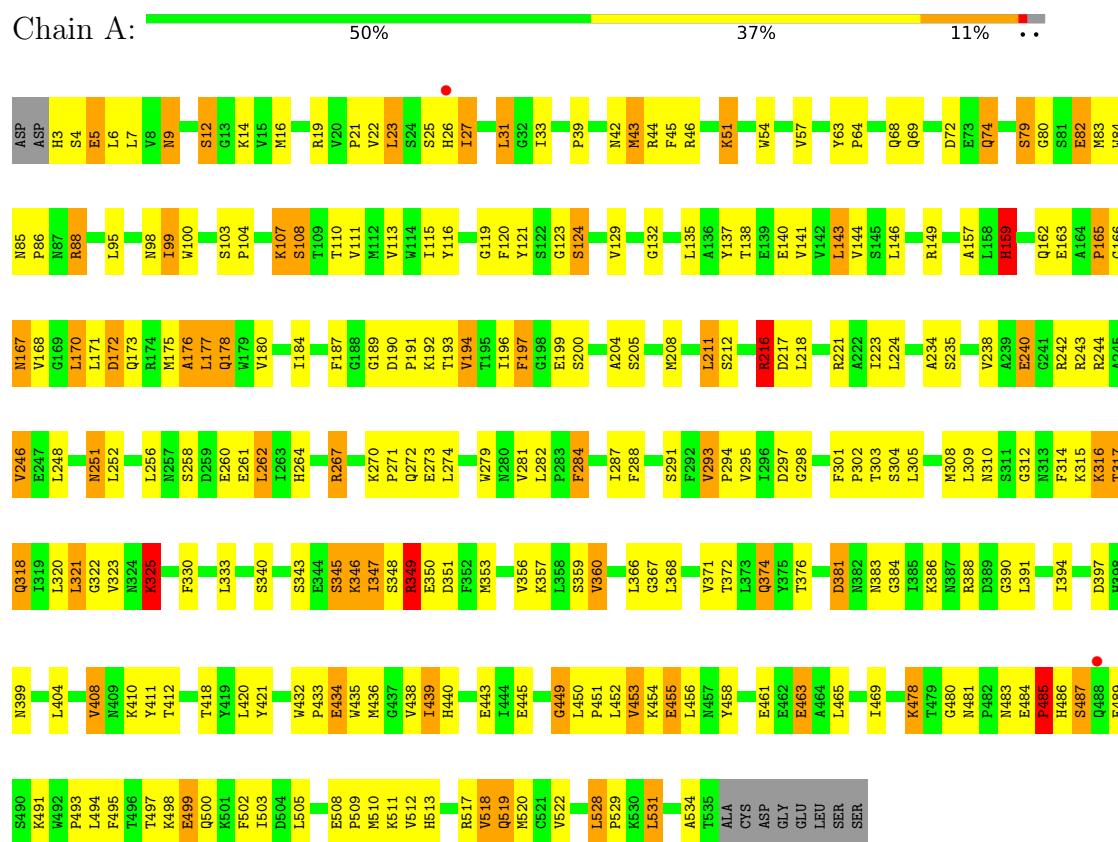
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		

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	114.00Å 114.00Å 138.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.94 – 2.85 18.94 – 2.88	Depositor EDS
% Data completeness (in resolution range)	95.6 (18.94-2.85) 95.3 (18.94-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.190 , 0.234 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4459	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: EBW, SO4, NAG

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	0.67	0/4379	1.19	49/5946 (0.8%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	MET	N-CA-C	-10.41	99.98	112.89
1	A	443	GLU	N-CA-C	-8.36	102.86	113.72
1	A	310	ASN	N-CA-C	8.20	120.30	111.36
1	A	291	SER	N-CA-C	7.39	119.03	110.97
1	A	439	ILE	N-CA-C	7.02	118.15	110.21
1	A	480	GLY	N-CA-C	-6.96	105.02	115.32
1	A	449	GLY	N-CA-C	6.95	125.60	114.90
1	A	157	ALA	N-CA-C	6.84	122.00	107.70
1	A	234	ALA	N-CA-C	6.71	121.63	113.17
1	A	481	ASN	CA-C-N	6.52	125.96	118.85
1	A	481	ASN	C-N-CA	6.52	125.96	118.85
1	A	218	LEU	N-CA-C	6.34	120.87	113.20
1	A	399	ASN	N-CA-C	6.09	120.79	113.23
1	A	374	GLN	N-CA-C	6.09	117.71	111.14
1	A	23	LEU	CB-CA-C	-6.00	109.67	116.63
1	A	159	HIS	N-CA-C	5.95	123.48	110.80
1	A	162	GLN	N-CA-C	-5.80	106.03	113.23
1	A	347	ILE	N-CA-C	5.79	116.28	108.17
1	A	511	LYS	N-CA-C	-5.78	100.36	109.50
1	A	165	PRO	N-CA-C	-5.77	100.75	111.03
1	A	346	LYS	N-CA-C	-5.76	101.09	110.20
1	A	187	PHE	N-CA-C	-5.76	105.45	112.88
1	A	99	ILE	N-CA-C	5.71	116.22	107.77
1	A	483	ASN	N-CA-C	5.71	118.51	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ALA	N-CA-C	-5.71	104.96	111.07
1	A	31	LEU	N-CA-C	5.62	118.40	109.24
1	A	217	ASP	N-CA-C	5.59	119.36	112.54
1	A	359	SER	N-CA-C	5.57	117.43	111.36
1	A	33	ILE	N-CA-C	-5.53	103.87	108.63
1	A	518	VAL	N-CA-C	5.51	116.29	110.72
1	A	297	ASP	N-CA-C	5.45	120.03	112.90
1	A	351	ASP	N-CA-C	-5.43	106.50	113.23
1	A	330	PHE	N-CA-C	5.39	117.15	111.28
1	A	381	ASP	N-CA-C	5.31	119.39	113.02
1	A	345	SER	N-CA-C	5.30	118.56	111.24
1	A	293	VAL	N-CA-CB	-5.27	103.83	111.21
1	A	434	GLU	N-CA-C	5.23	116.98	111.28
1	A	463	GLU	N-CA-C	-5.22	105.77	111.82
1	A	69	GLN	N-CA-C	5.20	116.11	107.73
