W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:17 pm GMT

PDB ID	:	3DKK
Title	:	Aged Form of Human Butyrylcholinesterase Inhibited by Tabun
Authors	:	Nachon, F.; Carletti, E.
Deposited on	:	2008-06-25
Resolution	:	2.31 Å(reported)

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	:	trunk28620
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)	:	recalc28949

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 2.31 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		10
Ramachandran outliers		1.3%
Sidechain outliers		6.4%
RSRZ outliers		3.2%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
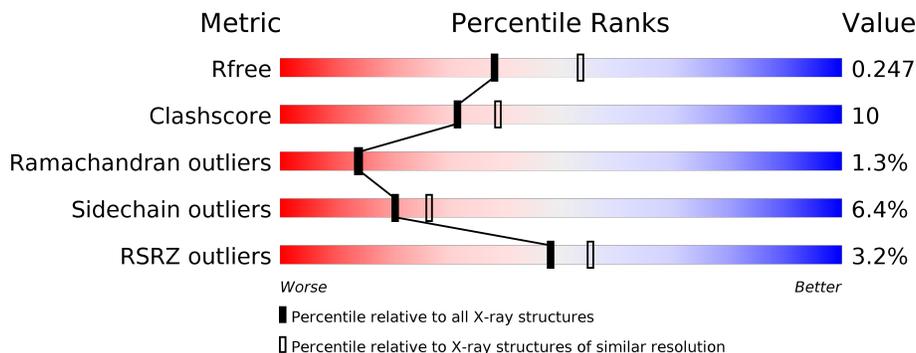
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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 <=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	529	3% 78% 18% ··

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
3	FUL	A	534	-	-	-	X
4	NAG	A	536	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4619 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 Cholinesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total 4215	C 2717	N 710	O 772	P 1	S 15	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED	UNP P06276
A	455	GLN	ASN	ENGINEERED	UNP P06276
A	481	GLN	ASN	ENGINEERED	UNP P06276
A	486	GLN	ASN	ENGINEERED	UNP P06276

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total 38	C 22	N 2	O 14	0	0
2	A	3	Total 38	C 22	N 2	O 14	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
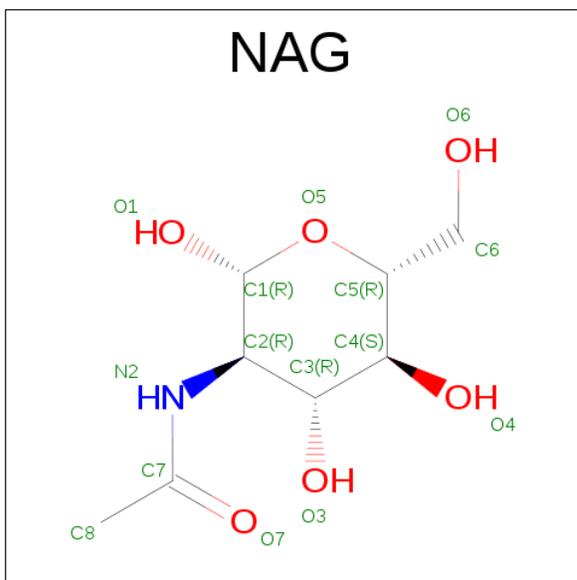
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Cl 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ —— S —— O⁻ O4

S

O

O2
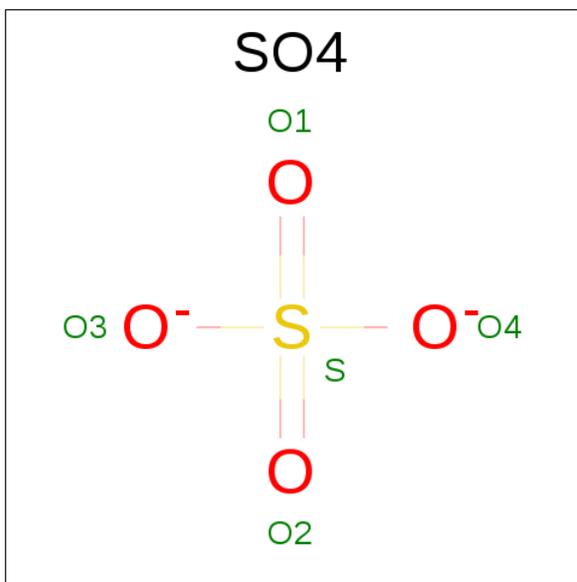
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	254	Total 254	O 254	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: Cholinesterase

