



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:33 PM GMT

PDB ID : 1U65
Title : Ache W. CPT-11
Authors : Harel, M.; Hyatt, J.L.; Brumshtein, B.; Morton, C.L.; Wadkins, R.W.; Silman, I.; Sussman, J.L.; Potter, P.M.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2004-07-29
Resolution : 2.61 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

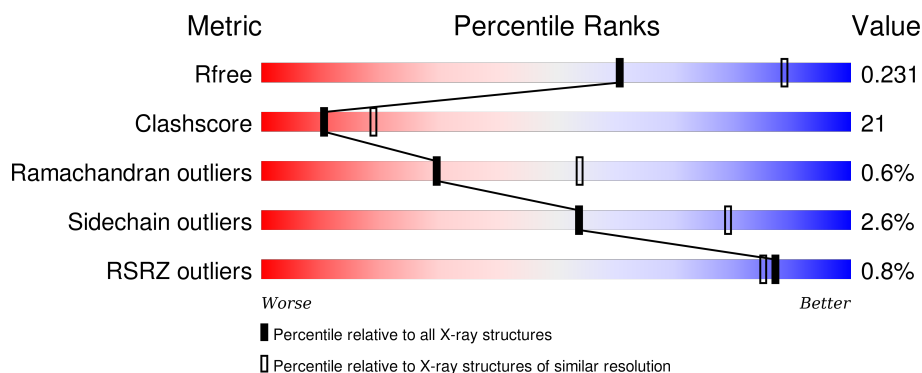
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div></div> <div>65%</div> <div>31%</div> <div>...</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	A	999	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	994	X	-	-	-
4	FUC	A	996	X	-	X	-
4	NAG	A	997	-	-	X	-
5	MAN	A	992	-	-	-	X
5	NAG	A	995	-	-	X	-
6	CP0	A	1000	-	-	-	X
7	IOD	A	1001	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

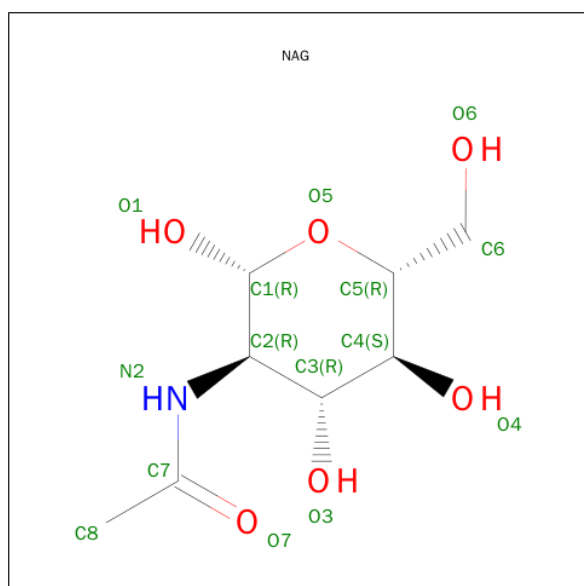
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4249	2724	721	782	22			

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

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

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



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

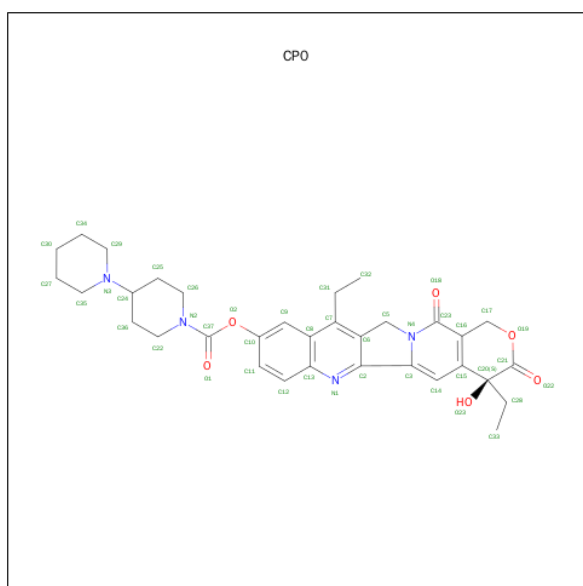
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is (4S)-4,11-DIETHYL-4-HYDROXY-3,14-DIOXO-3,4,12,14-TETRAHYDRO-1H-PYRANO[3',4':6,7]INDOLIZINO[1,2-B]QUINOLIN-9-YL 1,4'-BIPIPERIDINE-1'-CARBOXYLATE (three-letter code: CP0) (formula: C₃₃H₃₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	I	0	0
			1	1		