1	A	534	ALA	N-CA-C	-5.16	106.50	112.89
1	A	420	LEU	N-CA-C	5.14	116.77	108.34
1	A	360	VAL	CA-C-N	5.12	124.78	119.56
1	A	360	VAL	C-N-CA	5.12	124.78	119.56
1	A	172	ASP	N-CA-C	-5.11	105.14	111.33
1	A	108	SER	N-CA-C	-5.04	100.07	110.80
1	A	349	ARG	N-CA-C	-5.03	106.98	113.01
1	A	325	LYS	N-CA-C	5.02	117.14	111.11
1	A	212	SER	CA-C-N	5.01	124.18	118.97
1	A	212	SER	C-N-CA	5.01	124.18	118.97

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	4254	0	4093	215	0
2	A	30	0	38	1	0
3	A	5	0	0	0	0
4	A	42	0	39	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	128	0	0	9	1
All	All	4459	0	4170	218	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (218) 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:88:ARG:HB3	1:A:88:ARG:HH11	1.19	1.05
1:A:303:THR:HG22	1:A:304:SER:H	1.26	0.97
1:A:408:VAL:O	1:A:412:THR:HG23	1.72	0.89
1:A:519:GLN:CD	1:A:519:GLN:H	1.84	0.86
1:A:88:ARG:HB3	1:A:88:ARG:NH1	1.95	0.82
1:A:43:MET:HA	1:A:46:ARG:HH21	1.43	0.81
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.81	0.80
1:A:88:ARG:HH11	1:A:88:ARG:CB	1.92	0.80
1:A:107:LYS:H	1:A:107:LYS:HD2	1.47	0.79
1:A:110:THR:OG1	1:A:478:LYS:HB3	1.83	0.79
1:A:248:LEU:HD21	1:A:274:LEU:HD12	1.66	0.77
1:A:340:SER:HB2	1:A:343:SER:HB3	1.65	0.77
1:A:123:GLY:O	1:A:124:SER:HB2	1.86	0.76
1:A:9:ASN:HD21	1:A:14:LYS:HE2	1.50	0.76
1:A:487:SER:OG	1:A:489:GLU:HG2	1.86	0.76
1:A:21:PRO:HA	1:A:26:HIS:HD2	1.47	0.76
1:A:520:MET:HE2	1:A:520:MET:HA	1.69	0.75
1:A:433:PRO:HD2	1:A:436:MET:HE3	1.70	0.73
1:A:322:GLY:HA3	1:A:421:TYR:CZ	2.23	0.73
1:A:86:PRO:HD3	5:A:701:HOH:O	1.88	0.72
1:A:455:GLU:H	1:A:455:GLU:CD	1.97	0.72
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.71	0.72
1:A:321:LEU:HD11	1:A:408:VAL:HG23	1.70	0.72
1:A:303:THR:HG22	1:A:304:SER:N	2.05	0.71
1:A:216:ARG:HG3	1:A:315:LYS:HB2	1.71	0.71
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.73	0.71
1:A:518:VAL:O	1:A:522:VAL:HG13	1.89	0.71
1:A:6:LEU:O	1:A:16:MET:HE3	1.90	0.70
1:A:433:PRO:HG2	1:A:436:MET:HG3	1.71	0.70
1:A:5:GLU:OE2	1:A:104:PRO:HA	1.91	0.70
1:A:82:GLU:HA	1:A:85:ASN:HD22	1.57	0.69
1:A:107:LYS:HD2	1:A:107:LYS:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:CD	1:A:108:SER:H	2.07	0.67
1:A:107:LYS:CG	1:A:108:SER:H	2.07	0.67