Chain A:
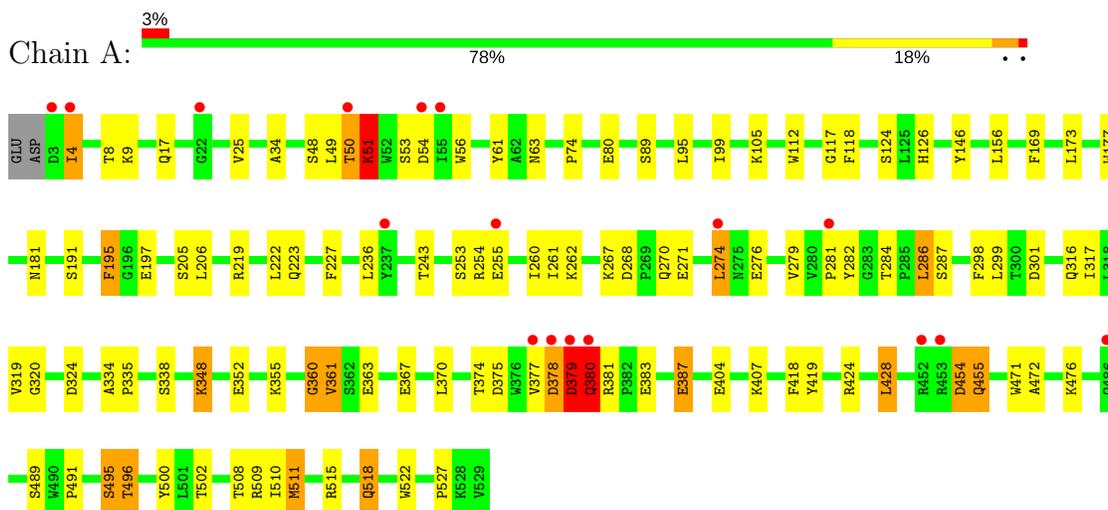
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	155.24Å 155.24Å 127.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.18 – 2.31 28.18 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.18-2.31) 99.0 (28.18-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.197 , 0.251 0.196 , 0.247	Depositor DCC
R_{free} test set	1700 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4619	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 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CL, NA, SO4, SEN, FUL

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	0.90	4/4327 (0.1%)	0.85	3/5873 (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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLU	CG-CD	7.15	1.62	1.51
1	A	146	TYR	CD2-CE2	6.82	1.49	1.39
1	A	363	GLU	CG-CD	6.27	1.61	1.51
1	A	404	GLU	CG-CD	5.12	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	515	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	324	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	380	GLN	Peptide

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	4215	0	4113	88	2
2	A	76	0	68	2	0
3	A	24	0	22	1	0
4	A	42	0	39	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
8	A	254	0	0	13	2
All	All	4619	0	4242	88	2

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 10.