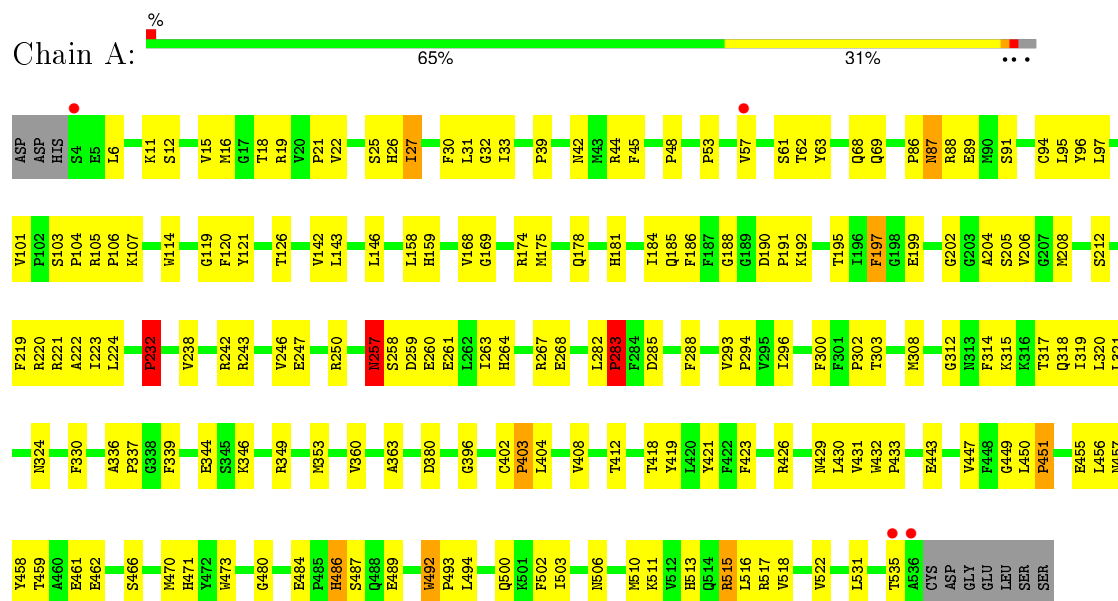
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	241	Total 241	O 241	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acetylcholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.87Å 137.87Å 70.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.88 – 2.61 27.87 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.2 (27.88-2.61) 99.3 (27.87-2.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.237 0.188 , 0.231	Depositor DCC
R_{free} test set	2377 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	EDS
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 23820 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4635	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, FUC, CP0, FUL, IOD, MAN

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	0.50	3/4372 (0.1%)	0.73	8/5936 (0.1%)

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	1
4	A	1	0
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	PRO	N-CD	-18.02	1.22	1.47
1	A	451	PRO	N-CD	5.34	1.55	1.47
1	A	493	PRO	N-CD	5.34	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	CA-N-CD	-18.49	85.61	111.50
1	A	337	PRO	CA-N-CD	-16.06	89.02	111.50
1	A	232	PRO	CA-N-CD	-11.97	94.74	111.50
1	A	283	PRO	N-CA-CB	6.30	110.86	103.30
1	A	283	PRO	N-CD-CG	6.13	112.39	103.20
1	A	337	PRO	N-CA-CB	5.71	110.15	103.30
1	A	403	PRO	N-CD-CG	5.51	111.47	103.20
1	A	283	PRO	CB-CA-C	-5.26	98.85	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	996	FUC	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	ARG	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	4249	0	4099	165	1
2	A	24	0	22	8	0
3	A	28	0	26	1	0
4	A	24	0	22	7	0
5	A	25	0	22	12	0
6	A	43	0	38	4	0
7	A	1	0	0	5	0
8	A	241	0	0	19	0
All	All	4635	0	4229	183	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 21.

