



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:25 PM BST

PDB ID : 2Y2U  
Title : Nonaged form of Mouse Acetylcholinesterase inhibited by VX-Update  
Authors : Akfur, C.; Artursson, E.; Ekstrom, F.  
Deposited on : 2010-12-16  
Resolution : 2.60 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

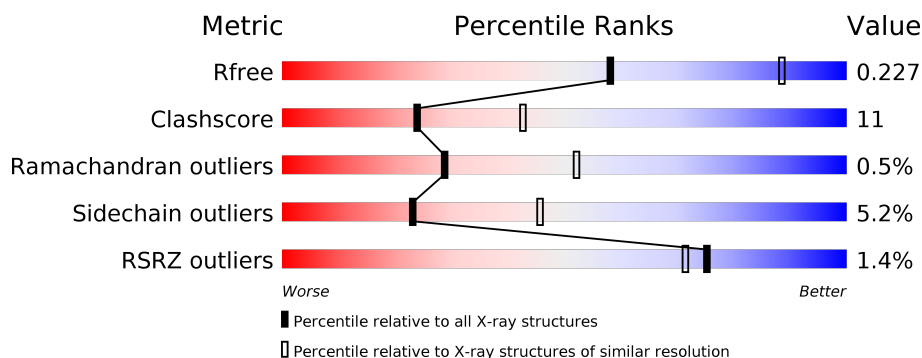
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	548	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <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	NAG	B	601	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8845 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	537	Total	C	N	O	P	S	0	3	1
			4211	2700	732	764	1	14			
1	B	532	Total	C	N	O	P	S	0	3	0
			4182	2683	724	760	1	14			

There are 10 discrepancies between the modelled and reference sequences:

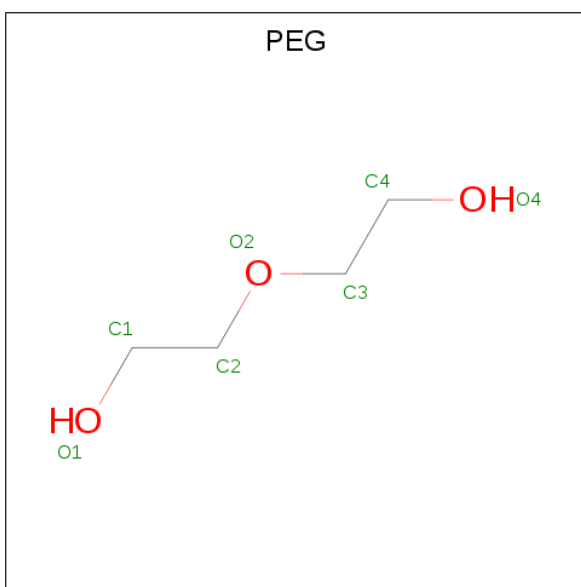
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLU	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



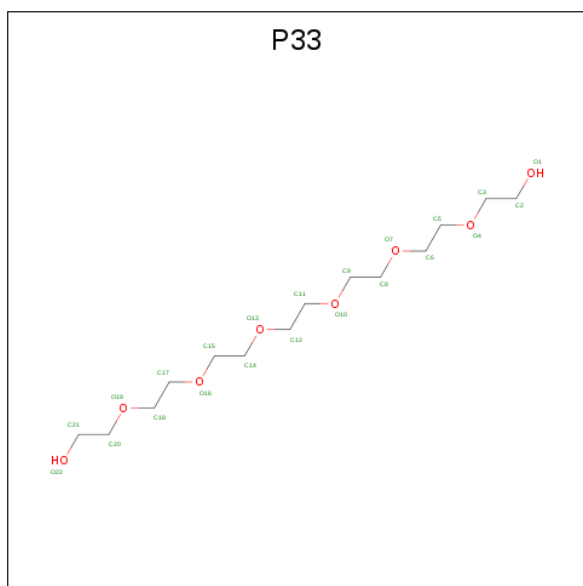
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	13	7		

