



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:52 PM GMT

PDB ID : 3DL7  
Title : Aged Form of Mouse Acetylcholinesterase Inhibited by Tabun- Update  
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Deposited on : 2008-06-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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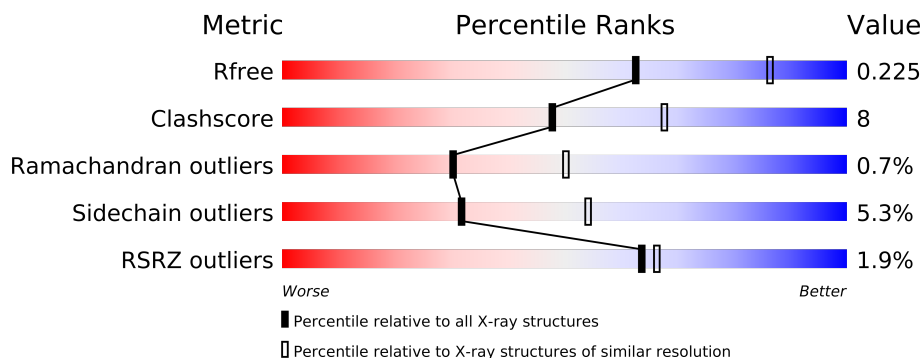
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8926 atoms, of which 0 are hydrogen and 0 are deuterium.

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	537	Total	C	N	O	P	S	0	3	0
			4229	2708	736	769	2	14			
1	B	533	Total	C	N	O	P	S	0	6	1
			4211	2700	732	762	2	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SEN	SER	MICROHETEROGENEITY	UNP P21836
A	203	SUN	SER	MICROHETEROGENEITY	UNP P21836
A	544	ALA	-	SEE REMARK 999	UNP P21836
A	545	THR	-	SEE REMARK 999	UNP P21836
A	546	GLU	-	SEE REMARK 999	UNP P21836
A	547	ALA	-	SEE REMARK 999	UNP P21836
A	548	PRO	-	SEE REMARK 999	UNP P21836
B	203	SEN	SER	MICROHETEROGENEITY	UNP P21836
B	203	SUN	SER	MICROHETEROGENEITY	UNP P21836
B	544	ALA	-	SEE REMARK 999	UNP P21836
B	545	THR	-	SEE REMARK 999	UNP P21836
B	546	GLU	-	SEE REMARK 999	UNP P21836
B	547	ALA	-	SEE REMARK 999	UNP P21836
B	548	PRO	-	SEE REMARK 999	UNP P21836

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

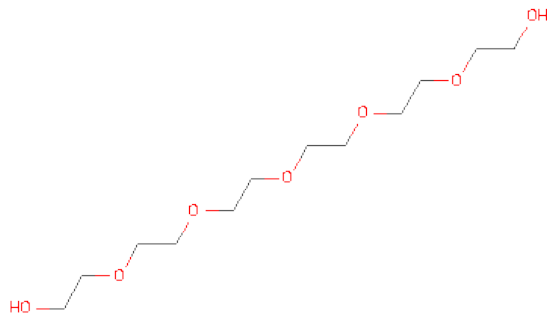


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

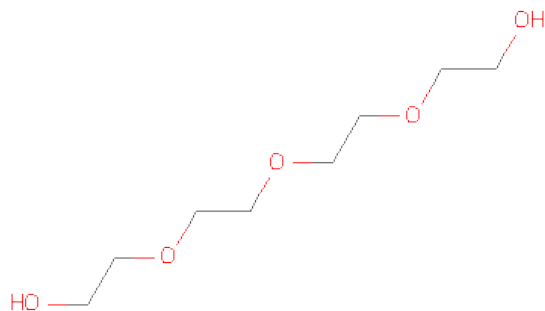
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		