All (183) 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:243:ARG:NH2	1:A:283:PRO:HD3	1.56	1.19
2:A:999:NDG:H5	5:A:995:NAG:H62	1.40	1.02
1:A:243:ARG:HH22	1:A:283:PRO:HD3	1.29	0.95
1:A:243:ARG:NH2	1:A:283:PRO:CD	2.35	0.88
2:A:999:NDG:H4	2:A:993:FUL:C6	2.07	0.84
1:A:107:LYS:HD2	1:A:188:GLY:HA2	1.59	0.84
2:A:999:NDG:C5	5:A:995:NAG:H62	2.08	0.82
1:A:268:GLU:OE1	7:A:1001:IOD:I	2.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:999:NDG:H4	2:A:993:FUL:H63	1.64	0.79
1:A:449:GLY:HA2	1:A:466:SER:OG	1.81	0.79
1:A:458:TYR:OH	5:A:992:MAN:H61	1.84	0.76
4:A:997:NAG:N2	4:A:996:FUC:H2	2.00	0.76
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.69	0.74
1:A:404:LEU:O	1:A:408:VAL:HG23	1.88	0.73
1:A:268:GLU:OE2	7:A:1001:IOD:I	2.78	0.72
1:A:264:HIS:NE2	7:A:1001:IOD:I	2.93	0.72
1:A:426:ARG:NH1	1:A:430:LEU:HD23	2.05	0.72
1:A:19:ARG:CZ	1:A:26:HIS:HB2	2.20	0.71
1:A:450:LEU:N	1:A:451:PRO:CD	2.54	0.70
1:A:303:THR:HA	8:A:1040:HOH:O	1.92	0.70
1:A:42:ASN:HB2	8:A:1101:HOH:O	1.92	0.69
1:A:268:GLU:CD	7:A:1001:IOD:I	3.00	0.69
1:A:500:GLN:NE2	1:A:515:ARG:HG2	2.09	0.68
1:A:178:GLN:O	1:A:181:HIS:HB3	1.94	0.67
1:A:259:ASP:O	1:A:263:ILE:HG12	1.95	0.67
1:A:87:ASN:C	1:A:87:ASN:HD22	1.99	0.66
2:A:999:NDG:C4	2:A:993:FUL:H63	2.25	0.66
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.32	0.65
1:A:402:CYS:N	1:A:403:PRO:HD2	2.12	0.64
1:A:107:LYS:HB3	8:A:1197:HOH:O	1.97	0.64
4:A:997:NAG:H83	4:A:996:FUC:H2	1.80	0.64
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.98	0.64
1:A:204:ALA:O	1:A:208:MET:HG3	1.98	0.63
1:A:506:ASN:HB2	8:A:1135:HOH:O	1.98	0.62
1:A:471:HIS:HB3	8:A:1219:HOH:O	1.99	0.62
1:A:285:ASP:HA	6:A:1000:CP0:H282	1.81	0.61
1:A:264:HIS:CD2	7:A:1001:IOD:I	3.23	0.61
1:A:451:PRO:HG2	1:A:466:SER:HB2	1.81	0.61
1:A:220:ARG:HH22	1:A:318:GLN:HE22	1.48	0.60
1:A:31:LEU:HB2	1:A:62:THR:O	2.01	0.60
1:A:457:ASN:HB2	5:A:995:NAG:C5	2.31	0.60
3:A:998:NAG:H61	3:A:994:NAG:C1	2.32	0.60
4:A:997:NAG:N2	4:A:996:FUC:C2	2.64	0.60
1:A:243:ARG:HH21	1:A:283:PRO:CD	2.15	0.59
1:A:302:PRO:HD2	1:A:308:MET:CE	2.32	0.59
1:A:48:PRO:HG2	1:A:175:MET:HE3	1.83	0.59
1:A:457:ASN:HB2	5:A:995:NAG:H5	1.84	0.59
1:A:344:GLU:OE1	1:A:346:LYS:HE3	2.01	0.59
1:A:264:HIS:HE1	8:A:1164:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:CZ	1:A:430:LEU:HD23	2.32	0.59
2:A:999:NDG:C6	5:A:995:NAG:H62	2.32	0.59
1:A:6:LEU:HB3	1:A:16:MET:HE3	1.85	0.58
1:A:232:PRO:HD3	8:A:1226:HOH:O	2.03	0.58
1:A:22:VAL:HG11	1:A:27:ILE:HD12	1.85	0.58
1:A:293:VAL:HB	1:A:294:PRO:HD2	1.86	0.58
4:A:997:NAG:C8	4:A:996:FUC:H2	2.34	0.58
2:A:999:NDG:H4	2:A:993:FUL:H61	1.87	0.57
1:A:221:ARG:HE	1:A:480:GLY:HA2	1.69	0.57
1:A:44:ARG:O	1:A:45:PHE:HB2	2.05	0.57
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.86	0.57
1:A:317:THR:OG1	1:A:318:GLN:N	2.38	0.57