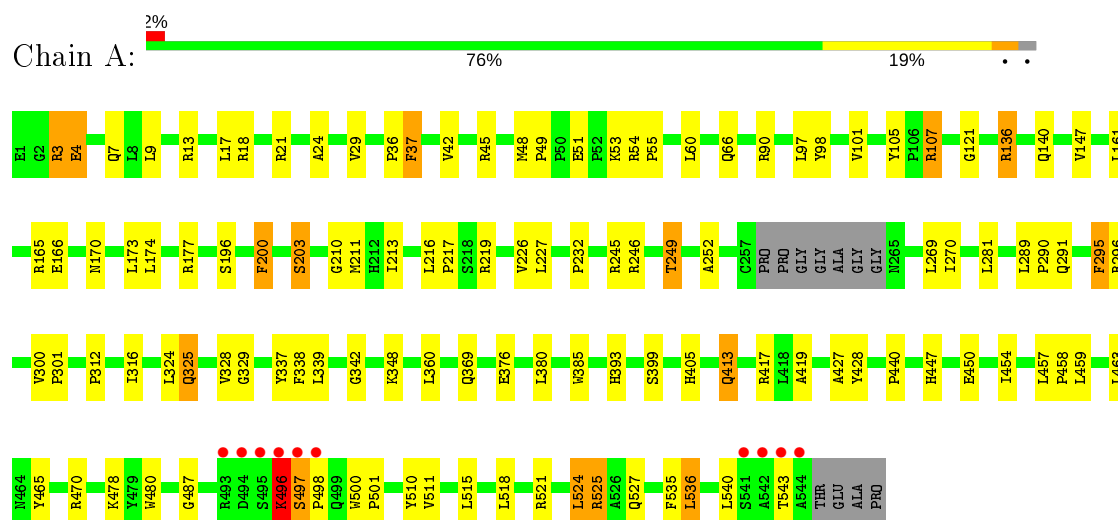
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total	O	0	0
			207	207		
5	B	150	Total	O	0	0
			150	150		

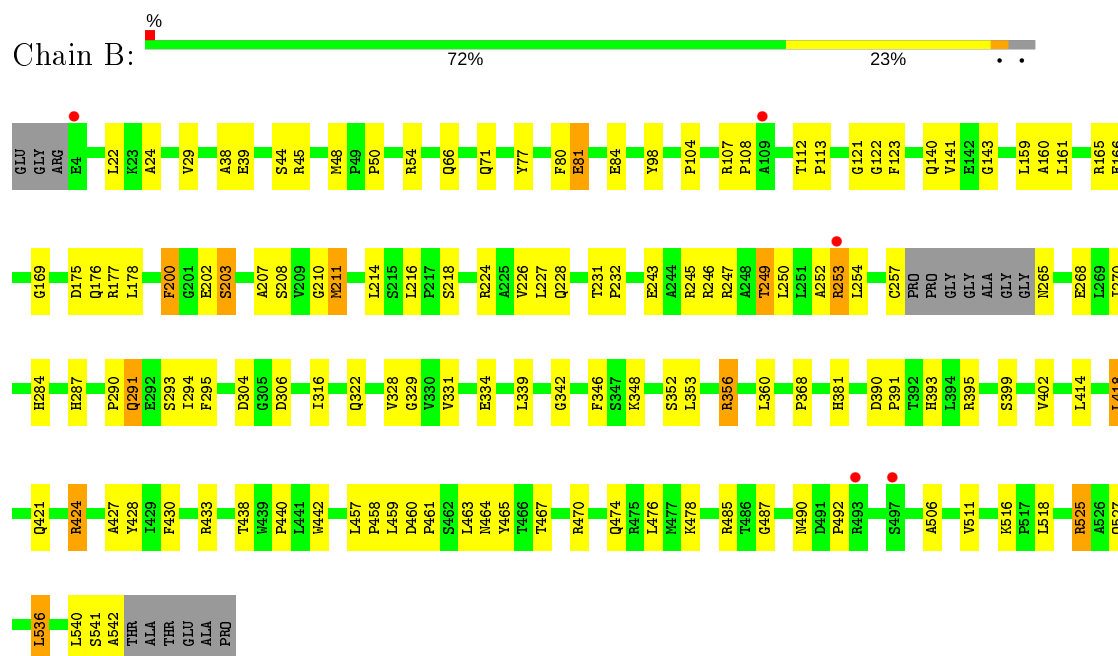
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	78.91Å 110.37Å 227.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 2.60 28.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.76-2.60) 99.8 (28.76-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, $R_{free}$	0.188 , 0.237 0.182 , 0.227	Depositor DCC
$R_{free}$ test set	1234 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P33, PEG, NAG, SVX

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	0.44	0/4326	0.60	0/5910
1	B	0.41	0/4294	0.58	0/5868
All	All	0.42	0/8620	0.59	0/11778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4211	0	4092	92	0
1	B	4182	0	4053	93	0
2	A	28	0	26	0	0
2	B	14	0	13	1	0
3	A	19	0	25	1	0
3	B	14	0	20	0	0
4	B	20	0	25	3	0
5	A	207	0	0	7	0
5	B	150	0	0	7	0
All	All	8845	0	8254	186	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 11.