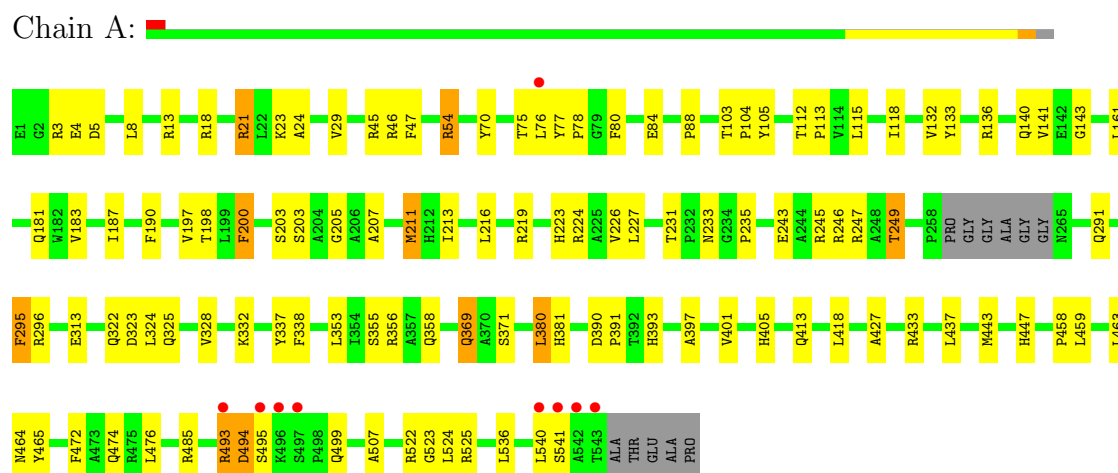
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	257	Total	O	0	0
			257	257		
6	B	182	Total	O	0	0
			182	182		

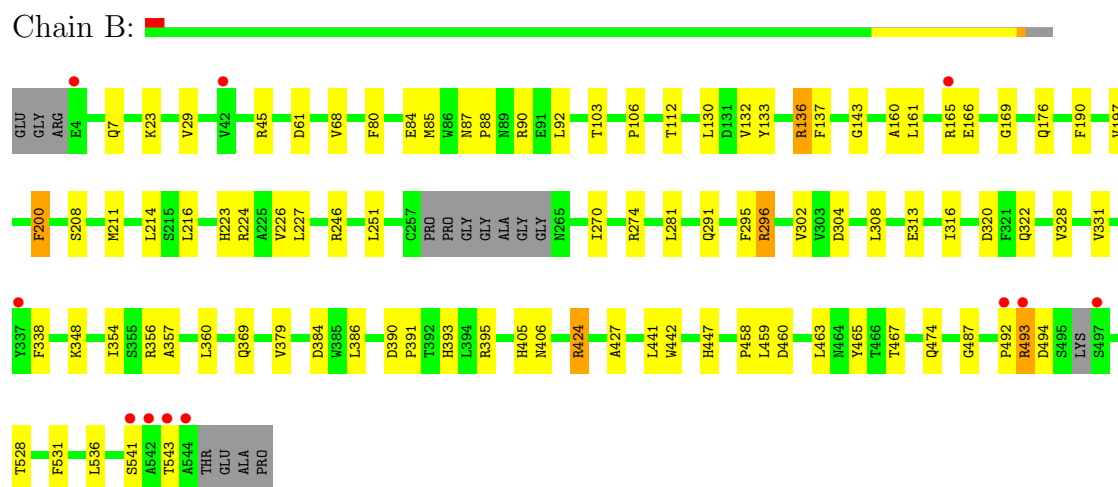
### 3 Residue-property plots

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



#### • Molecule 1: Acetylcholinesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.02Å 110.88Å 226.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.82 – 2.50 28.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.82-2.50) 99.2 (28.81-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.227 0.185 , 0.225	Depositor DCC
$R_{free}$ test set	1381 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 69037 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, SUN, PG4, P6G, SEN

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	0.63	0/4330	0.72	1/5915 (0.0%)
1	B	0.61	0/4320	0.69	1/5901 (0.0%)
All	All	0.62	0/8650	0.71	2/11816 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	CA-CB-CG	-6.66	99.98	115.30
1	B	161	LEU	CA-CB-CG	-5.09	103.58	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4229	0	4114	75	0
1	B	4211	0	4101	54	0
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	19	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	13	0	18	0	0
6	A	257	0	0	10	0
6	B	182	0	0	5	0
All	All	8926	0	8270	129	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:338:PHE:CZ	1:A:447[B]:HIS:HE1	1.51	1.28
1:A:338:PHE:CZ	1:A:447[B]:HIS:CE1	2.27	1.23
1:A:338:PHE:CE2	1:A:447[B]:HIS:CE1	2.29	1.20
1:A:338:PHE:CE2	1:A:447[B]:HIS:HE1	1.62	1.15
1:B:424:ARG:HH11	1:B:424:ARG:HG3	0.93	1.06
1:B:356:ARG:HD2	6:B:727:HOH:O	1.56	1.05
1:A:380:LEU:HB3	4:A:551:P6G:H61	1.40	0.98
1:B:197:VAL:H	1:B:223:HIS:HD2	1.11	0.97
1:B:424:ARG:HG3	1:B:424:ARG:NH1	1.71	0.90
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.72	0.88
1:B:424:ARG:CG	1:B:424:ARG:HH11	1.84	0.87
1:B:197:VAL:H	1:B:223:HIS:CD2	1.95	0.84
1:A:433:ARG:HD3	6:A:765:HOH:O	1.77	0.84
1:A:197:VAL:H	1:A:223:HIS:HD2	1.25	0.82
1:A:245:ARG:O	1:A:249:THR:HG23	1.88	0.73
1:B:338:PHE:CZ	1:B:447[B]:HIS:CE1	2.78	0.72
1:A:380:LEU:HB3	4:A:551:P6G:C6	2.19	0.70
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.72	0.70
1:A:369:GLN:HG3	6:A:795:HOH:O	1.92	0.69
1:B:338:PHE:CE2	1:B:447[B]:HIS:CE1	2.81	0.69
1:A:54:ARG:HG2	1:A:54:ARG:HH11	1.59	0.68
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.06	0.68
1:A:393:HIS:HD2	6:A:567:HOH:O	1.79	0.66
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.76	0.66
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.30	0.66
1:A:337:TYR:HA	1:A:443:MET:HE3	1.78	0.66
1:A:337:TYR:HA	1:A:443:MET:CE	2.27	0.64
1:B:160:ALA:HB2	1:B:169:GLY:HA3	1.81	0.63
1:A:76:LEU:HD23	1:A:77:TYR:CE2	2.34	0.63
1:B:112:THR:HG21	1:B:143:GLY:O	1.99	0.62
1:A:338:PHE:CE2	1:A:447[B]:HIS:ND1	2.66	0.61
1:A:338:PHE:HZ	1:A:447[B]:HIS:CE1	2.12	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.82	0.60
1:B:80:PHE:O	1:B:84:GLU:HG2	2.01	0.60
1:A:112:THR:HG21	1:A:143:GLY:O	2.02	0.58
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.69	0.58
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.86	0.57
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.34	0.57
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.87	0.57
1:A:54:ARG:CB	1:A:54:ARG:HH11	2.18	0.56
1:B:296:ARG:HG2	6:B:634:HOH:O	2.05	0.56
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.21	0.55
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.40	0.55
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.88	0.55
1:A:54:ARG:HG2	1:A:54:ARG:NH1	2.22	0.54
1:B:493:ARG:CB	1:B:494:ASP:HA	2.37	0.53
1:B:357:ALA:N	6:B:729:HOH:O	2.42	0.53
1:A:338:PHE:HE2	1:A:447[B]:HIS:ND1	2.04	0.53
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.92	0.52
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.90	0.52
1:A:88:PRO:HD3	6:A:618:HOH:O	2.08	0.52
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.91	0.52
1:A:197:VAL:H	1:A:223:HIS:CD2	2.17	0.52
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.90	0.52
1:A:207:ALA:O	1:A:211:MET:HG2	2.09	0.52
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.93	0.51
1:B:320:ASP:OD1	1:B:322:GLN:HG2	2.11	0.51
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.75	0.51
