



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 01:21 PM EDT

PDB ID : 3DL4  
Title : Non-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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.17.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

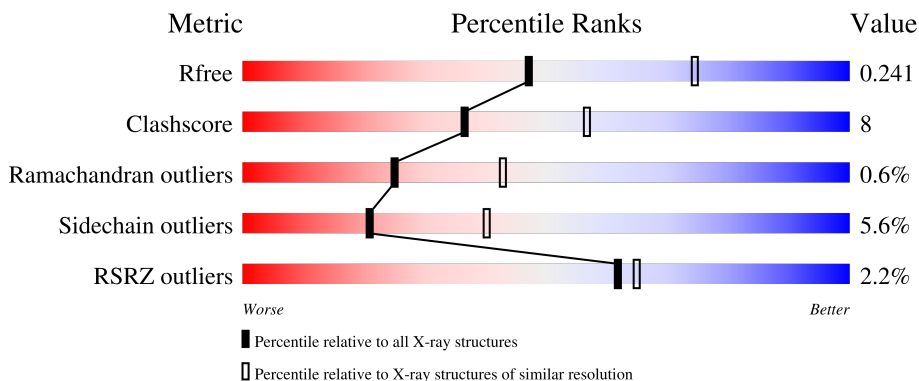
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	 2% 78% 17% ..
1	B	548	 2% 80% 17% ..

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	P6G	B	550	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8731 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.

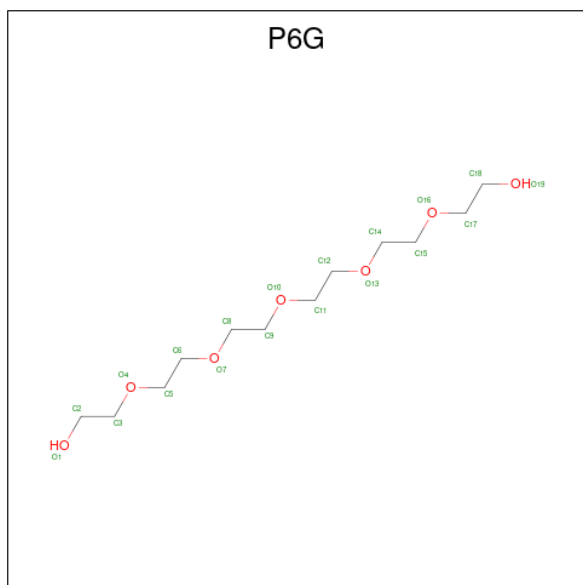
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	537	4240	2719	734	771	1	15	0	6	0
1	B	537	4220	2709	729	766	1	15	0	5	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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 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
2	B	1	Total	C O	0	0
			19	12 7		

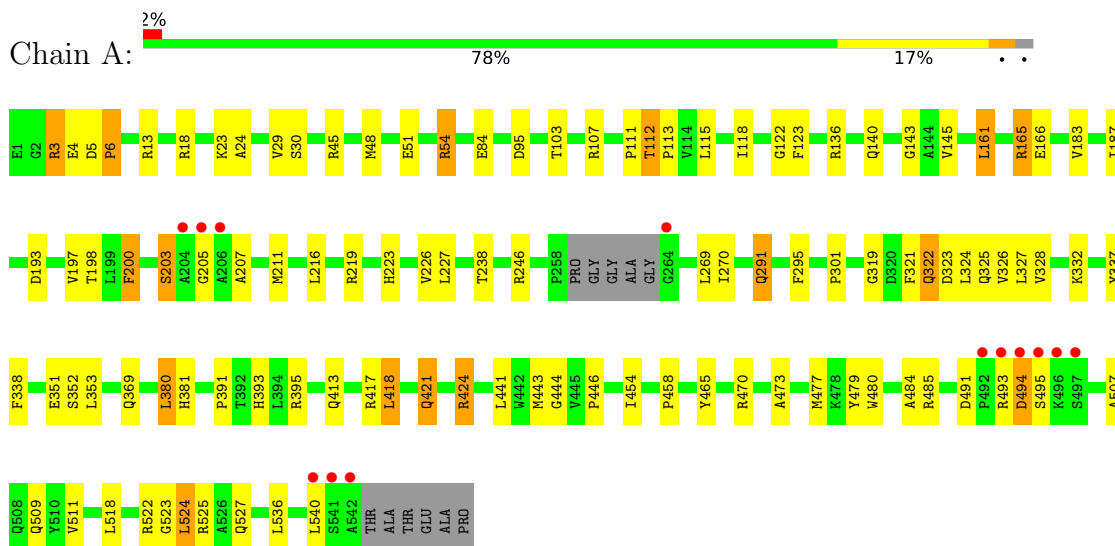
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total	O	0	0
			137	137		
3	B	115	Total	O	0	0
			115	115		