All (186) 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:3:ARG:HH11	1:A:3:ARG:HG3	1.13	1.10
1:B:424:ARG:HH11	1:B:424:ARG:HG2	0.86	1.02
1:A:48:MET:HE1	1:A:166:GLU:HA	1.45	0.96
1:B:424:ARG:CG	1:B:424:ARG:HH11	1.79	0.96
1:B:424:ARG:HG2	1:B:424:ARG:NH1	1.66	0.92
1:B:245:ARG:O	1:B:249:THR:HG23	1.77	0.84
1:A:3:ARG:NH1	1:A:3:ARG:HG3	1.93	0.84
1:B:48:MET:HE1	1:B:166:GLU:HA	1.58	0.84
1:A:210:GLY:HA3	1:A:232:PRO:HG3	1.60	0.83
1:A:245:ARG:O	1:A:249:THR:HG23	1.81	0.81
1:A:3:ARG:CG	1:A:3:ARG:HH11	1.98	0.75
1:A:497:SER:H	1:A:498:PRO:HA	1.51	0.75
2:B:601:NAG:H61	5:B:2147:HOH:O	1.85	0.74
1:B:348:LYS:O	1:B:440:PRO:HG3	1.89	0.73
1:A:497:SER:N	1:A:498:PRO:HA	2.04	0.72
1:B:390:ASP:OD2	1:B:393[A]:HIS:ND1	2.17	0.72
1:A:525:ARG:HG2	1:A:525:ARG:HH11	1.57	0.69
1:B:45:ARG:HG2	5:B:2024:HOH:O	1.90	0.69
1:A:447[B]:HIS:HE1	5:A:2187:HOH:O	1.75	0.68
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.73	0.68
1:A:45:ARG:HD2	1:A:51:GLU:OE1	1.95	0.66
1:A:497:SER:H	1:A:498:PRO:CA	2.09	0.65
1:A:338:PHE:CE1	1:A:447[B]:HIS:CD2	2.86	0.63
1:A:525:ARG:CG	1:A:525:ARG:HH11	2.13	0.62
1:A:49:PRO:HB3	1:A:174:LEU:HD12	1.81	0.62
1:B:207:ALA:O	1:B:211:MET:HG2	1.98	0.62
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.34	0.62
1:B:48:MET:HE1	1:B:166:GLU:CA	2.31	0.61
1:B:50:PRO:HG3	1:B:175:ASP:OD1	2.00	0.61
1:A:393[B]:HIS:CD2	5:A:2170:HOH:O	2.52	0.60
1:B:525:ARG:HH11	1:B:525:ARG:HG2	1.66	0.59
3:A:1546:PEG:H21	5:A:2169:HOH:O	2.02	0.59
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.39	0.58
1:A:36:PRO:O	1:A:97:LEU:O	2.22	0.58
1:A:497:SER:N	1:A:498:PRO:CA	2.67	0.58
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.86	0.57
1:A:338:PHE:CE1	1:A:447[B]:HIS:HD2	2.23	0.57
1:A:213:ILE:O	1:A:219:ARG:HD3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD12	1:A:470:ARG:HG2	1.87	0.56
1:A:216:LEU:HB3	1:A:217:PRO:HD3	1.88	0.56
1:B:346:PHE:HA	1:B:352:SER:OG	2.05	0.56
1:A:90:ARG:NE	5:A:2033:HOH:O	2.39	0.56
1:B:203:SVX:H1C1	5:B:2062:HOH:O	2.08	0.54
1:B:48:MET:HE1	1:B:165:ARG:O	2.07	0.54
1:B:253:ARG:HB3	1:B:253:ARG:NH1	2.22	0.54
1:A:210:GLY:CA	1:A:232:PRO:HG3	2.36	0.53
1:B:252:ALA:HB1	1:B:257:CYS:HB2	1.90	0.53
1:B:214:LEU:HD21	1:B:316:ILE:HG22	1.90	0.53
1:B:356:ARG:O	1:B:360:LEU:HG	2.08	0.53
1:B:81:GLU:HG2	1:B:438:THR:HG21	1.90	0.53
1:A:496:LYS:HD3	1:A:498:PRO:HA	1.89	0.53
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.91	0.53
1:A:252:ALA:HB1	1:A:269:LEU:HD11	1.90	0.52
1:A:527:GLN:HE21	4:B:1545:P33:H31	1.74	0.52
1:A:200:PHE:CB	1:A:226:VAL:HB	2.40	0.52
1:A:419:ALA:O	5:A:2176:HOH:O	2.19	0.52
1:B:80:PHE:O	1:B:84:GLU:HG2	2.10	0.52
1:A:21:ARG:HG3	1:A:105:TYR:CE2	2.45	0.52
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.44	0.52
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.39	0.52
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.45	0.51
1:B:541:SER:O	1:B:542:ALA:HB2	2.10	0.51
1:A:166:GLU:HG2	1:A:270:ILE:HD12	1.92	0.51
1:A:48:MET:HE1	1:A:165:ARG:O	2.10	0.51
1:A:203:SVX:OG	1:A:447[A]:HIS:NE2	2.43	0.51
1:B:231:THR:HG22	1:B:414:LEU:HD22	1.92	0.51
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.45	0.51
1:A:376:GLU:O	1:A:380:LEU:HG	2.11	0.51
1:A:393[B]:HIS:HD2	5:A:2170:HOH:O	1.90	0.51
1:B:203:SVX:H1C3	5:B:2114:HOH:O	2.11	0.51
1:A:48:MET:CE	1:A:166:GLU:HA	2.29	0.50
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.46	0.50
1:B:265:ASN:HB3	1:B:268:GLU:OE1	2.12	0.50
1:B:22:LEU:HB2	1:B:29:VAL:HG22	1.92	0.50
1:A:348:LYS:O	1:A:440:PRO:HG3	2.11	0.50
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.95	0.49
1:B:121:GLY:HA2	1:B:203:SVX:H1C2	1.95	0.49
1:B:112:THR:HG21	1:B:143:GLY:O	2.13	0.49
1:A:413:GLN:O	1:A:417:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ARG:CG	1:A:525:ARG:NH1	2.70	0.49
1:B:200:PHE:CB	1:B:226:VAL:HB	2.42	0.49
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.94	0.49
1:B:506:ALA:HB3	5:B:2126:HOH:O	2.13	0.49
1:A:535:PHE:CD2	4:B:1545:P33:H91	2.47	0.49
1:B:331:VAL:HG22	1:B:334:GLU:OE2	2.13	0.49
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.94	0.49
1:A:213:ILE:HD13	1:A:324:LEU:HD21	1.95	0.48
1:A:496:LYS:HE3	1:A:496:LYS:HA	1.94	0.48
1:B:122:GLY:O	1:B:123:PHE:HB2	2.13	0.48
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.95	0.48
1:B:166:GLU:HB2	1:B:270:ILE:HD13	1.94	0.48
1:A:3:ARG:CG	1:A:3:ARG:NH1	2.63	0.48
1:A:48:MET:HE1	1:A:166:GLU:CA	2.32	0.48
1:B:293:SER:HB3	1:B:368:PRO:HG3	1.94	0.48
1:B:243:GLU:O	1:B:247:ARG:HG3	2.14	0.48
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.96	0.48
1:B:284:HIS:HD2	1:B:287:HIS:HD2	1.61	0.48
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.49	0.48
1:B:414:LEU:HG	1:B:418:LEU:HD22	1.95	0.48
1:A:227:LEU:N	1:A:227:LEU:HD12	2.30	0.47
1:A:457:LEU:N	1:A:458:PRO:CD	2.78	0.47
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.94	0.47
1:B:253:ARG:HH11	1:B:253:ARG:HB3	1.78	0.47
1:A:338:PHE:CZ	1:A:447[B]:HIS:CD2	3.02	0.47
1:B:433:ARG:NH2	1:B:440:PRO:O	2.47	0.47
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.96	0.47
1:B:390:ASP:HA	1:B:391:PRO:HD3	1.75	0.47
1:A:450:GLU:OE1	1:A:450:GLU:N	2.36	0.47
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.97	0.47
1:A:447[B]:HIS:ND1	1:A:447[B]:HIS:C	2.69	0.46
1:B:328:VAL:O	1:B:427:ALA:HA	2.14	0.46
1:B:457:LEU:O	1:B:463:LEU:HD12	2.16	0.46
1:B:165:ARG:O	1:B:165:ARG:HG2	2.15	0.46
1:B:177:ARG:HD2	5:B:2066:HOH:O	2.15	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.50	0.46
1:A:121:GLY:HA2	1:A:203:SVX:H1C2	1.98	0.46
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.15	0.46
1:B:202:GLU:HA	1:B:228:GLN:O	2.15	0.46
1:B:525:ARG:HH11	1:B:525:ARG:CG	2.29	0.46
1:B:430:PHE:HE2	1:B:476:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.98	0.45
1:A:312:PRO:O	1:A:316:ILE:HG23	2.17	0.45
1:B:160:ALA:HB2	1:B:169:GLY:HA2	1.99	0.45
1:A:203:SVX:H2C2	1:A:203:SVX:H4C1	1.87	0.45
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.99	0.45
1:A:166:GLU:HG2	1:A:270:ILE:CD1	2.47	0.44
1:A:325:GLN:OE1	1:A:487:GLY:HA3	2.16	0.44
1:A:7[A]:GLN:OE1	1:A:107:ARG:HG2	2.17	0.44
1:B:141:VAL:HG21	1:B:459:LEU:HD23	1.99	0.44
1:A:369:GLN:HE22	1:A:405:HIS:CE1	2.36	0.44
1:A:42:VAL:O	1:A:45:ARG:HB2	2.17	0.44
1:B:200:PHE:HB3	1:B:226:VAL:HB	2.00	0.44
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.64	0.44
1:B:470:ARG:O	1:B:474:GLN:HG3	2.17	0.44
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.00	0.44
1:B:107:ARG:HB3	5:B:2047:HOH:O	2.17	0.44
1:A:177:ARG:NH1	5:A:2088:HOH:O	2.02	0.43
1:A:385:TRP:HD1	1:B:527:GLN:OE1	2.01	0.43
1:A:540:LEU:HA	1:A:540:LEU:HD23	1.85	0.43
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.54	0.43
1:B:460:ASP:HA	1:B:461:PRO:HD3	1.89	0.43
1:A:328:VAL:O	1:A:427:ALA:HA	2.18	0.43
1:A:360:LEU:HD23	1:A:360:LEU:N	2.33	0.43
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.54	0.43
1:A:17:LEU:HD23	1:A:60:LEU:HB3	2.00	0.43
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.80	0.43
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.18	0.42
1:B:470:ARG:HB3	1:B:470:ARG:HE	1.75	0.42
1:B:490:ASN:O	1:B:492:PRO:HD3	2.18	0.42
1:A:295:PHE:CE2	1:A:338:PHE:CE1	3.07	0.42
1:A:536:LEU:HD22	1:A:536:LEU:HA	1.77	0.42
1:B:294:ILE:HD11	1:B:402:VAL:HG21	2.01	0.42
1:B:457:LEU:N	1:B:458:PRO:CD	2.81	0.42
1:A:289:LEU:HA	1:A:290:PRO:HD3	1.91	0.42
1:B:39:GLU:OE1	1:B:54:ARG:HD3	2.19	0.42
1:B:113:PRO:HG2	1:B:485:ARG:HG2	2.01	0.42
1:A:161:LEU:HD12	1:A:270:ILE:HD11	2.02	0.42
1:A:500:TRP:HA	1:A:501:PRO:HD3	1.85	0.42
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.86	0.42
1:B:141:VAL:HG21	1:B:459:LEU:CD2	2.50	0.42
1:A:101:VAL:HG22	1:A:147:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:HIS:HD2	1:B:287:HIS:CD2	2.37	0.42
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.55	0.42
1:B:458:PRO:HA	1:B:465:TYR:HD2	1.83	0.42
1:B:159:LEU:C	1:B:159:LEU:HD23	2.40	0.41
1:A:4:GLU:HG2	1:A:9:LEU:HD21	2.00	0.41
1:B:381:HIS:HA	4:B:1545:P33:H32	2.01	0.41
1:B:227:LEU:N	1:B:227:LEU:HD12	2.35	0.41
1:B:210:GLY:CA	1:B:232:PRO:HG3	2.46	0.41
1:B:463:LEU:O	1:B:464:ASN:HB2	2.20	0.41
1:A:339:LEU:HD11	1:A:399:SER:HA	2.03	0.41
1:A:54:ARG:HA	1:A:55:PRO:HD3	1.96	0.41
1:B:243:GLU:OE2	1:B:290:PRO:HG3	2.20	0.41
1:B:540:LEU:HA	1:B:540:LEU:HD23	1.72	0.41
1:A:36:PRO:HB2	1:A:53:LYS:HG2	2.03	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.21	0.41
1:B:200:PHE:H	1:B:200:PHE:HD1	1.67	0.41
1:B:424:ARG:CG	1:B:424:ARG:NH1	2.50	0.41
1:A:252:ALA:CB	1:A:269:LEU:HD11	2.51	0.41
1:B:250:LEU:O	1:B:254:LEU:HG	2.21	0.41
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.20	0.41
1:B:339:LEU:HD11	1:B:399:SER:HA	2.03	0.41
1:A:463:LEU:HA	1:A:463:LEU:HD23	1.88	0.40
1:A:524:LEU:HD13	1:A:524:LEU:HA	1.84	0.40
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.52	0.40
1:A:13:ARG:HG3	1:A:13:ARG:O	2.22	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	535/548 (98%)	506 (95%)	25 (5%)	4 (1%)	22 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	530/548 (97%)	506 (96%)	23 (4%)	1 (0%)	47 71
All	All	1065/1096 (97%)	1012 (95%)	48 (4%)	5 (0%)	29 52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	497	SER
1	A	496	LYS
1	A	342	GLY
1	B	342	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	441/445 (99%)	418 (95%)	23 (5%)	23 46
1	B	438/445 (98%)	416 (95%)	22 (5%)	24 47
All	All	879/890 (99%)	834 (95%)	45 (5%)	23 46

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	37	PHE
1	A	107	ARG
1	A	136	ARG
1	A	173	LEU
1	A	196	SER
1	A	200	PHE
1	A	246	ARG
1	A	249	THR
1	A	281	LEU

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	295	PHE
1	A	296	ARG
1	A	325	GLN
1	A	337	TYR
1	A	413	GLN
1	A	478	LYS
1	A	496	LYS
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	A	543	THR
1	B	44	SER
1	B	71	GLN
1	B	81	GLU
1	B	200	PHE
1	B	211	MET
1	B	216	LEU
1	B	218	SER
1	B	246	ARG
1	B	249	THR
1	B	253	ARG
1	B	291	GLN
1	B	295	PHE
1	B	322	GLN
1	B	356	ARG
1	B	418	LEU
1	B	421	GLN
1	B	424	ARG
1	B	467	THR
1	B	478	LYS
1	B	516	LYS
1	B	525	ARG
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	B	287	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	SVX	B	203	1	10,11,12	1.30	1 (10%)	9,14,16	2.00	3 (33%)
1	SVX	A	203	1	10,11,12	1.21	1 (10%)	9,14,16	2.44	2 (22%)

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	SVX	B	203	1	-	2/9/12/14	-
1	SVX	A	203	1	-	3/9/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	SVX	P1-OG	2.71	1.61	1.58
1	A	203	SVX	P1-OG	2.53	1.61	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	SVX	OG-CB-CA	5.94	113.92	108.14
1	B	203	SVX	OG-CB-CA	4.43	112.46	108.14
1	A	203	SVX	O5-P1-O6	-2.41	106.19	113.10
1	B	203	SVX	OG-P1-O6	-2.07	107.17	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	SVX	O5-P1-C4	2.01	110.97	105.41