1:A:325:LYS:HE3	5:A:707:HOH:O	1.95	0.67
1:A:39:PRO:HD3	1:A:95:LEU:HD12	1.77	0.66
1:A:107:LYS:HG2	1:A:108:SER:N	2.13	0.64
1:A:240:GLU:HA	1:A:243:ARG:HH11	1.63	0.64
1:A:9:ASN:ND2	1:A:14:LYS:HE2	2.13	0.63
1:A:165:PRO:HA	5:A:702:HOH:O	1.99	0.62
4:A:603:NAG:H83	5:A:773:HOH:O	1.99	0.62
1:A:258:SER:HB3	1:A:261:GLU:HG3	1.81	0.62
1:A:107:LYS:CG	1:A:108:SER:N	2.63	0.62
1:A:322:GLY:HA3	1:A:421:TYR:CE2	2.35	0.61
1:A:83:MET:HE2	1:A:84:TRP:CZ2	2.36	0.61
1:A:433:PRO:CD	1:A:436:MET:HE3	2.31	0.61
1:A:68:GLN:HE21	1:A:68:GLN:HA	1.65	0.61
1:A:503:ILE:HD12	1:A:510:MET:HE2	1.83	0.60
1:A:44:ARG:O	1:A:45:PHE:HB2	2.02	0.60
1:A:383:ASN:HB3	1:A:386:LYS:HB2	1.83	0.60
1:A:43:MET:CA	1:A:46:ARG:HH21	2.14	0.59
1:A:22:VAL:O	1:A:22:VAL:HG13	2.02	0.59
1:A:205:SER:HA	1:A:208:MET:HE2	1.84	0.59
1:A:374:GLN:OE1	1:A:520:MET:HE1	2.04	0.58
1:A:116:TYR:CD1	1:A:116:TYR:C	2.81	0.58
1:A:284:PHE:HD2	5:A:810:HOH:O	1.86	0.58
1:A:111:VAL:HB	1:A:194:VAL:HG12	1.86	0.58
1:A:6:LEU:HB3	1:A:16:MET:CE	2.35	0.57
1:A:107:LYS:H	1:A:107:LYS:CD	2.14	0.57
1:A:246:VAL:HA	1:A:262:LEU:HD11	1.87	0.57
1:A:21:PRO:HA	1:A:26:HIS:CD2	2.35	0.57
1:A:216:ARG:CG	1:A:315:LYS:HB2	2.35	0.57
1:A:221:ARG:NH1	1:A:318:GLN:OE1	2.37	0.57
1:A:302:PRO:HD2	1:A:308:MET:SD	2.45	0.57
1:A:270:LYS:HB2	1:A:273:GLU:HG3	1.88	0.56
1:A:353:MET:O	1:A:357:LYS:HG3	2.05	0.56
1:A:149:ARG:NH2	1:A:168:VAL:CG1	2.69	0.56
1:A:43:MET:HA	1:A:46:ARG:NH2	2.17	0.55
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.41	0.55
1:A:284:PHE:O	1:A:284:PHE:HD1	1.89	0.55
1:A:190:ASP:OD1	1:A:192:LYS:CG	2.52	0.55
1:A:204:ALA:O	1:A:208:MET:HG3	2.06	0.55
4:A:603:NAG:H3	5:A:773:HOH:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD12	1:A:410:LYS:HB2	1.87	0.54
1:A:135:LEU:HD23	1:A:143:LEU:HD21	1.90	0.54
1:A:251:ASN:N	1:A:251:ASN:HD22	2.05	0.54
1:A:503:ILE:CD1	1:A:510:MET:HE2	2.37	0.54
1:A:68:GLN:HA	1:A:68:GLN:NE2	2.22	0.54
1:A:345:SER:O	1:A:388:ARG:HG3	2.08	0.54
1:A:519:GLN:CD	1:A:519:GLN:N	2.61	0.54
1:A:325:LYS:HB3	1:A:438:VAL:HB	1.91	0.53
1:A:223:ILE:HA	1:A:320:LEU:O	2.08	0.53
1:A:349:ARG:NH1	1:A:353:MET:HE2	2.23	0.53
1:A:258:SER:HB3	1:A:261:GLU:CG	2.38	0.53
1:A:349:ARG:HD2	1:A:381:ASP:O	2.07	0.53
1:A:113:VAL:HB	1:A:196:ILE:HG22	1.90	0.53
1:A:170:LEU:O	1:A:173:GLN:HB2	2.08	0.53
1:A:197:PHE:CB	1:A:223:ILE:HB	2.38	0.53
1:A:433:PRO:CG	1:A:436:MET:HE3	2.39	0.53
1:A:491:LYS:O	1:A:493:PRO:HD3	2.08	0.53
1:A:258:SER:HB3	1:A:261:GLU:CD	2.34	0.53
1:A:51:LYS:C	1:A:51:LYS:HD3	2.34	0.52
1:A:320:LEU:HD23	1:A:320:LEU:C	2.35	0.52
1:A:499:GLU:C	1:A:500:GLN:HG2	2.34	0.52
1:A:240:GLU:OE1	1:A:244:ARG:NE	2.42	0.52
1:A:121:TYR:CD1	1:A:121:TYR:C	2.87	0.52
1:A:165:PRO:CA	5:A:702:HOH:O	2.56	0.52
1:A:321:LEU:HD11	1:A:408:VAL:CG2	2.39	0.52
4:A:605:NAG:O3	4:A:605:NAG:H82	2.09	0.51
1:A:439:ILE:HG22	1:A:440:HIS:N	2.24	0.51
1:A:445:GLU:HB2	1:A:450:LEU:HD12	1.91	0.51
1:A:166:GLY:C	1:A:168:VAL:H	2.19	0.50
1:A:372:THR:HG22	1:A:376:THR:OG1	2.11	0.50
1:A:279:TRP:CE2	2:A:601:EBW:H262	2.46	0.50
1:A:107:LYS:HG2	1:A:108:SER:H	1.71	0.50
1:A:211:LEU:O	1:A:216:ARG:NH1	2.45	0.50
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.47	0.50
1:A:224:LEU:HD12	1:A:224:LEU:N	2.27	0.50
1:A:484:GLU:OE1	1:A:485:PRO:HD2	2.11	0.50
1:A:412:THR:HG22	1:A:418:THR:OG1	2.11	0.50
1:A:303:THR:CG2	1:A:304:SER:H	2.07	0.49
1:A:439:ILE:CG2	1:A:440:HIS:N	2.74	0.49
1:A:314:PHE:CE1	1:A:411:TYR:CE1	3.01	0.49
1:A:519:GLN:O	1:A:522:VAL:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CE1	1:A:123:GLY:HA3	2.48	0.48
1:A:163:GLU:CD	1:A:267:ARG:HH22	2.21	0.48
1:A:322:GLY:HA3	1:A:421:TYR:CE1	2.48	0.48
1:A:383:ASN:ND2	1:A:386:LYS:HG3	2.28	0.48
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.96	0.48
1:A:98:ASN:O	1:A:144:VAL:HA	2.13	0.48
1:A:135:LEU:HD23	1:A:143:LEU:CD2	2.43	0.47
1:A:197:PHE:HB2	1:A:223:ILE:HB	1.96	0.47
1:A:531:LEU:HD12	1:A:531:LEU:O	2.14	0.47
1:A:115:ILE:HG23	1:A:146:LEU:HD11	1.97	0.47
1:A:63:TYR:HD1	1:A:64:PRO:HD2	1.79	0.47
1:A:72:ASP:OD1	1:A:74:GLN:HB2	2.14	0.47
1:A:149:ARG:NH2	1:A:168:VAL:HG13	2.28	0.47
1:A:449:GLY:O	1:A:452:LEU:HB2	2.13	0.47
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.49	0.47
1:A:44:ARG:O	1:A:45:PHE:CB	2.63	0.47
1:A:508:GLU:HB2	1:A:509:PRO:HD2	1.97	0.47
1:A:346:LYS:HB3	1:A:384:GLY:HA3	1.97	0.47
1:A:284:PHE:N	1:A:284:PHE:CD1	2.80	0.46
1:A:321:LEU:HD23	1:A:321:LEU:H	1.80	0.46
1:A:356:VAL:HG12	1:A:368:LEU:HD23	1.96	0.46
1:A:19:ARG:HD2	1:A:26:HIS:HB3	1.97	0.46
1:A:159:HIS:ND1	5:A:704:HOH:O	2.36	0.46
1:A:298:GLY:HA2	1:A:301:PHE:O	2.16	0.46