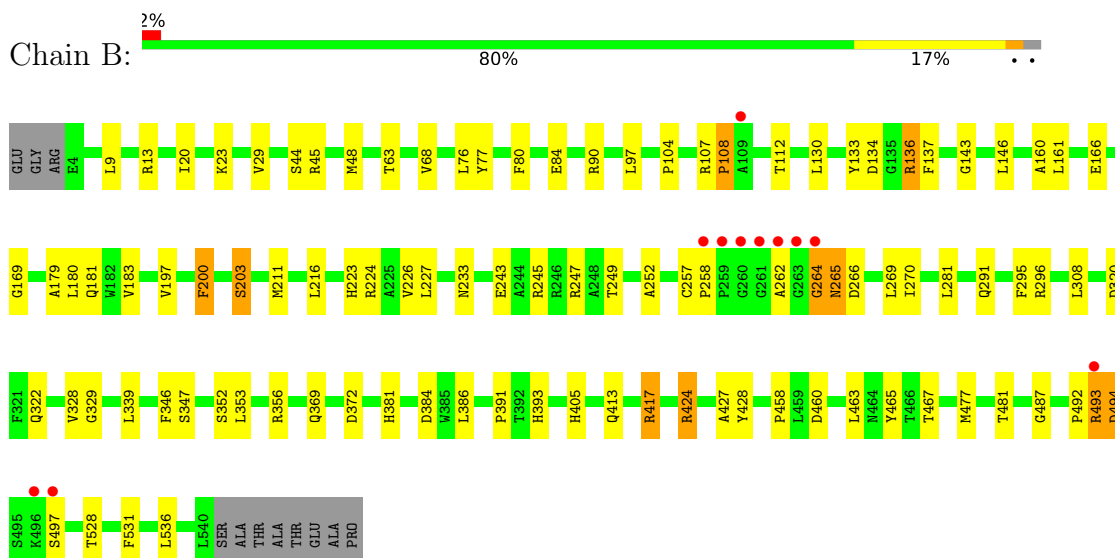
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acetylcholinesterase



- Molecule 1: Acetylcholinesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.62Å 112.94Å 226.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.17 – 2.50 29.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.17-2.50) 99.5 (29.17-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.245 0.191 , 0.241	Depositor DCC
$R_{free}$ test set	1422 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SUN, P6G

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	0.72	0/4364	0.76	2/5958 (0.0%)
1	B	0.70	0/4346	0.73	0/5938
All	All	0.71	0/8710	0.75	2/11896 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	95	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	161	LEU	CA-CB-CG	-5.00	103.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	497	SER	Peptide

### 5.2 Too-close contacts [i](#)

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	4240	0	4142	74	0
1	B	4220	0	4122	58	0
2	B	19	0	24	4	0
3	A	137	0	0	11	0
3	B	115	0	0	4	0
All	All	8731	0	8288	132	0

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 8.