1:B:328:VAL:O	1:B:427:ALA:HA	2.11	0.51
1:A:507:ALA:HA	1:A:522[A]:ARG:HH12	1.76	0.51
1:A:213:ILE:O	1:A:219:ARG:HD3	2.10	0.51
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.93	0.51
1:A:393:HIS:CD2	6:A:567:HOH:O	2.58	0.50
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.94	0.49
1:B:493:ARG:HB3	1:B:494:ASP:HA	1.95	0.49
1:B:224:ARG:HD3	1:B:487:GLY:CA	2.42	0.49
1:B:214:LEU:HD21	1:B:316:ILE:HG22	1.94	0.49
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.48	0.49
1:A:447[B]:HIS:CD2	1:A:447[B]:HIS:C	2.86	0.48
1:A:203[A]:SEN:HBA	1:A:447[A]:HIS:NE2	2.28	0.48
1:A:296:ARG:HH21	1:A:369:GLN:NE2	2.11	0.48
1:A:105:TYR:HA	6:A:561:HOH:O	2.13	0.47
1:A:397:ALA:O	1:A:401:VAL:HG23	2.14	0.47
1:B:200:PHE:CB	1:B:226:VAL:HB	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:GLN:HG2	6:A:610:HOH:O	2.14	0.47
1:A:459:LEU:HD11	1:A:474:GLN:HG3	1.95	0.47
1:B:459:LEU:HD11	1:B:474:GLN:HG3	1.97	0.47
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.97	0.46
1:B:360:LEU:HD22	1:B:379:VAL:HG11	1.98	0.46
1:B:348:LYS:HD2	6:B:706:HOH:O	2.15	0.46
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.46	0.46
1:A:393:HIS:HB2	6:A:751:HOH:O	2.15	0.46
1:A:499:GLN:NE2	6:A:557:HOH:O	2.47	0.46
1:A:75:THR:O	1:A:78:PRO:HD3	2.16	0.45
1:B:354:ILE:O	1:B:391:PRO:HB3	2.17	0.45
1:A:447[B]:HIS:O	1:A:447[B]:HIS:CD2	2.70	0.45
1:B:528:THR:O	1:B:531:PHE:HB3	2.17	0.45
1:B:136:ARG:HG2	1:B:137:PHE:N	2.32	0.45
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.52	0.45
1:A:80:PHE:O	1:A:84:GLU:HG2	2.17	0.45
1:B:302:VAL:HG13	1:B:304:ASP:HB3	1.99	0.45
1:B:85:MET:CE	1:B:132:VAL:HG11	2.48	0.44
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.36	0.44
1:A:328:VAL:O	1:A:427:ALA:HA	2.17	0.44
1:A:183:VAL:HG13	1:A:187:ILE:HB	1.99	0.44
1:A:295:PHE:CE2	1:A:338:PHE:CE2	3.06	0.44
1:A:115:LEU:HD23	1:A:198:THR:HB	2.00	0.43
1:A:219:ARG:NH2	1:A:324:LEU:HD13	2.33	0.43
1:B:338:PHE:CE2	1:B:447[B]:HIS:ND1	2.86	0.43
1:A:105:TYR:CD2	1:A:105:TYR:C	2.92	0.43
1:B:384:ASP:HB2	1:B:393[B]:HIS:CE1	2.54	0.43
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.52	0.43
1:A:21:ARG:HG3	1:A:105:TYR:CE1	2.53	0.43
1:B:390:ASP:OD2	1:B:393[A]:HIS:ND1	2.28	0.42
1:A:243:GLU:O	1:A:247:ARG:HG3	2.20	0.42
1:A:231:THR:HB	1:A:233:ASN:OD1	2.19	0.42
1:A:5:ASP:HB3	1:A:8:LEU:HD12	2.02	0.42
1:A:493:ARG:O	1:A:494:ASP:HB2	2.20	0.42
1:A:381:HIS:HA	4:A:551:P6G:H31	2.01	0.42
1:B:45[B]:ARG:HD2	1:B:45[B]:ARG:HA	1.92	0.42
1:A:355:SER:OG	1:A:358:GLN:HG3	2.20	0.42
1:A:118:ILE:O	1:A:205:GLY:HA3	2.20	0.42
1:A:463:LEU:O	1:A:464:ASN:HB2	2.19	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.41
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.55	0.41
1:B:274:ARG:NH1	6:B:693:HOH:O	2.37	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:313:GLU:HG3	6:A:807:HOH:O	2.21	0.41
1:B:88:PRO:HG2	1:B:92:LEU:HD21	2.02	0.41
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.50	0.41
1:B:7:GLN:OE1	1:B:106:PRO:HA	2.20	0.41
1:B:103:THR:HG21	1:B:190:PHE:HB3	2.03	0.41
1:A:141:VAL:HG21	1:A:459:LEU:HD23	2.02	0.41
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.21	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.91	0.40
1:A:132:VAL:HG23	1:A:133:TYR:CD1	2.56	0.40
1:A:46:ARG:HD3	1:A:47:PHE:CZ	2.57	0.40
1:B:331:VAL:HG21	1:B:447[B]:HIS:HA	2.04	0.40
1:A:235:PRO:HG3	1:A:405:HIS:CE1	2.56	0.40
1:B:68:VAL:HG23	1:B:90:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

## 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	534/549 (97%)	515 (96%)	15 (3%)	4 (1%)	30	50
1	B	531/549 (97%)	506 (95%)	22 (4%)	3 (1%)	33	55
All	All	1065/1098 (97%)	1021 (96%)	37 (4%)	7 (1%)	30	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	PRO
1	A	494	ASP
1	A	541	SER
1	B	543	THR
1	A	371	SER
1	B	541	SER
1	A	523	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	442/445 (99%)	415 (94%)	27 (6%)	26	46
1	B	441/445 (99%)	422 (96%)	19 (4%)	40	65
All	All	883/890 (99%)	837 (95%)	46 (5%)	32	55

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	13	ARG
1	A	21	ARG
1	A	23	LYS
1	A	45	ARG
1	A	54	ARG
1	A	70	TYR
1	A	200	PHE
1	A	211	MET
1	A	216	LEU
1	A	249	THR
1	A	291	GLN
1	A	295	PHE
1	A	322	GLN
1	A	323	ASP
1	A	332	LYS
1	A	356	ARG
1	A	369	GLN
1	A	380	LEU
1	A	413	GLN
1	A	418	LEU
1	A	493	ARG
1	A	495	SER
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	A	540	LEU
1	B	23	LYS
1	B	61	ASP

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Mol	Chain	Res	Type
1	B	136	ARG
1	B	165	ARG
1	B	200	PHE
1	B	216	LEU
1	B	246	ARG
1	B	251	LEU
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	313	GLU
1	B	386	LEU
1	B	424	ARG
1	B	441	LEU
1	B	467	THR
1	B	493	ARG
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	287	HIS
1	A	291	GLN
1	A	369	GLN
1	A	509	GLN
1	B	87	ASN
1	B	223	HIS
1	B	291	GLN
1	B	387	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	SEN	A	203[A]	-	11,11,12	5.57	3 (27%)	13,15,17	1.99	3 (23%)
1	SUN	A	203[B]	-	13,13,14	5.07	3 (23%)	15,17,19	3.28	7 (46%)
1	SEN	B	203[A]	-	11,11,12	5.46	3 (27%)	13,15,17	2.45	5 (38%)
1	SUN	B	203[B]	-	13,13,14	4.95	4 (30%)	15,17,19	2.81	5 (33%)

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	203[A]	-	-	0/10/14/16	0/0/0/0
1	SUN	A	203[B]	-	-	0/16/18/20	0/0/0/0
1	SEN	B	203[A]	-	-	0/10/14/16	0/0/0/0
1	SUN	B	203[B]	-	-	0/16/18/20	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203[A]	SEN	O-C	17.32	1.23	1.11
1	A	203[B]	SUN	O-C	17.32	1.23	1.11
1	B	203[A]	SEN	O-C	17.00	1.23	1.11
1	B	203[B]	SUN	O-C	17.00	1.23	1.11
1	A	203[A]	SEN	CA-C	4.69	1.57	1.48
1	A	203[B]	SUN	CA-C	4.69	1.57	1.48
1	B	203[A]	SEN	P-OG	4.18	1.61	1.57
1	B	203[A]	SEN	CA-C	3.95	1.55	1.48
1	B	203[B]	SUN	CA-C	3.95	1.55	1.48
1	A	203[A]	SEN	P-OG	3.86	1.61	1.57
1	A	203[B]	SUN	P1-O2	2.50	1.65	1.57
1	B	203[B]	SUN	P1-O1	2.16	1.48	1.46
1	B	203[B]	SUN	P1-O2	2.03	1.63	1.57

