



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 05:54 PM EDT

PDB ID : 1E3Q  
Title : TORPEDO CALIFORNICA ACETYLCHOLINESTERASE COMPLEXED  
WITH BW284C51  
Authors : Felder, C.E.; Harel, M.; Silman, I.; Sussman, J.L.  
Deposited on : unknown  
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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

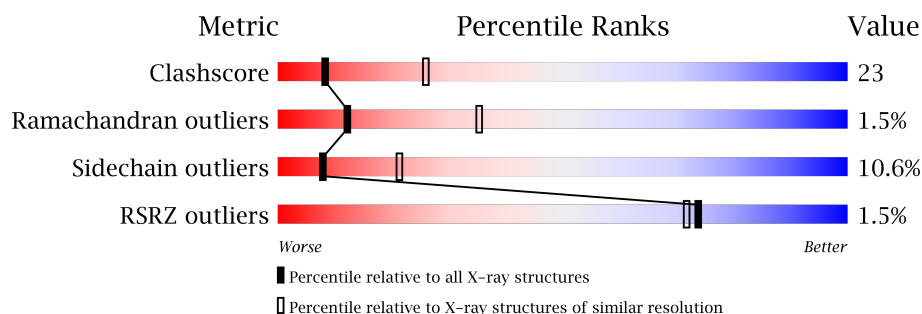
# 1 Overall quality at a glance

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	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	

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](#)

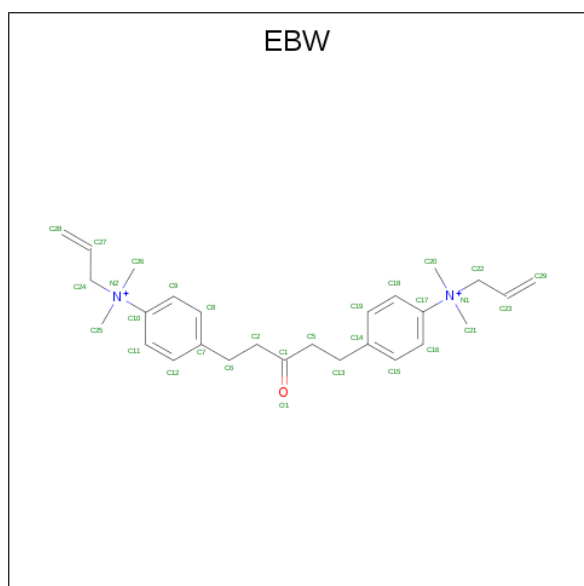
There are 5 unique types of molecules in this entry. The entry contains 4459 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-OXOPEN TYL)-N,N-DIMETHYL-N-PROP-2-ENYLBENZENAMINIUM (three-letter code: EBW) (formula: C<sub>27</sub>H<sub>38</sub>N<sub>2</sub>O).



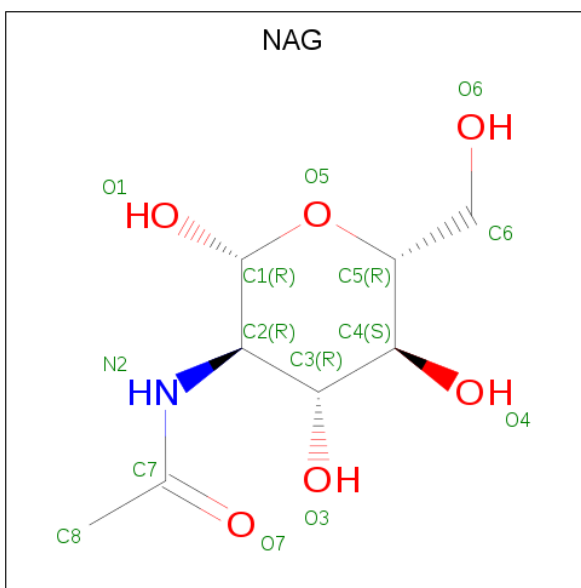
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	27	2	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: 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		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

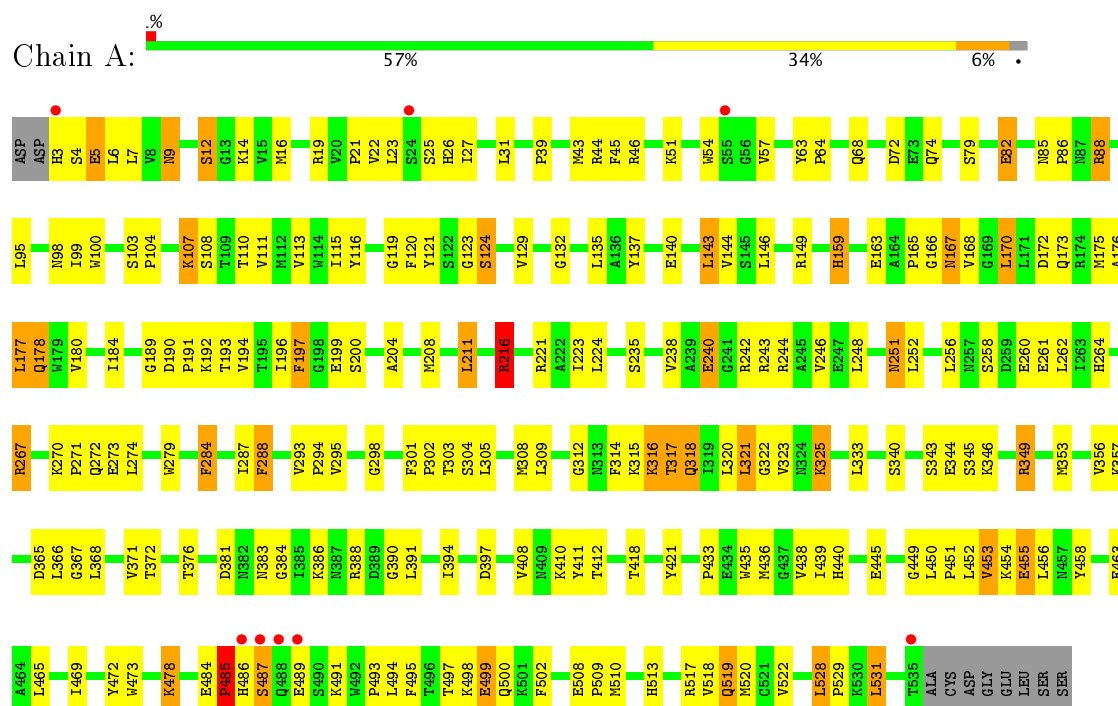
- Molecule 5 is water.

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

### 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 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, $\alpha$ , $\beta$ , $\gamma$	114.00Å 114.00Å 138.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.94 – 2.85 23.03 – 2.88	Depositor EDS
% Data completeness (in resolution range)	95.6 (18.94-2.85) 95.6 (23.03-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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.	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 74.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EBW, NAG, SO4

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	0.54	0/4379	0.78	0/5946

There are no bond length outliers.

There are no bond angle outliers.

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	195	0
2	A	30	0	38	1	0
3	A	5	0	0	0	0
4	A	42	0	39	3	0
5	A	128	0	0	9	1
All	All	4459	0	4170	198	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 23.

All (198) 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:88:ARG:NH1	1:A:88:ARG:HB3	1.95	0.82
1:A:519:GLN:CD	1:A:519:GLN:H	1.84	0.81
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:CB	1:A:88:ARG:HH11	1.92	0.80
1:A:433:PRO:HD2	1:A:436:MET:HE3	1.65	0.79
1:A:107:LYS:HD2	1:A:107:LYS:H	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: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: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: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
1:A:455:GLU:CD	1:A:455:GLU:H	1.97	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:HA	1:A:68:GLN:HE21	1.65	0.61
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: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:CD	1:A:107:LYS:H	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:433:PRO:CD	1:A:436:MET:HE3	2.33	0.56
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:HD1	1:A:284:PHE:O	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
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:345:SER:O	1:A:388:ARG:HG3	2.08	0.54
1:A:68:GLN:HA	1:A:68:GLN:NE2	2.22	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:116:TYR:C	1:A:116:TYR:CD1	2.81	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:6:LEU:HB3	1:A:16:MET:HE2	1.89	0.53
1:A:197:PHE:CB	1:A:223:ILE:HB	2.38	0.53
1:A:491:LYS:O	1:A:493:PRO:HD3	2.08	0.53
1:A:240:GLU:OE1	1:A:244:ARG:NE	2.42	0.52
1:A:165:PRO:CA	5:A:702:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD11	1:A:408:VAL:CG2	2.39	0.52
1:A:472:TYR:OH	1:A:510:MET:HE3	2.10	0.51
4:A:605:NAG:O3	4:A:605:NAG:H82	2.09	0.51
1:A:333:LEU:HG	1:A:436:MET:HE1	1.92	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: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:519:GLN:CD	1:A:519:GLN:N	2.61	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
1:A:116:TYR:CE1	1:A:123:GLY:HA3	2.48	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:499:GLU:C	1:A:500:GLN:HG2	2.34	0.48
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.96	0.48
1:A:258:SER:HB3	1:A:261:GLU:CD	2.34	0.48
1:A:98:ASN:O	1:A:144:VAL:HA	2.13	0.48
1:A:51:LYS:C	1:A:51:LYS:HD3	2.34	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:320:LEU:C	1:A:320:LEU:HD23	2.35	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:317:THR:OG1	1:A:318:GLN:N	2.46	0.47
1:A:63:TYR:HD1	1:A:64:PRO:HD2	1.79	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:72:ASP:OD1	1:A:74:GLN:HB2	2.14	0.47
1:A:349:ARG:NH1	1:A:353:MET:HE2	2.29	0.47
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.49	0.47
1:A:121:TYR:C	1:A:121:TYR:CD1	2.87	0.47
1:A:44:ARG:O	1:A:45:PHE:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:465:LEU:O	1:A:469:ILE:HG12	2.15	0.46
1:A:520:MET:CE	1:A:520:MET:HA	2.46	0.46
1:A:98:ASN:O	1:A:144:VAL:HG23	2.16	0.46
1:A:193:THR:HG22	1:A:193:THR:O	2.15	0.46
1:A:199:GLU:O	1:A:200:SER:HB3	2.16	0.46
1:A:107:LYS:HD2	1:A:108:SER:H	1.78	0.46
1:A:166:GLY:C	1:A:168:VAL:H	2.19	0.46
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: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:178:GLN:HE21	1:A:178:GLN:CA	2.30	0.45
1:A:316:LYS:H	1:A:316:LYS:HG2	1.63	0.45
1:A:163:GLU:OE1	1:A:163:GLU:HA	2.16	0.44
1:A:367:GLY:O	1:A:371:VAL:HG23	2.17	0.44
1:A:176:ALA:O	1:A:180:VAL:HG23	2.17	0.44
1:A:498:LYS:HB2	1:A:499:GLU:H	1.65	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:163:GLU:CD	1:A:267:ARG:HH22	2.21	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:95:LEU:HD23	1:A:95:LEU:HA	1.80	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:3:HIS:ND1	1:A:4:SER:N	2.63	0.43
1:A:68:GLN:CA	1:A:68:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:OD2	1:A:517:ARG:NH2	2.52	0.42
1:A:166:GLY:N	5:A:702:HOH:O	2.35	0.42
1:A:25:SER:HB3	1:A:137:TYR:CE1	2.54	0.42
1:A:235:SER:HA	1:A:294:PRO:O	2.19	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD12	1.82	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
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:103:SER:HA	1:A:104:PRO:C	2.41	0.41
1:A:390:GLY:O	1:A:394:ILE:HG13	2.20	0.41
1:A:454:LYS:H	1:A:454:LYS:HG3	1.52	0.41
1:A:166:GLY:C	1:A:168:VAL:N	2.74	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:177:LEU:HD11	1:A:196:ILE:HG21	2.01	0.41
1:A:82:GLU:HG3	1:A:85:ASN:HD22	1.85	0.41
1:A:7:LEU:HD13	1:A:7:LEU:C	2.41	0.41
1:A:184:ILE:HA	1:A:184:ILE:HD12	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:N	1:A:321:LEU:CD2	2.84	0.40
1:A:498:LYS:HG3	1:A:498:LYS:H	1.74	0.40
1:A:98:ASN:C	1:A:99:ILE:HG13	2.41	0.40
1:A:256:LEU:H	1:A:256:LEU:HD22	1.86	0.40
1:A:177:LEU:HA	1:A:177:LEU:HD12	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%)	12	35

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 [i](#)

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%)	414 (89%)	49 (11%)	8	21

All (49) 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

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	31	LEU
1	A	79	SER
1	A	82	GLU
1	A	88	ARG
1	A	107	LYS
1	A	129	VAL
1	A	140	GLU
1	A	143	LEU
1	A	170	LEU
1	A	172	ASP
1	A	175	MET
1	A	177	LEU
1	A	178	GLN
1	A	197	PHE
1	A	211	LEU
1	A	216	ARG
1	A	238	VAL
1	A	240	GLU
1	A	251	ASN
1	A	267	ARG
1	A	284	PHE
1	A	287	ILE
1	A	288	PHE
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	344	GLU
1	A	349	ARG
1	A	365	ASP
1	A	453	VAL
1	A	473	TRP
1	A	478	LYS
1	A	485	PRO
1	A	494	LEU
1	A	497	THR

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Mol	Chain	Res	Type
1	A	499	GLU
1	A	519	GLN
1	A	528	LEU
1	A	531	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	514	GLN
1	A	526	GLN

### 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 carbohydrates 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
2	EBW	A	601	-	29,31,31	0.67	0	39,43,43	0.45	0
3	SO4	A	602	-	4,4,4	0.39	0	6,6,6	0.09	0
4	NAG	A	603	1	14,14,15	0.90	0	15,19,21	1.14	2 (13%)
4	NAG	A	604	1	14,14,15	0.68	0	15,19,21	0.66	0
4	NAG	A	605	1	14,14,15	1.15	1 (7%)	15,19,21	0.84	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
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	NAG	A	603	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	605	1	-	0/6/23/26	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	3.76	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C2-N2-C7	-2.16	119.79	122.94
4	A	603	NAG	C3-C4-C5	2.50	114.63	110.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	603	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EBW	1	0
4	A	603	NAG	2	0
4	A	605	NAG	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	533/543 (98%)	-0.62	8 (1%) 74 72	14, 33, 61, 90	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	GLN	6.8
1	A	487	SER	4.0
1	A	486	HIS	3.8
1	A	3	HIS	3.3
1	A	489	GLU	2.7
1	A	24	SER	2.4
1	A	55	SER	2.1
1	A	535	THR	2.1

### 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 carbohydrates 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. 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( $\text{\AA}^2$ )	Q<0.9
2	EBW	A	601	30/30	0.96	0.15	1.57	27,49,54,54	0
3	SO4	A	602	5/5	0.96	0.12	0.19	91,91,91,91	0
4	NAG	A	605	14/15	0.86	0.44	-	84,88,90,90	0
4	NAG	A	604	14/15	0.91	0.36	-	70,75,76,77	0
4	NAG	A	603	14/15	0.89	0.31	-	78,81,84,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.