All (132) 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:B:197:VAL:H	1:B:223:HIS:HD2	1.13	0.95
1:B:45[A]:ARG:NH1	1:B:48[A]:MET:SD	2.46	0.88
1:A:351[A]:GLU:OE2	3:A:552:HOH:O	1.91	0.87
1:A:197:VAL:H	1:A:223:HIS:HD2	1.23	0.83
1:A:54:ARG:HH11	1:A:54:ARG:CG	1.95	0.79
1:B:197:VAL:H	1:B:223:HIS:CD2	2.01	0.78
1:A:54:ARG:HH11	1:A:54:ARG:HG2	1.50	0.75
1:B:493:ARG:O	1:B:494:ASP:HB2	1.85	0.75
1:A:291:GLN:HE22	1:A:369:GLN:NE2	1.89	0.70
1:A:369:GLN:HB2	3:A:658:HOH:O	1.91	0.70
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.74	0.70
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.75	0.68
1:A:197:VAL:H	1:A:223:HIS:CD2	2.10	0.67
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.77	0.67
1:A:319:GLY:O	1:A:421:GLN:HG2	1.96	0.65
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.79	0.65
1:A:54:ARG:HH11	1:A:54:ARG:CB	2.10	0.64
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.33	0.63
1:B:320:ASP:OD1	1:B:322:GLN:HG2	1.98	0.62
1:B:245:ARG:O	1:B:249:THR:HG23	1.99	0.62
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.83	0.61
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.65	0.61
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.83	0.60
1:B:477:MET:O	1:B:481:THR:OG1	2.16	0.60
1:A:338:PHE:HB2	3:A:559:HOH:O	2.03	0.59
1:A:493:ARG:HB2	3:A:675:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:HD2	3:B:587:HOH:O	2.02	0.58
1:B:258:PRO:HD2	1:B:262:ALA:HB1	1.85	0.58
1:B:203:SUN:H3C2	3:B:655:HOH:O	2.03	0.57
1:B:112:THR:HG21	1:B:143:GLY:O	2.03	0.57
1:B:233:ASN:HD22	1:B:413:GLN:HE21	1.53	0.56
1:A:207:ALA:O	1:A:211:MET:HG2	2.06	0.56
1:A:493:ARG:O	1:A:495:SER:N	2.39	0.56
1:B:417:ARG:HA	1:B:417:ARG:HE	1.68	0.56
1:A:45:ARG:HH12	1:A:51:GLU:CD	2.09	0.56
1:B:107:ARG:HB3	3:B:570:HOH:O	2.05	0.55
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.88	0.55
1:A:54:ARG:HG2	1:A:54:ARG:NH1	2.16	0.55
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.89	0.55
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.42	0.55
1:B:20:ILE:HB	1:B:63:THR:HB	1.88	0.54
1:B:424:ARG:HH11	1:B:424:ARG:CG	2.21	0.54
1:A:527:GLN:HE21	2:B:550:P6G:H171	1.72	0.54
1:A:393:HIS:HD2	3:A:661:HOH:O	1.92	0.53
1:A:112:THR:HG21	1:A:143:GLY:O	2.09	0.53
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.39	0.52
1:A:48[B]:MET:SD	1:A:166:GLU:HA	2.49	0.51
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.93	0.51
1:A:319:GLY:O	1:A:421:GLN:CG	2.59	0.50
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.76	0.50
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.93	0.50
1:A:381:HIS:HA	2:B:550:P6G:H31	1.93	0.50
1:A:473:ALA:O	1:A:477:MET:HG3	2.12	0.50
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.93	0.50
1:B:393:HIS:HB3	3:B:616:HOH:O	2.12	0.50
1:B:136:ARG:HG2	1:B:137:PHE:N	2.27	0.49
1:B:424:ARG:HG3	1:B:424:ARG:NH1	2.27	0.49
1:A:29:VAL:CG1	1:A:140:GLN:HB2	2.43	0.48
1:A:291:GLN:HE22	1:A:369:GLN:HE22	1.61	0.48
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.94	0.48
1:A:337:TYR:HA	1:A:443:MET:CE	2.43	0.48
1:A:352:SER:O	1:A:395:ARG:HG3	2.14	0.48
1:B:328:VAL:O	1:B:427:ALA:HA	2.13	0.47
1:A:424:ARG:HD2	3:A:666:HOH:O	2.14	0.47
1:B:528:THR:O	1:B:531:PHE:HB3	2.14	0.47
1:A:107:ARG:HG3	3:A:554:HOH:O	2.14	0.47