1:A:89:GLU:HG3	8:A:1200:HOH:O	2.05	0.57
1:A:450:LEU:N	1:A:451:PRO:HD3	2.20	0.56
1:A:402:CYS:N	1:A:403:PRO:CD	2.68	0.56
1:A:159:HIS:CB	1:A:238:VAL:HG13	2.34	0.56
1:A:199:GLU:HG3	1:A:443:GLU:OE2	2.05	0.56
1:A:257:ASN:HD22	1:A:257:ASN:N	2.03	0.56
1:A:146:LEU:C	1:A:146:LEU:HD12	2.26	0.56
1:A:45:PHE:O	1:A:168:VAL:HG11	2.06	0.56
1:A:19:ARG:NH2	1:A:26:HIS:HB2	2.22	0.55
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.42	0.55
4:A:997:NAG:C7	4:A:996:FUC:H2	2.37	0.54
1:A:257:ASN:HD22	1:A:258:SER:H	1.56	0.54
1:A:103:SER:HA	1:A:104:PRO:C	2.28	0.54
1:A:451:PRO:HD2	1:A:466:SER:OG	2.08	0.53
1:A:518:VAL:O	1:A:522:VAL:HG23	2.09	0.53
1:A:16:MET:HB2	1:A:57:VAL:CG1	2.39	0.53
1:A:466:SER:O	1:A:470:MET:HG3	2.09	0.53
1:A:159:HIS:HB3	1:A:238:VAL:HG13	1.90	0.53
1:A:336:ALA:HB3	1:A:339:PHE:CD1	2.43	0.53
1:A:455:GLU:N	1:A:455:GLU:OE2	2.37	0.52
1:A:431:VAL:HG22	8:A:1014:HOH:O	2.09	0.52
1:A:447:VAL:O	1:A:470:MET:HG2	2.10	0.52
1:A:39:PRO:HD3	1:A:95:LEU:HD12	1.90	0.52
1:A:531:LEU:HD23	1:A:531:LEU:C	2.28	0.52
1:A:293:VAL:HB	1:A:294:PRO:CD	2.39	0.52
1:A:107:LYS:HE3	1:A:185:GLN:O	2.10	0.52
1:A:106:PRO:HB3	8:A:1092:HOH:O	2.09	0.52
1:A:87:ASN:C	1:A:87:ASN:ND2	2.63	0.52
1:A:16:MET:HG2	8:A:1215:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.40	0.51
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.45	0.51
1:A:486:HIS:HB3	8:A:1153:HOH:O	2.10	0.51
1:A:15:VAL:HG11	1:A:33:ILE:HD12	1.91	0.51
6:A:1000:CP0:H11	6:A:1000:CP0:O1	2.10	0.51
1:A:158:LEU:HD12	1:A:263:ILE:CD1	2.38	0.51
1:A:471:HIS:ND1	8:A:1110:HOH:O	2.34	0.51
1:A:302:PRO:HD2	1:A:308:MET:HE1	1.93	0.51
1:A:242:ARG:O	1:A:246:VAL:HG23	2.11	0.51
1:A:457:ASN:HB2	5:A:995:NAG:H61	1.93	0.51
1:A:263:ILE:O	1:A:267:ARG:HG3	2.10	0.51
1:A:487:SER:OG	1:A:489:GLU:HG3	2.12	0.51
1:A:432:TRP:HB3	1:A:433:PRO:HD2	1.92	0.50
1:A:6:LEU:HB3	1:A:16:MET:CE	2.41	0.50
1:A:114:TRP:HB2	1:A:197:PHE:CE1	2.46	0.50
1:A:471:HIS:NE2	1:A:484:GLU:OE1	2.45	0.50
1:A:142:VAL:HG11	1:A:184:ILE:HD11	1.94	0.49
1:A:260:GLU:CD	1:A:260:GLU:H	2.15	0.49
1:A:30:PHE:CD1	1:A:30:PHE:N	2.81	0.49
1:A:219:PHE:O	1:A:315:LYS:HE3	2.13	0.49
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.48	0.49
1:A:429:ASN:HB2	5:A:995:NAG:O4	2.13	0.49
1:A:257:ASN:HD21	1:A:261:GLU:CB	2.25	0.49
6:A:1000:CP0:H352	8:A:1137:HOH:O	2.12	0.48
1:A:221:ARG:HE	1:A:480:GLY:CA	2.25	0.48
1:A:324:ASN:OD1	1:A:423:PHE:HB3	2.13	0.48
1:A:68:GLN:HA	1:A:68:GLN:NE2	2.28	0.48
1:A:458:TYR:OH	5:A:992:MAN:C6	2.57	0.48
1:A:6:LEU:HD22	1:A:18:THR:N	2.29	0.48
1:A:257:ASN:ND2	1:A:257:ASN:N	2.61	0.48
4:A:997:NAG:H83	4:A:996:FUC:O4	2.13	0.48
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.13	0.48
1:A:202:GLY:O	1:A:205:SER:HB2	2.14	0.48
1:A:268:GLU:HG2	8:A:1027:HOH:O	2.14	0.47
1:A:238:VAL:HG23	1:A:296:ILE:O	2.13	0.47
1:A:21:PRO:HA	1:A:25:SER:O	2.14	0.47