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	203	SVX	N-CA-CB-OG
1	A	203	SVX	N-CA-CB-OG
1	A	203	SVX	C2-O5-P1-C4
1	A	203	SVX	C2-O5-P1-O6
1	B	203	SVX	C2-O5-P1-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	203	SVX	3	0
1	A	203	SVX	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	601	1	14,14,15	0.63	0	17,19,21	1.04	1 (5%)
2	NAG	A	701	1	14,14,15	0.45	0	17,19,21	0.96	0
3	PEG	A	1547	-	4,4,6	0.38	0	3,3,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	P33	B	1545	-	19,19,21	0.52	0	18,18,20	1.49	1 (5%)
3	PEG	B	1543	-	6,6,6	0.52	0	5,5,5	1.78	2 (40%)
3	PEG	A	1546	-	6,6,6	0.51	0	5,5,5	1.70	1 (20%)
3	PEG	B	1544	-	6,6,6	0.51	0	5,5,5	1.42	0
2	NAG	A	601	1	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
3	PEG	A	1545	-	6,6,6	0.48	0	5,5,5	1.39	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	B	601	1	-	4/6/23/26	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	PEG	A	1547	-	-	1/2/2/4	-
4	P33	B	1545	-	-	3/17/17/19	-
3	PEG	B	1543	-	-	1/4/4/4	-
3	PEG	A	1546	-	-	1/4/4/4	-
3	PEG	B	1544	-	-	0/4/4/4	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	PEG	A	1545	-	-	1/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C1-O5-C5	4.08	117.72	112.19
2	B	601	NAG	C4-C3-C2	2.24	114.31	111.02
3	A	1546	PEG	O2-C3-C4	2.23	119.85	110.07
3	B	1543	PEG	O2-C2-C1	2.17	119.61	110.07
3	B	1543	PEG	O2-C3-C4	2.04	119.05	110.07
4	B	1545	P33	O4-C3-C2	2.04	119.04	110.07

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	NAG	C8-C7-N2-C2

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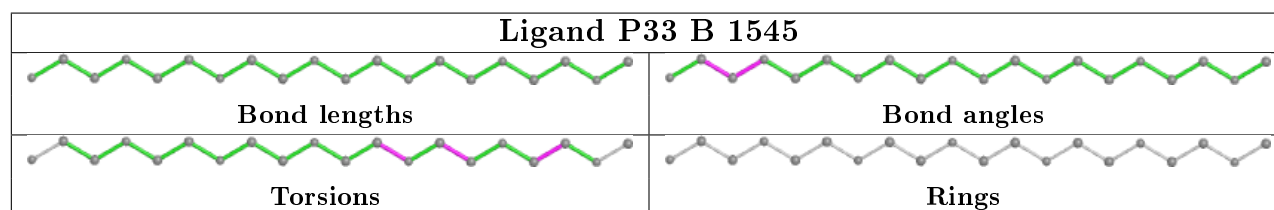
Mol	Chain	Res	Type	Atoms
2	A	701	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
2	A	701	NAG	O7-C7-N2-C2
3	B	1543	PEG	O2-C3-C4-O4
2	B	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
4	B	1545	P33	O13-C14-C15-O16
2	A	601	NAG	O5-C5-C6-O6
3	A	1545	PEG	O1-C1-C2-O2
2	B	601	NAG	C4-C5-C6-O6
4	B	1545	P33	C11-C12-O13-C14
4	B	1545	P33	O16-C17-C18-O19
3	A	1547	PEG	O2-C3-C4-O4
3	A	1546	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAG	1	0
4	B	1545	P33	3	0
3	A	1546	PEG	1	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

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, 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%)	-0.33	10 (1%) 66 62	35, 50, 71, 127	0
1	B	531/548 (96%)	-0.33	5 (0%) 84 82	37, 54, 76, 116	0
All	All	1067/1096 (97%)	-0.33	15 (1%) 75 71	35, 52, 75, 127	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	LYS	4.9
1	B	493	ARG	4.8
1	A	497	SER	4.0
1	A	495	SER	3.7
1	A	543	THR	3.4
1	A	541	SER	3.4
1	A	544	ALA	3.3
1	A	494	ASP	3.3
1	A	493	ARG	3.3
1	B	109	ALA	3.0
1	A	498	PRO	2.4
1	B	497	SER	2.3
1	B	253	ARG	2.1
1	A	542	ALA	2.1
1	B	4	GLU	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( $\text{\AA}^2$ )	Q<0.9
1	SVX	B	203	12/13	0.97	0.15	43,54,63,68	0
1	SVX	A	203	12/13	0.97	0.19	42,50,62,67	0