1:A:115:LEU:HD23	1:A:198:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:OD2	1:B:136:ARG:HD2	2.14	0.47
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.47
1:B:233:ASN:ND2	1:B:413:GLN:HE21	2.13	0.47
1:B:252:ALA:HB2	1:B:269:LEU:HD21	1.97	0.47
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.50	0.47
1:B:76:LEU:HD23	1:B:77:TYR:CE2	2.49	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.50	0.47
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.32	0.47
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.97	0.47
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.97	0.46
1:B:264:GLY:HA2	1:B:265:ASN:HA	1.66	0.46
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.49	0.46
1:B:381:HIS:CE1	2:B:550:P6G:H181	2.51	0.46
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.16	0.46
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.51	0.45
1:A:23:LYS:HG2	3:A:563:HOH:O	2.16	0.45
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.99	0.45
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.98	0.45
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.98	0.45
1:A:122:GLY:O	1:A:123:PHE:HB2	2.17	0.44
1:A:507:ALA:O	1:A:522:ARG:NH1	2.50	0.44
1:A:183:VAL:HG13	1:A:187:ILE:HB	1.99	0.44
1:A:111:PRO:HB2	1:A:193:ASP:HB2	1.98	0.44
1:A:107:ARG:CG	3:A:554:HOH:O	2.64	0.44
1:B:80:PHE:O	1:B:84:GLU:HG2	2.19	0.43
1:A:291:GLN:NE2	1:A:369:GLN:NE2	2.63	0.43
1:A:24:ALA:HB3	1:A:140:GLN:HG3	2.01	0.43
1:B:257:CYS:HA	1:B:258:PRO:HA	1.85	0.43
1:A:479:TYR:OH	1:A:518:LEU:HG	2.18	0.43
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.54	0.43
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.70	0.43
1:A:203:SUN:H4C2	1:A:338:PHE:HZ	1.84	0.43
1:A:161:LEU:HD12	1:A:270:ILE:HD11	2.01	0.43
1:A:238:THR:HA	1:A:301:PRO:O	2.19	0.43
1:B:424:ARG:CG	1:B:424:ARG:NH1	2.81	0.43
1:A:219:ARG:HD2	1:A:219:ARG:HA	1.73	0.42
1:A:491:ASP:HB3	1:A:494:ASP:HB3	2.01	0.42
1:A:227:LEU:HD12	1:A:227:LEU:N	2.33	0.42
1:B:243:GLU:O	1:B:247:ARG:HG3	2.19	0.42
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.82	0.42
1:A:324:LEU:HG	1:A:326:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:PRO:HD2	1:B:108:PRO:HD3	2.00	0.42
1:B:179:ALA:O	1:B:183:VAL:HG23	2.19	0.42
1:B:493:ARG:O	1:B:494:ASP:CB	2.60	0.42
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.02	0.42
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.50	0.42
1:A:84:GLU:HA	1:A:84:GLU:OE1	2.19	0.42
1:A:511:VAL:HG11	1:A:518:LEU:HD13	2.01	0.42
1:B:384:ASP:C	1:B:384:ASP:OD1	2.58	0.42
1:A:321:PHE:CD2	1:A:418:LEU:HD12	2.54	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD2	1.87	0.41
1:A:118:ILE:O	1:A:205:GLY:HA3	2.19	0.41
1:A:444:GLY:O	1:A:446:PRO:HD3	2.20	0.41
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.32	0.41
1:A:291:GLN:HE21	1:A:291:GLN:HB2	1.62	0.41
1:A:413[B]:GLN:NE2	3:A:624:HOH:O	2.54	0.41
1:B:424:ARG:HH11	1:B:424:ARG:HB2	1.86	0.41
1:B:265:ASN:CG	1:B:266:ASP:H	2.24	0.41
1:A:165:ARG:CZ	1:A:165:ARG:HB3	2.51	0.41
1:A:380:LEU:HB3	2:B:550:P6G:H51	2.02	0.41
1:A:509:GLN:HB2	3:A:681:HOH:O	2.21	0.40
1:A:524:LEU:O	1:A:525:ARG:C	2.59	0.40
1:B:97:LEU:HD23	1:B:97:LEU:HA	1.90	0.40
1:A:326:VAL:HG12	1:A:328:VAL:HG13	2.04	0.40
1:B:200:PHE:CB	1:B:226:VAL:HB	2.51	0.40

There are no symmetry-related clashes.

## 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	538/548 (98%)	511 (95%)	24 (4%)	3 (1%)	25 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	539/548 (98%)	508 (94%)	28 (5%)	3 (1%)	25	43
All	All	1077/1096 (98%)	1019 (95%)	52 (5%)	6 (1%)	25	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	ASP
1	B	494	ASP
1	A	322	GLN
1	A	523	GLY
1	B	108	PRO
1	B	264	GLY

### 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	446/445 (100%)	422 (95%)	24 (5%)	22	42
1	B	443/445 (100%)	418 (94%)	25 (6%)	21	40
All	All	889/890 (100%)	840 (94%)	49 (6%)	21	41

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	6	PRO
1	A	13	ARG
1	A	30	SER
1	A	54	ARG
1	A	112	THR
1	A	165	ARG
1	A	200	PHE
1	A	216	LEU
1	A	246	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	291	GLN
1	A	295	PHE
1	A	322	GLN
1	A	323	ASP
1	A	325	GLN
1	A	332	LYS
1	A	380	LEU
1	A	418	LEU
1	A	421	GLN
1	A	424	ARG
1	A	441	LEU
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	9	LEU
1	B	23	LYS
1	B	44	SER
1	B	136	ARG
1	B	146	LEU
1	B	180	LEU
1	B	181	GLN
1	B	200	PHE
1	B	216	LEU
1	B	265	ASN
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	347	SER
1	B	352	SER
1	B	356	ARG
1	B	372	ASP
1	B	386	LEU
1	B	417	ARG
1	B	424	ARG
1	B	467	THR
1	B	492	PRO
1	B	493	ARG
1	B	536	LEU

Sometimes 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	509	GLN
1	B	223	HIS
1	B	265	ASN
1	B	291	GLN
1	B	405	HIS
1	B	413	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](#)

2 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	SUN	B	203	1	11,13,14	0.65	0	11,17,19	2.32	4 (36%)
1	SUN	A	203	1	11,13,14	0.59	0	11,17,19	2.26	4 (36%)

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	SUN	B	203	1	-	2/15/18/20	-
1	SUN	A	203	1	-	2/15/18/20	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	SUN	OG-CB-CA	4.80	112.81	108.14
1	A	203	SUN	O1-P1-N1	4.07	119.64	113.28
1	A	203	SUN	OG-P1-O1	-3.84	102.99	115.61
1	B	203	SUN	OG-P1-O1	-3.83	103.04	115.61
1	A	203	SUN	OG-CB-CA	3.21	111.27	108.14
1	A	203	SUN	O2-P1-OG	2.75	109.63	100.53
1	B	203	SUN	O2-P1-OG	2.72	109.54	100.53
1	B	203	SUN	P1-O2-C3	-2.71	113.22	120.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	SUN	C4-C3-O2-P1
1	A	203	SUN	N-CA-CB-OG
1	B	203	SUN	N-CA-CB-OG
1	B	203	SUN	C1-N1-P1-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203	SUN	1	0
1	A	203	SUN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand 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
2	P6G	B	550	-	18,18,18	1.72	5 (27%)	17,17,17	2.36	9 (52%)