1:A:22:VAL:CG1	1:A:27:ILE:HD12	2.42	0.47
1:A:456:LEU:C	5:A:995:NAG:H61	2.35	0.47
1:A:11:LYS:HG3	1:A:186:PHE:HE2	1.80	0.47
4:A:997:NAG:HN2	4:A:996:FUC:C2	2.27	0.47
1:A:15:VAL:HG11	1:A:33:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HD12	1:A:517:ARG:HG3	1.96	0.47
1:A:302:PRO:HD2	1:A:308:MET:SD	2.55	0.46
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.75	0.46
1:A:91:SER:O	1:A:94:CYS:HB3	2.16	0.46
1:A:221:ARG:NE	1:A:480:GLY:HA2	2.31	0.46
1:A:450:LEU:H	1:A:451:PRO:HD3	1.80	0.46
1:A:119:GLY:O	1:A:120:PHE:HB2	2.16	0.46
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.98	0.45
1:A:459:THR:HG23	1:A:462:GLU:OE1	2.15	0.45
1:A:396:GLY:HA3	8:A:1063:HOH:O	2.15	0.45
1:A:44:ARG:O	1:A:45:PHE:CB	2.63	0.45
1:A:510:MET:HG2	1:A:511:LYS:N	2.31	0.45
1:A:69:GLN:CD	1:A:86:PRO:HG3	2.36	0.45
1:A:412:THR:HG22	1:A:412:THR:O	2.15	0.45
1:A:257:ASN:HD22	1:A:258:SER:N	2.15	0.45
1:A:121:TYR:HB3	8:A:1047:HOH:O	2.16	0.45
1:A:212:SER:HB2	1:A:300:PHE:CE1	2.51	0.44
1:A:247:GLU:HA	1:A:250:ARG:NH1	2.31	0.44
1:A:349:ARG:O	1:A:353:MET:HG2	2.17	0.44
1:A:344:GLU:CD	1:A:346:LYS:HE3	2.37	0.44
1:A:282:LEU:HD12	6:A:1000:CP0:O23	2.17	0.44
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.53	0.44
2:A:999:NDG:H5	5:A:995:NAG:C6	2.28	0.44
1:A:22:VAL:HG13	1:A:22:VAL:O	2.17	0.44
1:A:511:LYS:HE3	8:A:1217:HOH:O	2.18	0.44
1:A:257:ASN:HD21	1:A:261:GLU:HG3	1.83	0.43
1:A:206:VAL:HG11	1:A:222:ALA:HB1	1.99	0.43
1:A:223:ILE:HA	1:A:320:LEU:O	2.19	0.43
1:A:12:SER:O	1:A:53:PRO:HA	2.18	0.43
1:A:264:HIS:CE1	8:A:1164:HOH:O	2.67	0.43
1:A:174:ARG:NH2	1:A:212:SER:OG	2.52	0.43
1:A:195:THR:OG1	1:A:221:ARG:HG3	2.19	0.43
1:A:190:ASP:OD1	1:A:192:LYS:CG	2.67	0.42
1:A:88:ARG:HD3	1:A:88:ARG:HA	1.94	0.42
1:A:461:GLU:CD	1:A:461:GLU:H	2.21	0.42
1:A:360:VAL:HG12	1:A:363:ALA:HB2	2.00	0.42
1:A:101:VAL:HG11	1:A:105:ARG:HG3	2.02	0.42
1:A:18:THR:CG2	1:A:61:SER:HA	2.50	0.42
1:A:168:VAL:HG23	1:A:169:GLY:N	2.34	0.42
1:A:457:ASN:HB2	5:A:995:NAG:C6	2.49	0.42
1:A:421:TYR:C	1:A:421:TYR:CD1	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:O	1:A:319:ILE:HG13	2.20	0.42
1:A:492:TRP:CD2	1:A:503:ILE:HD11	2.55	0.41
1:A:190:ASP:HA	1:A:191:PRO:HD2	1.93	0.41
1:A:404:LEU:HD23	1:A:404:LEU:C	2.41	0.41
1:A:32:GLY:O	1:A:96:TYR:HD2	2.03	0.41
1:A:418:THR:O	1:A:494:LEU:HD12	2.21	0.41
1:A:224:LEU:N	1:A:224:LEU:HD12	2.35	0.41
1:A:97:LEU:HD12	1:A:97:LEU:C	2.41	0.41
1:A:257:ASN:ND2	1:A:261:GLU:HG3	2.36	0.41
1:A:221:ARG:NE	1:A:480:GLY:CA	2.85	0.40
1:A:461:GLU:OE1	1:A:461:GLU:N	2.48	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)
1:A:535:THR:CG2	1:A:535:THR:CG2[5_675]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	531/543 (98%)	480 (90%)	48 (9%)	3 (1%)	30 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	486	HIS
1	A	380	ASP

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	465/474 (98%)	453 (97%)	12 (3%)	54 79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	87	ASN
1	A	143	LEU
1	A	197	PHE
1	A	232	PRO
1	A	257	ASN
1	A	283	PRO
1	A	288	PHE
1	A	321	LEU
1	A	330	PHE
1	A	473	TRP
1	A	492	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	66	ASN
1	A	68	GLN
1	A	87	ASN
1	A	181	HIS
1	A	257	ASN
1	A	280	ASN
1	A	382	ASN
1	A	500	GLN
1	A	519	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

6 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MAN	A	992	5	11,11,12	0.37	0	14,15,17	0.63	0
2	FUL	A	993	2	10,10,11	0.73	0	14,14,16	1.47	3 (21%)
5	NAG	A	995	5	14,14,15	0.60	0	15,19,21	1.01	1 (6%)
4	FUC	A	996	4	10,10,11	0.51	0	14,14,16	0.69	0
4	NAG	A	997	1,4	14,14,15	0.69	0	15,19,21	0.64	0
2	NDG	A	999	1,2	14,14,15	0.70	0	15,19,21	0.81	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	992	5	-	0/2/19/22	1/1/1/1
2	FUL	A	993	2	-	0/0/17/20	0/1/1/1
5	NAG	A	995	5	-	0/6/23/26	0/1/1/1
4	FUC	A	996	4	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	A	997	1,4	-	1/6/23/26	0/1/1/1
2	NDG	A	999	1,2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	995	NAG	C4-C3-C2	-2.49	107.36	111.23
2	A	999	NDG	C2-N2-C7	-2.16	120.27	123.04
2	A	993	FUL	O5-C5-C4	2.09	113.15	109.53
2	A	993	FUL	C1-C2-C3	2.72	112.75	109.54
2	A	993	FUL	C1-O5-C5	3.72	118.12	112.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	996	FUC	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	997	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	992	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	992	MAN	2	0
2	A	993	FUL	4	0
5	A	995	NAG	10	0
4	A	996	FUC	7	0
4	A	997	NAG	7	0
2	A	999	NDG	8	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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
6	CP0	A	1000	-	45,49,49	3.45	26 (57%)	48,74,74	2.89	18 (37%)
3	NAG	A	994	3	14,14,15	0.62	0	15,19,21	0.73	0
3	NAG	A	998	1,3	14,14,15	0.53	0	15,19,21	0.73	1 (6%)