All (88) 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:380:GLN:N	1:A:380:GLN:HE21	1.67	0.93
1:A:4:ILE:H	1:A:4:ILE:HD12	1.33	0.92
1:A:518:GLN:H	1:A:518:GLN:HE21	1.12	0.92
1:A:518:GLN:H	1:A:518:GLN:NE2	1.71	0.88
1:A:379:ASP:O	1:A:380:GLN:HB2	1.75	0.86
1:A:4:ILE:N	1:A:4:ILE:HD12	1.94	0.82
1:A:379:ASP:HB3	1:A:381:ARG:HG3	1.63	0.80
1:A:355:LYS:HD3	8:A:743:HOH:O	1.81	0.79
1:A:495:SER:HA	8:A:713:HOH:O	1.83	0.77
1:A:380:GLN:HE21	1:A:380:GLN:CA	1.97	0.75
1:A:282:TYR:CB	8:A:700:HOH:O	2.35	0.74
1:A:53:SER:O	8:A:729:HOH:O	2.06	0.72
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.72	0.70
1:A:378:ASP:OD1	1:A:378:ASP:C	2.31	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:SER:O	1:A:496:THR:OG1	2.08	0.68
1:A:378:ASP:O	1:A:380:GLN:NE2	2.27	0.68
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.75	0.68
1:A:375:ASP:HB2	8:A:720:HOH:O	1.95	0.66
1:A:496:THR:N	8:A:713:HOH:O	2.21	0.65
1:A:380:GLN:H	1:A:381:ARG:HB2	1.59	0.65
1:A:4:ILE:HG12	1:A:17:GLN:OE1	1.98	0.63
1:A:518:GLN:HE21	1:A:518:GLN:N	1.90	0.63
1:A:227:PHE:CD2	1:A:227:PHE:C	2.72	0.63
1:A:378:ASP:O	1:A:380:GLN:N	2.32	0.62
1:A:377:VAL:O	1:A:377:VAL:HG13	2.00	0.61
1:A:495:SER:CA	8:A:713:HOH:O	2.47	0.60
1:A:48:SER:CB	8:A:732:HOH:O	2.50	0.60
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.36	0.60
1:A:370:LEU:HD12	1:A:374:THR:HG21	1.83	0.59
1:A:54:ASP:HB2	8:A:729:HOH:O	2.01	0.59
1:A:383:GLU:O	1:A:387:GLU:HG2	2.04	0.57
1:A:522:TRP:O	1:A:527:PRO:HD3	2.04	0.56
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.21	0.56
1:A:495:SER:O	1:A:496:THR:CB	2.53	0.55
1:A:253:SER:O	1:A:254:ARG:HD3	2.06	0.55
1:A:454:ASP:O	1:A:455:GLN:HB2	2.06	0.55
1:A:380:GLN:N	1:A:381:ARG:HB2	2.23	0.53
1:A:267:LYS:HE3	1:A:271:GLU:OE1	2.08	0.53
1:A:48:SER:HA	8:A:732:HOH:O	2.10	0.52
1:A:219:ARG:HD3	1:A:316:GLN:OE1	2.10	0.51
1:A:48:SER:HB3	8:A:732:HOH:O	2.11	0.51
1:A:206:LEU:HD21	1:A:227:PHE:HB2	1.93	0.51
1:A:281:PRO:HG3	2:A:538:NAG:H83	1.94	0.50
1:A:380:GLN:NE2	1:A:380:GLN:CA	2.71	0.50
1:A:74:PRO:HA	1:A:80:GLU:OE1	2.13	0.49
1:A:126:HIS:HD2	8:A:752:HOH:O	1.94	0.49
1:A:383:GLU:O	1:A:387:GLU:CG	2.61	0.48
1:A:495:SER:O	1:A:496:THR:HG23	2.13	0.48
1:A:49:LEU:HD12	1:A:50:THR:H	1.79	0.48
1:A:112:TRP:HA	1:A:195:PHE:O	2.14	0.47
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.47
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.50	0.47
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.82	0.47
1:A:377:VAL:N	1:A:378:ASP:HA	2.30	0.47
1:A:472:ALA:O	1:A:476:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:HA	1:A:348:LYS:HD2	1.66	0.46
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.50	0.46
1:A:25:VAL:HG13	1:A:99:ILE:O	2.15	0.46
1:A:284:THR:C	1:A:286:LEU:H	2.19	0.46
1:A:63:ASN:HB3	1:A:89:SER:HB3	1.98	0.46
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.98	0.46
1:A:454:ASP:O	1:A:455:GLN:CB	2.63	0.45
1:A:191:SER:HB2	3:A:534:FUL:H3	1.98	0.45
1:A:177:TRP:O	1:A:181:ASN:HB2	2.17	0.45
1:A:270:GLN:O	1:A:274:LEU:HB2	2.17	0.45
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.98	0.45
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.99	0.44
1:A:276:GLU:O	1:A:279:VAL:HG22	2.16	0.44
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.65	0.44
1:A:338:SER:HB2	2:A:530:NAG:H62	1.99	0.44
1:A:4:ILE:N	1:A:4:ILE:CD1	2.61	0.43
1:A:317:ILE:HD12	1:A:319:VAL:HG21	1.99	0.43
1:A:317:ILE:HD12	1:A:319:VAL:CG2	2.49	0.43
1:A:50:THR:O	1:A:51:LYS:CB	2.67	0.43
1:A:56:TRP:C	1:A:56:TRP:CD1	2.92	0.43
1:A:95:LEU:HD12	1:A:95:LEU:C	2.39	0.43
1:A:502:THR:O	1:A:508:THR:HB	2.19	0.42
1:A:378:ASP:OD1	1:A:380:GLN:NE2	2.52	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.55	0.42
1:A:169:PHE:CZ	1:A:298:PHE:HB2	2.55	0.42
1:A:156:LEU:HD22	1:A:261:ILE:HD11	2.02	0.42
1:A:48:SER:CA	8:A:732:HOH:O	2.65	0.41
1:A:117:GLY:O	1:A:118:PHE:HB2	2.21	0.41
1:A:254:ARG:HB2	1:A:260:ILE:CG1	2.50	0.41
1:A:50:THR:O	1:A:51:LYS:HB3	2.21	0.41
1:A:197:GLU:HA	1:A:223:GLN:O	2.21	0.41
1:A:284:THR:C	1:A:286:LEU:N	2.75	0.40
1:A:491:PRO:CD	1:A:510:ILE:HD12	2.52	0.40