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203[B]	SUN	OG-P1-O1	-7.38	101.96	115.95
1	A	203[B]	SUN	O2-P1-OG	6.33	115.35	99.93
1	B	203[A]	SEN	P-N1-C1	-5.87	107.39	119.86
1	B	203[B]	SUN	O2-P1-OG	5.39	113.06	99.93
1	B	203[B]	SUN	P1-N1-C1	-5.32	108.55	119.86
1	B	203[B]	SUN	OG-P1-O1	-5.25	105.99	115.95
1	A	203[A]	SEN	P-N1-C1	-4.67	109.95	119.86
1	A	203[B]	SUN	P1-N1-C2	-4.56	110.17	119.86
1	B	203[B]	SUN	P1-N1-C2	-4.29	110.74	119.86
1	A	203[B]	SUN	P1-N1-C1	-4.17	111.00	119.86
1	B	203[A]	SEN	P-N1-C2	-3.78	111.83	119.86
1	A	203[A]	SEN	P-N1-C2	-3.61	112.19	119.86
1	A	203[B]	SUN	O2-P1-O1	-2.94	110.38	115.95
1	B	203[A]	SEN	O2-P-O3	2.66	118.52	109.84
1	A	203[A]	SEN	OG-P-O3	-2.65	110.92	115.95
1	B	203[A]	SEN	C-CA-N	-2.63	111.20	113.83
1	B	203[B]	SUN	C-CA-N	-2.63	111.20	113.83
1	B	203[A]	SEN	OG-P-O3	-2.62	110.99	115.95
1	A	203[B]	SUN	P1-O2-C3	2.60	127.84	120.70
1	A	203[B]	SUN	O2-P1-N1	2.03	112.17	105.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
2	NAG	A	549	1	12,14,15	0.62	0	15,19,21	2.60	4 (26%)
4	P6G	A	551	-	18,18,18	1.72	5 (27%)	17,17,17	2.12	8 (47%)
5	PG4	B	549	-	12,12,12	0.92	0	11,11,11	0.34	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	NAG	A	549	1	-	0/6/23/26	0/1/1/1
4	P6G	A	551	-	-	0/16/16/16	0/0/0/0
5	PG4	B	549	-	-	0/10/10/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	551	P6G	C17-C18	-2.95	1.33	1.49
4	A	551	P6G	C3-C2	-2.81	1.34	1.49
4	A	551	P6G	C9-C8	-2.80	1.34	1.48
4	A	551	P6G	C15-C14	-2.67	1.34	1.48
4	A	551	P6G	C6-C5	-2.66	1.34	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	549	NAG	O5-C5-C6	8.00	115.38	106.98
2	A	549	NAG	C3-C4-C5	-3.52	103.91	110.20
4	A	551	P6G	O7-C8-C9	3.28	125.37	110.47
4	A	551	P6G	O13-C14-C15	3.12	124.65	110.47
4	A	551	P6G	O16-C15-C14	3.10	124.54	110.47
2	A	549	NAG	O5-C5-C4	-3.02	106.82	110.65
4	A	551	P6G	O7-C6-C5	2.85	123.42	110.47
4	A	551	P6G	O10-C9-C8	2.84	123.33	110.47
2	A	549	NAG	C3-C2-N2	-2.80	107.50	111.76
4	A	551	P6G	O4-C5-C6	2.65	122.48	110.47
4	A	551	P6G	C5-O4-C3	2.27	123.38	113.38
4	A	551	P6G	O4-C3-C2	2.12	120.81	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	538/549 (97%)	-0.24	9 (1%) 67 69	30, 45, 67, 92	6 (1%)
1	B	534/549 (97%)	-0.13	11 (2%) 60 63	33, 50, 71, 97	4 (0%)
All	All	1072/1098 (97%)	-0.19	20 (1%) 64 66	30, 47, 70, 97	10 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	THR	6.3
1	B	544	ALA	5.1
1	A	496	LYS	4.3
1	B	541	SER	3.9
1	A	540	LEU	3.7
1	A	543	THR	3.6
1	A	495	SER	3.3
1	A	541	SER	3.1
1	B	542	ALA	3.0
1	A	76	LEU	2.9
1	A	497	SER	2.9
1	B	497	SER	2.9
1	A	493	ARG	2.7
1	A	542	ALA	2.6
1	B	493	ARG	2.6
1	B	4	GLU	2.5
1	B	42	VAL	2.3
1	B	492	PRO	2.2
1	B	337	TYR	2.2
1	B	165	ARG	2.0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEN	A	203[A]	12/13	0.19	-	38,39,39,39	12
1	SEN	B	203[A]	12/13	0.12	-	38,40,40,41	12
1	SUN	B	203[B]	14/15	0.15	-	38,40,41,42	14
1	SUN	A	203[B]	14/15	0.22	-	39,39,40,40	14

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PG4	B	549	13/13	0.40	-	96,102,110,110	0
2	NAG	A	549	14/15	0.40	-	85,92,93,94	0
4	P6G	A	551	19/19	0.24	-	67,72,78,78	0
3	CL	A	550	1/1	0.14	-	87,87,87,87	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.