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
6	CP0	A	1000	-	-	0/17/60/60	0/5/7/7
3	NAG	A	994	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	998	1,3	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1000	CP0	C3-C2	-3.29	1.40	1.47
6	A	1000	CP0	O1-C37	-2.29	1.17	1.21
6	A	1000	CP0	C2-C6	2.23	1.45	1.40
6	A	1000	CP0	C30-C27	2.36	1.61	1.51
6	A	1000	CP0	C16-C15	2.37	1.42	1.38
6	A	1000	CP0	C22-N2	2.40	1.51	1.47
6	A	1000	CP0	C17-C16	2.44	1.56	1.50
6	A	1000	CP0	C24-N3	2.66	1.55	1.48
6	A	1000	CP0	C9-C10	2.67	1.41	1.37
6	A	1000	CP0	C36-C24	2.71	1.59	1.52
6	A	1000	CP0	C20-C21	2.89	1.60	1.53
6	A	1000	CP0	C20-C15	3.00	1.59	1.53
6	A	1000	CP0	O19-C17	3.16	1.48	1.45
6	A	1000	CP0	C36-C22	3.20	1.61	1.52
6	A	1000	CP0	O19-C21	3.33	1.38	1.34
6	A	1000	CP0	C7-C8	3.52	1.49	1.43
6	A	1000	CP0	C13-N1	3.81	1.44	1.37
6	A	1000	CP0	C9-C8	3.85	1.49	1.42
6	A	1000	CP0	O2-C37	4.28	1.46	1.36
6	A	1000	CP0	C12-C13	5.33	1.51	1.41
6	A	1000	CP0	C29-N3	5.83	1.59	1.47
6	A	1000	CP0	C14-C15	5.97	1.48	1.39
6	A	1000	CP0	C8-C13	7.02	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1000	CP0	C6-C7	7.40	1.47	1.38
6	A	1000	CP0	C11-C10	7.56	1.54	1.38
6	A	1000	CP0	C23-N4	8.67	1.51	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1000	CP0	C36-C22-N2	-6.94	101.01	111.07
6	A	1000	CP0	C11-C12-C13	-6.63	113.68	120.88
6	A	1000	CP0	C26-N2-C37	-6.56	103.36	121.81
6	A	1000	CP0	C25-C26-N2	-4.65	104.33	111.07
6	A	1000	CP0	C12-C13-N1	-3.55	113.09	118.73
6	A	1000	CP0	C2-C3-N4	-3.39	108.41	113.62
6	A	1000	CP0	C2-C6-C7	-3.01	116.23	121.90
6	A	1000	CP0	O2-C37-O1	-2.62	119.39	123.93
6	A	1000	CP0	C34-C29-N3	-2.62	106.66	111.15
3	A	998	NAG	C2-N2-C7	-2.35	120.02	123.04
6	A	1000	CP0	C5-C6-C7	2.05	133.07	128.62
6	A	1000	CP0	C9-C8-C7	2.62	127.53	121.75
6	A	1000	CP0	C32-C31-C7	2.86	118.00	112.21
6	A	1000	CP0	C3-C2-N1	3.47	121.79	117.79
6	A	1000	CP0	C14-C3-C2	3.49	130.75	124.67
6	A	1000	CP0	C12-C11-C10	4.35	125.55	120.14
6	A	1000	CP0	C12-C13-C8	4.43	124.06	119.07
6	A	1000	CP0	C10-O2-C37	4.97	126.11	117.30
6	A	1000	CP0	C22-N2-C37	8.01	144.35	121.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	994	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1000	CP0	4	0
3	A	994	NAG	1	0
3	A	998	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.50	4 (0%) 87 85	19, 36, 59, 81	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ALA	4.3
1	A	535	THR	3.7
1	A	4	SER	3.0
1	A	57	VAL	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
5	MAN	A	992	11/12	0.73	0.34	6.16	97,99,102,104	0
2	NDG	A	999	14/15	0.82	0.29	-	73,78,81,83	0
4	NAG	A	997	14/15	0.79	0.34	-	87,91,95,96	0
5	NAG	A	995	14/15	0.73	0.53	-	103,105,107,108	0
2	FUL	A	993	10/11	0.85	0.41	-	85,87,88,88	0
4	FUC	A	996	10/11	0.87	0.34	-	94,95,95,95	0

6.4 Ligands

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	CP0	A	1000	43/43	0.80	0.26	3.69	44,76,89,91	0
7	IOD	A	1001	1/1	0.93	0.06	-	66,66,66,66	1
3	NAG	A	994	14/15	0.81	0.34	-	113,114,114,114	0
3	NAG	A	998	14/15	0.90	0.20	-	62,64,67,67	0

6.5 Other polymers

There are no such residues in this entry.