### 6.3 Carbohydrates [i](#)

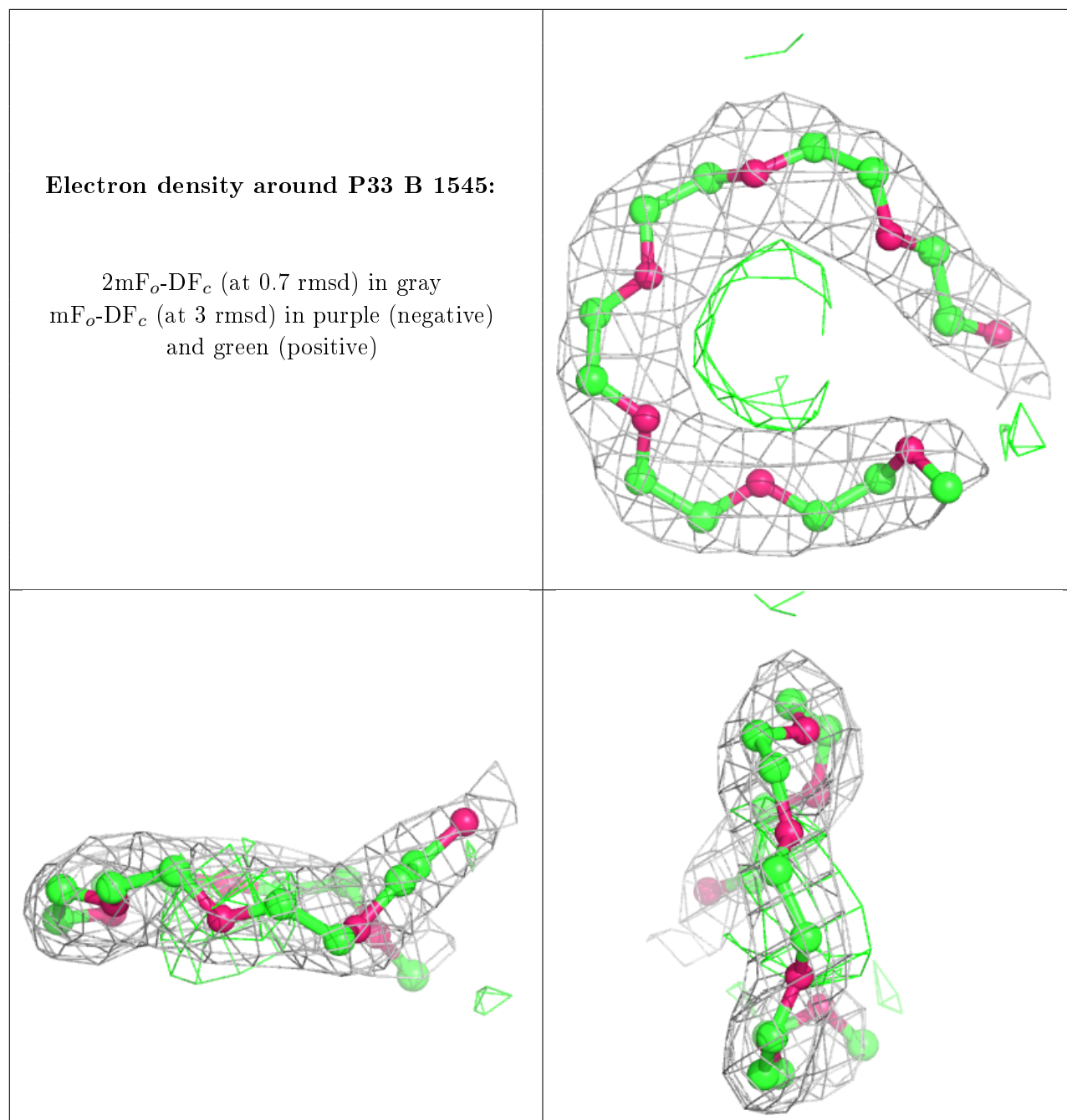
There are no monosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	601	14/15	0.63	0.41	73,95,104,110	0
3	PEG	B	1544	7/7	0.76	0.28	65,72,83,88	0
2	NAG	A	701	14/15	0.77	0.39	95,105,110,112	3
2	NAG	A	601	14/15	0.86	0.31	74,78,87,88	0
3	PEG	B	1543	7/7	0.86	0.25	60,70,74,77	0
3	PEG	A	1547	5/7	0.86	0.21	73,73,78,81	0
3	PEG	A	1545	7/7	0.93	0.33	62,70,80,83	0
3	PEG	A	1546	7/7	0.94	0.18	58,63,66,67	0
4	P33	B	1545	20/22	0.96	0.15	48,59,73,74	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 ⓘ

There are no such residues in this entry.