All (2) 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:379:ASP:CG	8:A:747:HOH:O[7_555]	2.10	0.10
1:A:379:ASP:OD2	8:A:747:HOH:O[7_555]	2.18	0.02

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	526/529 (99%)	494 (94%)	25 (5%)	7 (1%)	14	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	A	496	THR
1	A	51	LYS
1	A	361	VAL
1	A	378	ASP
1	A	380	GLN
1	A	360	GLY

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	452/453 (100%)	423 (94%)	29 (6%)	20	26

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	THR
1	A	9	LYS
1	A	50	THR

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Mol	Chain	Res	Type
1	A	51	LYS
1	A	105	LYS
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	274	LEU
1	A	286	LEU
1	A	287	SER
1	A	348	LYS
1	A	361	VAL
1	A	379	ASP
1	A	380	GLN
1	A	387	GLU
1	A	407	LYS
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN
1	A	471	TRP
1	A	489	SER
1	A	495	SER
1	A	509	ARG
1	A	511	MET
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	275	ASN
1	A	380	GLN
1	A	517	GLN
1	A	518	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#|Z| > 2$
1	SEN	A	198	1	11,11,12	2.00	2 (18%)	9,15,17	3.09	6 (66%)

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
1	SEN	A	198	1	-	0/9/14/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEN	P-N1	3.29	1.70	1.63
1	A	198	SEN	CA-C	5.21	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEN	OG-P-O3	-5.39	105.49	115.84
1	A	198	SEN	O3-P-N1	-2.81	108.81	113.30
1	A	198	SEN	O-C-CA	-2.12	119.16	125.02
1	A	198	SEN	OG-P-N1	2.27	112.91	105.83
1	A	198	SEN	O2-P-O3	3.78	119.04	109.74
1	A	198	SEN	OG-CB-CA	4.86	112.96	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