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	P6G	B	550	-	-	8/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	550	P6G	C9-C8	-2.87	1.34	1.49
2	B	550	P6G	C17-C18	-2.81	1.34	1.49
2	B	550	P6G	C3-C2	-2.77	1.34	1.49
2	B	550	P6G	C15-C14	-2.75	1.34	1.49
2	B	550	P6G	C6-C5	-2.47	1.36	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	P6G	O7-C8-C9	3.55	126.39	110.39
2	B	550	P6G	O7-C6-C5	3.30	125.29	110.39
2	B	550	P6G	O16-C15-C14	3.06	124.17	110.39
2	B	550	P6G	O13-C14-C15	2.98	123.83	110.39
2	B	550	P6G	O10-C9-C8	2.89	123.42	110.39
2	B	550	P6G	O4-C3-C2	2.78	122.29	110.07
2	B	550	P6G	C5-O4-C3	2.71	125.05	113.29
2	B	550	P6G	O4-C5-C6	2.64	122.28	110.39
2	B	550	P6G	O16-C17-C18	2.32	120.25	110.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	550	P6G	O7-C8-C9-O10
2	B	550	P6G	O13-C14-C15-O16
2	B	550	P6G	O4-C5-C6-O7
2	B	550	P6G	O10-C11-C12-O13
2	B	550	P6G	C6-C5-O4-C3

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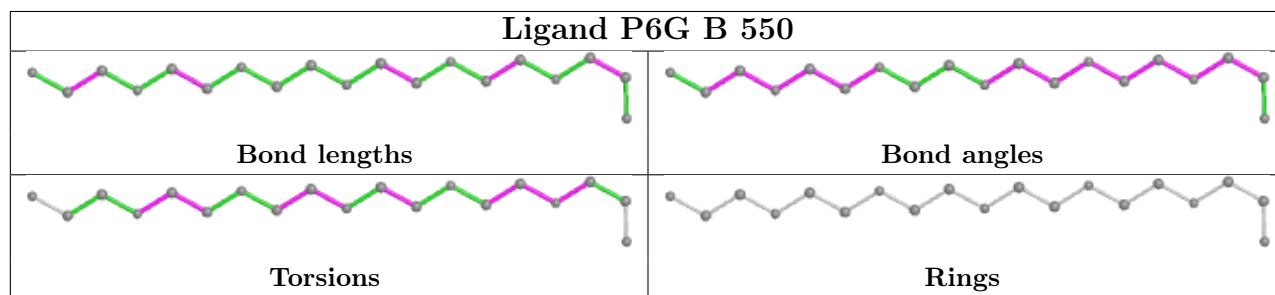
Mol	Chain	Res	Type	Atoms
2	B	550	P6G	C2-C3-O4-C5
2	B	550	P6G	C14-C15-O16-C17
2	B	550	P6G	C12-C11-O10-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	550	P6G	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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

### 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	536/548 (97%)	-0.30	13 (2%) 59 62	28, 42, 64, 90	0
1	B	536/548 (97%)	-0.17	11 (2%) 63 66	29, 47, 68, 98	0
All	All	1072/1096 (97%)	-0.24	24 (2%) 62 65	28, 44, 68, 98	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ALA	7.4
1	B	260	GLY	6.8
1	B	259	PRO	6.8
1	B	261	GLY	6.2
1	B	264	GLY	5.3
1	A	495	SER	5.0
1	A	496	LYS	4.8
1	A	493	ARG	3.9
1	B	496	LYS	3.9
1	A	541	SER	3.3
1	B	258	PRO	3.3
1	B	497	SER	3.3
1	A	264	GLY	3.1
1	A	497	SER	3.1
1	B	109	ALA	2.9
1	B	263	GLY	2.8
1	B	493	ARG	2.8
1	A	492	PRO	2.7
1	A	540	LEU	2.5
1	A	494	ASP	2.4
1	A	542	ALA	2.3
1	A	206	ALA	2.1
1	A	204	ALA	2.0
1	A	205	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	SUN	A	203	14/15	0.99	0.20	34,39,43,45	0
1	SUN	B	203	14/15	0.99	0.11	36,42,50,50	0

## 6.3 Carbohydrates [i](#)

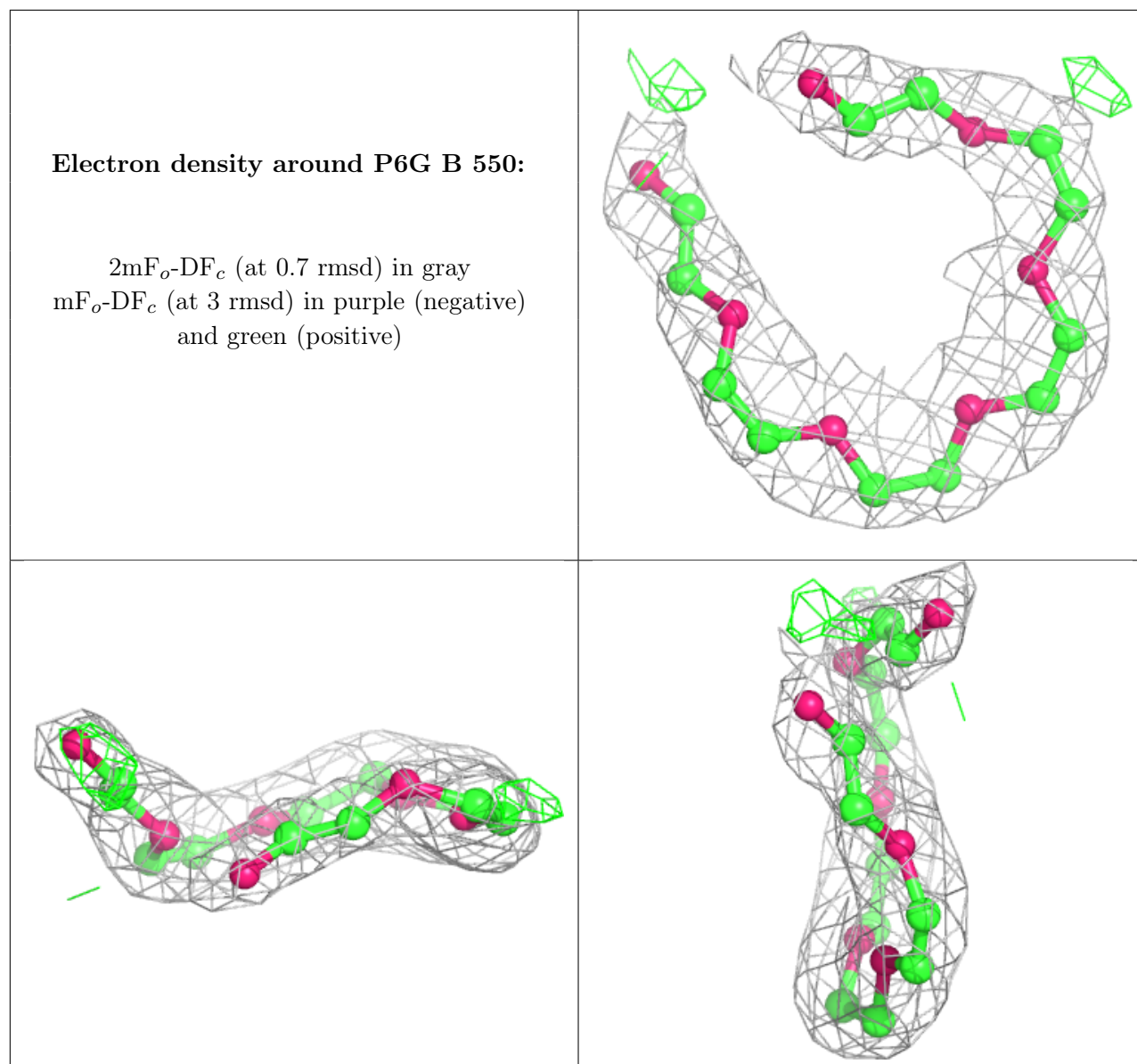
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	P6G	B	550	19/19	0.93	0.19	61,68,77,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.