1:A:103:SER:HA	1:A:104:PRO:C	2.41	0.46
1:A:465:LEU:O	1:A:469:ILE:HG12	2.15	0.46
1:A:98:ASN:O	1:A:144:VAL:HG23	2.16	0.46
1:A:166:GLY:C	1:A:168:VAL:N	2.74	0.46
1:A:193:THR:HG22	1:A:193:THR:O	2.15	0.46
1:A:107:LYS:HD2	1:A:108:SER:H	1.78	0.46
1:A:7:LEU:HD13	1:A:7:LEU:C	2.41	0.45
1:A:260:GLU:O	1:A:264[B]:HIS:CD2	2.69	0.45
1:A:450:LEU:O	1:A:453:VAL:HG13	2.16	0.45
1:A:461:GLU:H	1:A:461:GLU:CD	2.24	0.45
1:A:199:GLU:O	1:A:200:SER:HB3	2.16	0.45
1:A:242:ARG:O	1:A:246:VAL:HG13	2.16	0.45
1:A:252:LEU:CD1	1:A:274:LEU:HD13	2.45	0.45
1:A:495:PHE:CE2	1:A:500:GLN:HB2	2.51	0.45
1:A:98:ASN:C	1:A:99:ILE:HG13	2.41	0.45
1:A:178:GLN:CA	1:A:178:GLN:HE21	2.30	0.45
1:A:316:LYS:H	1:A:316:LYS:HG2	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TRP:CE3	1:A:436:MET:HE1	2.52	0.45
1:A:163:GLU:HA	1:A:163:GLU:OE1	2.16	0.44
1:A:281:VAL:O	1:A:282:LEU:C	2.60	0.44
1:A:367:GLY:O	1:A:371:VAL:HG23	2.17	0.44
1:A:171:LEU:O	1:A:172:ASP:C	2.58	0.44
1:A:346:LYS:C	1:A:347:ILE:HD12	2.43	0.44
1:A:176:ALA:O	1:A:180:VAL:HG23	2.17	0.44
1:A:317:THR:OG1	1:A:318:GLN:N	2.46	0.44
1:A:498:LYS:HB2	1:A:499:GLU:H	1.65	0.44
1:A:208:MET:HE1	1:A:294:PRO:HG2	2.00	0.44
1:A:486:HIS:O	1:A:487:SER:C	2.60	0.44
1:A:6:LEU:HB3	1:A:16:MET:HE2	1.99	0.44
1:A:178:GLN:HE21	1:A:178:GLN:C	2.26	0.44
1:A:271:PRO:HG2	1:A:272:GLN:H	1.83	0.44
1:A:349:ARG:NH1	1:A:353:MET:CE	2.81	0.44
1:A:12:SER:HB3	1:A:54:TRP:CH2	2.53	0.43
1:A:434:GLU:C	1:A:436:MET:N	2.75	0.43
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.80	0.43
1:A:113:VAL:HG13	1:A:144:VAL:HG13	1.99	0.43
1:A:450:LEU:N	1:A:451:PRO:CD	2.80	0.43
1:A:119:GLY:O	1:A:120:PHE:HB2	2.17	0.43
1:A:453:VAL:CG2	1:A:456:LEU:HG	2.44	0.43
1:A:166:GLY:O	1:A:168:VAL:N	2.51	0.43
1:A:146:LEU:HD12	1:A:146:LEU:C	2.43	0.43
1:A:404:LEU:HD23	1:A:404:LEU:C	2.44	0.43
1:A:348:SER:C	1:A:350:GLU:N	2.77	0.43
1:A:3:HIS:ND1	1:A:4:SER:N	2.63	0.43
1:A:68:GLN:HE21	1:A:68:GLN:CA	2.27	0.43
1:A:298:GLY:CA	1:A:301:PHE:O	2.67	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.79	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.90	0.42
1:A:397:ASP:OD2	1:A:517:ARG:NH2	2.52	0.42
1:A:25:SER:HB3	1:A:137:TYR:CE1	2.54	0.42
1:A:166:GLY:N	5:A:702:HOH:O	2.35	0.42
1:A:79:SER:O	1:A:80:GLY:C	2.61	0.42
1:A:235:SER:HA	1:A:294:PRO:O	2.19	0.42
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.82	0.42
1:A:348:SER:C	1:A:350:GLU:H	2.26	0.42
1:A:452:LEU:HD12	1:A:463:GLU:HG2	2.01	0.42
1:A:508:GLU:HB2	1:A:509:PRO:CD	2.49	0.42
1:A:189:GLY:O	1:A:191:PRO:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:HB2	1:A:487:SER:CB	2.49	0.42
1:A:100:TRP:CE3	1:A:132:GLY:HA3	2.55	0.42
1:A:167:ASN:O	1:A:170:LEU:HB2	2.20	0.41
1:A:357:LYS:HA	1:A:368:LEU:HD21	2.02	0.41
1:A:27:ILE:HG21	1:A:137:TYR:HB2	2.02	0.41
1:A:333:LEU:HD23	1:A:435:TRP:HZ2	1.84	0.41
1:A:484:GLU:O	1:A:486:HIS:N	2.54	0.41
1:A:390:GLY:O	1:A:394:ILE:HG13	2.20	0.41
1:A:450:LEU:C	1:A:452:LEU:N	2.78	0.41
1:A:454:LYS:H	1:A:454:LYS:HG3	1.52	0.41
1:A:224:LEU:O	1:A:321:LEU:HA	2.20	0.41
1:A:333:LEU:HG	1:A:436:MET:CE	2.51	0.41
1:A:528:LEU:HB3	1:A:529:PRO:CD	2.48	0.41
1:A:82:GLU:HG3	1:A:85:ASN:HD22	1.85	0.41
1:A:177:LEU:HD11	1:A:196:ILE:HG21	2.01	0.41
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.95	0.40
1:A:113:VAL:HA	1:A:144:VAL:O	2.21	0.40
1:A:318:GLN:HE21	1:A:318:GLN:HB3	1.72	0.40
1:A:321:LEU:CD2	1:A:321:LEU:N	2.84	0.40
1:A:498:LYS:H	1:A:498:LYS:HG3	1.74	0.40
1:A:256:LEU:HD22	1:A:256:LEU:H	1.86	0.40
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.91	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:809:HOH:O	5:A:814:HOH:O[3_564]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/543 (98%)	473 (89%)	51 (10%)	8 (2%)	8	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	SER
1	A	124	SER
1	A	455	GLU
1	A	167	ASN
1	A	216	ARG
1	A	288	PHE
1	A	159	HIS
1	A	485	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	463/474 (98%)	406 (88%)	57 (12%)	4	8

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	9	ASN
1	A	12	SER
1	A	23	LEU
1	A	27	ILE
1	A	31	LEU
1	A	42	ASN
1	A	51	LYS
1	A	74	GLN
1	A	79	SER
1	A	82	GLU
1	A	88	ARG
1	A	107	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	VAL
1	A	138	THR
1	A	140	GLU
1	A	141	VAL
1	A	143	LEU
1	A	170	LEU
1	A	175	MET
1	A	177	LEU
1	A	178	GLN
1	A	194	VAL
1	A	197	PHE
1	A	211	LEU
1	A	216	ARG
1	A	238	VAL
1	A	240	GLU
1	A	246	VAL
1	A	251	ASN
1	A	262	LEU
1	A	267	ARG
1	A	284	PHE
1	A	287	ILE
1	A	293	VAL
1	A	295	VAL
1	A	305	LEU
1	A	316	LYS
1	A	317	THR
1	A	318	GLN
1	A	321	LEU
1	A	323	VAL
1	A	325	LYS
1	A	349	ARG
1	A	360	VAL
1	A	408	VAL
1	A	453	VAL
1	A	478	LYS
1	A	485	PRO
1	A	494	LEU
1	A	497	THR
1	A	499	GLU
1	A	505	LEU
1	A	512	VAL
1	A	519	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	528	LEU
1	A	531	LEU

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	HIS
1	A	66	ASN
1	A	68	GLN
1	A	74	GLN
1	A	178	GLN
1	A	209	HIS
1	A	251	ASN
1	A	310	ASN
1	A	488	GLN
1	A	514	GLN
1	A	519	GLN
1	A	526	GLN
1	A	533	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](#)

5 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
4	NAG	A	605	1	14,14,15	1.19	1 (7%)	17,19,21	0.82	0
4	NAG	A	603	1	14,14,15	0.94	0	17,19,21	1.09	2 (11%)
2	EBW	A	601	-	29,31,31	0.67	0	41,43,43	0.59	0
3	SO4	A	602	-	4,4,4	0.42	0	6,6,6	0.10	0
4	NAG	A	604	1	14,14,15	0.72	0	17,19,21	0.63	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	EBW	A	601	-	-	0/30/30/30	0/2/2/2
4	NAG	A	605	1	-	5/6/23/26	0/1/1/1
4	NAG	A	603	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	604	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	NAG	C1-C2	3.88	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C3-C4-C5	2.43	114.63	110.23
4	A	603	NAG	C2-N2-C7	-2.32	119.79	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	603	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	A	605	NAG	C3-C2-N2-C7
4	A	605	NAG	C8-C7-N2-C2
4	A	605	NAG	O7-C7-N2-C2
4	A	604	NAG	C8-C7-N2-C2
4	A	604	NAG	O7-C7-N2-C2
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	A	605	NAG	C4-C5-C6-O6
4	A	605	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	NAG	1	0
4	A	603	NAG	2	0
2	A	601	EBW	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 [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	533/543 (98%)	-0.54	2 (0%) 88 87	14, 33, 60, 90	6 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	GLN	2.3
1	A	26	HIS	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](#)

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
4	NAG	A	605	14/15	0.60	0.17	84,88,90,90	0
4	NAG	A	603	14/15	0.78	0.13	78,81,84,85	0
4	NAG	A	604	14/15	0.87	0.12	70,75,76,77	0
3	SO4	A	602	5/5	0.95	0.09	91,91,91,91	0
2	EBW	A	601	30/30	0.96	0.09	27,49,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.