8 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	#$|Z| > 2$
2	NAG	A	530	1,2	14,14,15	0.96	1 (7%)	15,19,21	2.00	6 (40%)
2	NAG	A	531	2	14,14,15	0.73	0	15,19,21	0.88	0
2	FUL	A	532	2	9,10,11	0.94	0	13,14,16	2.56	5 (38%)
3	NAG	A	533	1,3	14,14,15	1.06	1 (7%)	15,19,21	2.09	7 (46%)
3	FUL	A	534	3	9,10,11	0.92	0	13,14,16	2.11	4 (30%)
2	NAG	A	538	1,2	14,14,15	0.60	0	15,19,21	1.95	4 (26%)
2	NAG	A	539	2	14,14,15	0.67	0	15,19,21	2.90	7 (46%)
2	FUL	A	540	2	9,10,11	0.81	0	13,14,16	2.50	6 (46%)

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	NAG	A	530	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	531	2	-	0/6/23/26	0/1/1/1
2	FUL	A	532	2	-	0/0/17/20	0/1/1/1
3	NAG	A	533	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	534	3	-	0/0/17/20	0/1/1/1
2	NAG	A	538	1,2	-	1/6/23/26	0/1/1/1
2	NAG	A	539	2	-	0/6/23/26	0/1/1/1
2	FUL	A	540	2	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	530	NAG	O5-C1	-2.16	1.40	1.43
3	A	533	NAG	C1-C2	2.81	1.56	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	539	NAG	C4-C3-C2	-6.20	101.94	111.02
2	A	540	FUL	C1-C2-C3	-5.68	102.45	109.65
2	A	532	FUL	O5-C1-C2	-5.46	102.23	110.79
2	A	539	NAG	C3-C4-C5	-4.41	102.45	110.22
3	A	534	FUL	C1-C2-C3	-4.13	104.42	109.65
3	A	534	FUL	O5-C1-C2	-3.90	104.68	110.79
2	A	532	FUL	C1-O5-C5	-3.57	104.50	112.39
2	A	530	NAG	O5-C1-C2	-3.33	106.84	111.47
3	A	533	NAG	O5-C1-C2	-2.99	107.31	111.47
2	A	540	FUL	C1-O5-C5	-2.98	105.80	112.39
2	A	532	FUL	C1-C2-C3	-2.87	106.02	109.65
2	A	540	FUL	O5-C1-C2	-2.82	106.38	110.79
2	A	538	NAG	O5-C1-C2	-2.69	107.72	111.47
3	A	533	NAG	C3-C4-C5	-2.69	105.48	110.22
2	A	530	NAG	C3-C4-C5	-2.51	105.80	110.22
2	A	538	NAG	O7-C7-C8	-2.21	118.04	122.06
2	A	530	NAG	O4-C4-C3	-2.16	105.66	110.36
3	A	534	FUL	C1-O5-C5	-2.14	107.66	112.39
3	A	533	NAG	O6-C6-C5	2.05	118.24	111.34
2	A	538	NAG	C8-C7-N2	2.06	119.82	116.11
2	A	540	FUL	O3-C3-C4	2.08	114.88	110.36
2	A	530	NAG	C6-C5-C4	2.36	118.53	113.00
3	A	533	NAG	O3-C3-C2	2.46	114.66	109.39
2	A	539	NAG	O3-C3-C4	2.74	116.32	110.36
3	A	533	NAG	C8-C7-N2	2.76	121.09	116.11
2	A	539	NAG	O4-C4-C3	2.77	116.39	110.36
3	A	534	FUL	C3-C4-C5	2.78	114.04	109.68
2	A	540	FUL	O2-C2-C1	2.78	114.82	109.18
3	A	533	NAG	C1-O5-C5	2.89	116.15	112.17
2	A	530	NAG	C2-N2-C7	2.90	127.17	122.94
2	A	539	NAG	O3-C3-C2	2.98	115.78	109.39
2	A	532	FUL	C2-C3-C4	3.02	116.15	110.88
3	A	533	NAG	O4-C4-C5	3.15	117.21	109.28
2	A	530	NAG	O6-C6-C5	3.29	122.42	111.34
2	A	539	NAG	C1-C2-N2	3.61	116.66	110.49
2	A	532	FUL	C3-C4-C5	4.13	116.17	109.68
2	A	540	FUL	C3-C4-C5	4.25	116.37	109.68
2	A	539	NAG	C1-O5-C5	4.44	118.28	112.17
2	A	538	NAG	C1-O5-C5	5.47	119.70	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	538	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	530	NAG	1	0
3	A	534	FUL	1	0
2	A	538	NAG	1	0

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#|Z| > 2$
4	NAG	A	535	1	14,14,15	0.63	0	15,19,21	2.32	4 (26%)
4	NAG	A	536	1	14,14,15	0.80	0	15,19,21	1.35	2 (13%)
4	NAG	A	537	1	14,14,15	0.65	0	15,19,21	1.40	2 (13%)
7	SO4	A	544	-	4,4,4	0.31	0	6,6,6	0.45	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
4	NAG	A	535	1	-	0/6/23/26	0/1/1/1
4	NAG	A	536	1	-	0/6/23/26	0/1/1/1
4	NAG	A	537	1	-	1/6/23/26	0/1/1/1
7	SO4	A	544	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	535	NAG	O5-C1-C2	-6.53	102.38	111.47
4	A	535	NAG	C2-N2-C7	-3.39	118.00	122.94
4	A	536	NAG	O5-C1-C2	-3.28	106.91	111.47
4	A	536	NAG	O7-C7-C8	-2.22	118.01	122.06
4	A	537	NAG	C8-C7-N2	2.01	119.73	116.11
4	A	535	NAG	C1-C2-N2	2.58	114.90	110.49
4	A	535	NAG	C1-O5-C5	2.95	116.24	112.17
4	A	537	NAG	C2-N2-C7	3.36	127.85	122.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	537	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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	526/529 (99%)	-0.13	17 (3%)	48	55	19, 36, 62, 82	9 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.7
1	A	237	TYR	4.6
1	A	453	ARG	4.2
1	A	379	ASP	4.0
1	A	255	GLU	3.4
1	A	377	VAL	3.3
1	A	281	PRO	3.2
1	A	4	ILE	2.9
1	A	486	GLN	2.9
1	A	378	ASP	2.8
1	A	50	THR	2.8
1	A	452	ARG	2.7
1	A	54	ASP	2.6
1	A	22	GLY	2.5
1	A	380	GLN	2.2
1	A	55	ILE	2.1
1	A	274	LEU	2.1

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

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
1	SEN	A	198	12/13	0.98	0.15	-	24,25,27,28	0

6.3 Carbohydrates ⓘ

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
3	FUL	A	534	10/11	0.74	0.33	4.42	44,46,48,49	10
2	FUL	A	540	10/11	0.89	0.22	0.50	73,75,77,77	0
2	NAG	A	530	14/15	0.95	0.12	-0.20	47,54,63,66	0
3	NAG	A	533	14/15	0.87	0.30	-	56,62,64,65	0
2	NAG	A	539	14/15	0.77	0.41	-	85,89,91,91	0
2	FUL	A	532	10/11	0.88	0.24	-	71,74,76,76	0
2	NAG	A	531	14/15	0.83	0.24	-	69,73,76,76	0
2	NAG	A	538	14/15	0.82	0.24	-	74,78,83,83	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
4	NAG	A	536	14/15	0.67	0.28	9.50	60,73,76,76	0
5	CL	A	541	1/1	0.98	0.08	-	63,63,63,63	0
4	NAG	A	537	14/15	0.71	0.43	-	90,95,97,97	0
7	SO4	A	544	5/5	0.97	0.10	-	40,42,46,47	5
4	NAG	A	535	14/15	0.72	0.34	-	74,79,80,80	0
6	NA	A	543	1/1	0.80	0.09	-	57,57,57,57	1
5	CL	A	542	1/1	0.92	0.13	-	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK