



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 2C0Q / pdb_00002c0q
Title : non-aged form of mouse acetylcholinesterase inhibited by tabun
Authors : Ekstrom, F.; Akfur, C.; Tunemalm, A.-K.; Lundberg, S.
Deposited on : 2005-09-07
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

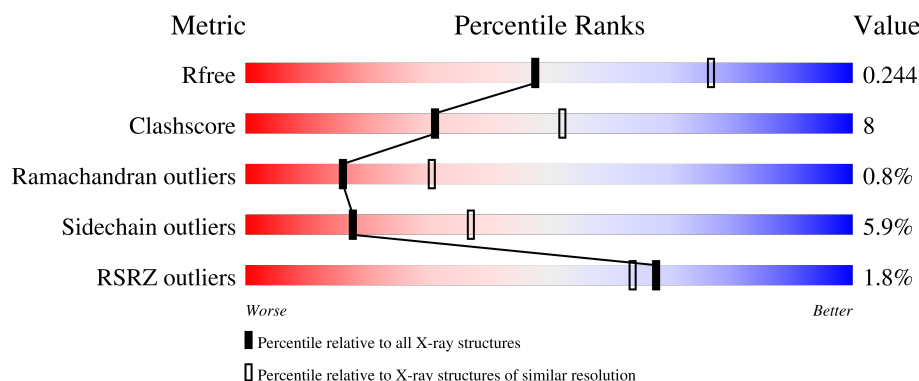
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	% 79% 16% ..
1	B	548	2% 77% 19% ..

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	P6G	B	1545	-	X	-	-

2 Entry composition [i](#)

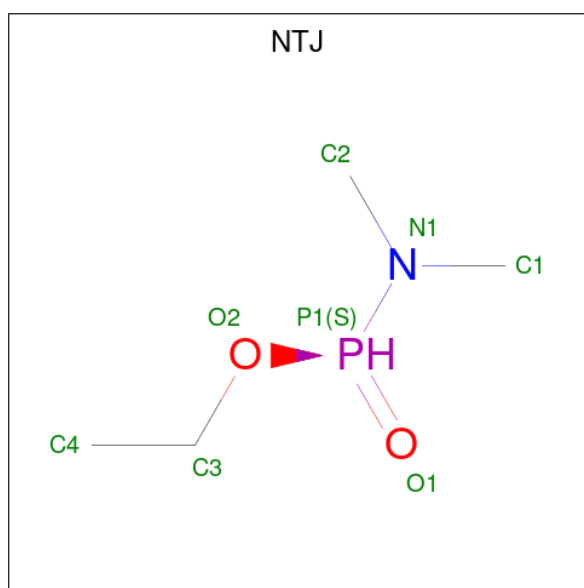
There are 4 unique types of molecules in this entry. The entry contains 8602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

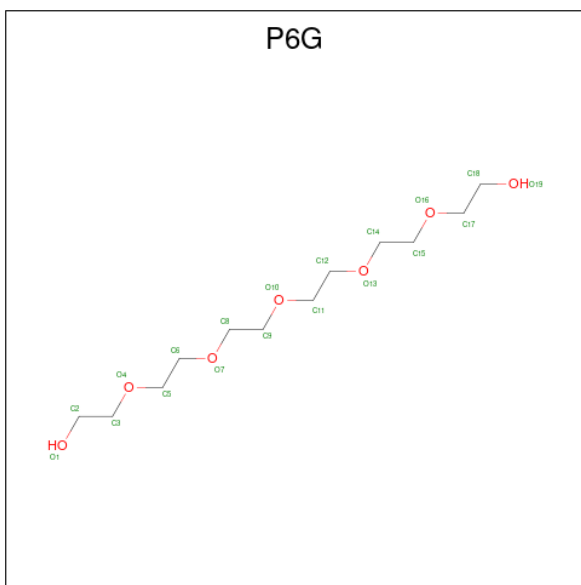
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	534	Total	C	N	O	S	0	0	1
			4159	2670	719	756	14			

- Molecule 2 is R-ETHYL N,N-DIMETHYLPHOSPHONAMIDATE (CCD ID: NTJ) (formula: $C_4H_{12}NO_2P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
2	B	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			19	12	7		

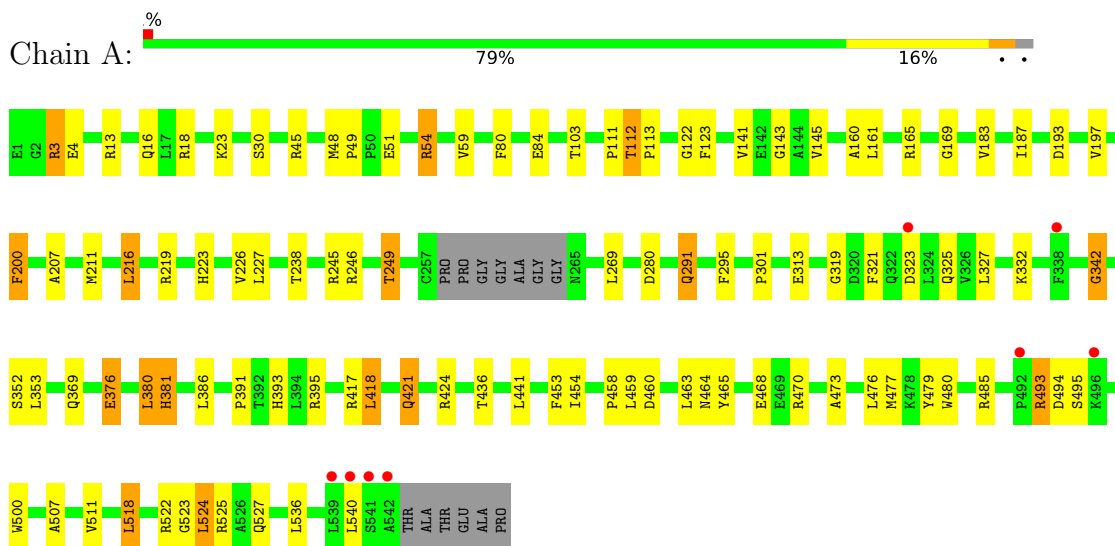
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	134	Total O 134 134	0	0
4	B	97	Total O 97 97	0	0

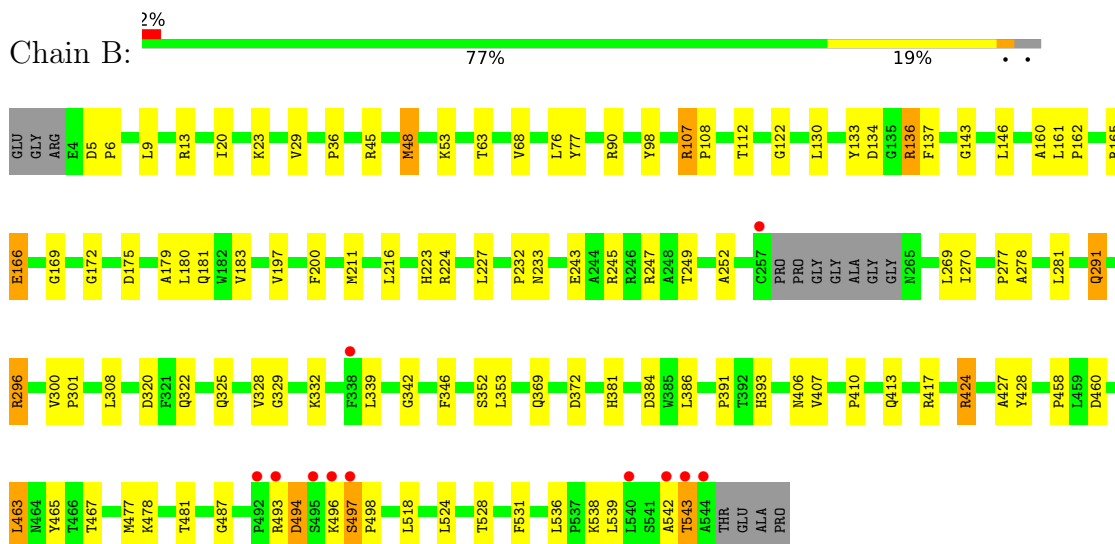
3 Residue-property plots

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, α , β , γ	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) 99.4 (29.17-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.246 0.196 , 0.244	Depositor DCC
R_{free} test set	1422 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8602	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NTJ, 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	0.76	0/4300	0.96	5/5875 (0.1%)
1	B	0.78	1/4282 (0.0%)	0.96	4/5853 (0.1%)
All	All	0.77	1/8582 (0.0%)	0.96	9/11728 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	THR	C-N	-5.68	1.25	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	SER	CA-C-N	8.45	130.40	119.84
1	B	497	SER	C-N-CA	8.45	130.40	119.84
1	B	107	ARG	CA-C-N	5.19	126.33	119.84
1	B	107	ARG	C-N-CA	5.19	126.33	119.84
1	A	342	GLY	CA-C-N	-5.19	117.62	123.02
1	A	342	GLY	C-N-CA	-5.19	117.62	123.02
1	A	216	LEU	CA-C-N	-5.11	114.35	119.56
1	A	216	LEU	C-N-CA	-5.11	114.35	119.56
1	A	381	HIS	N-CA-C	5.10	116.84	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	LYS	Peptide
1	B	497	SER	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	4177	0	4064	68	0
1	B	4159	0	4046	68	0
2	A	8	0	11	1	0
2	B	8	0	11	1	0
3	B	19	0	24	5	0
4	A	134	0	0	6	0
4	B	97	0	0	4	0
All	All	8602	0	8156	135	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 (135) 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:376:GLU:OE2	1:B:538:LYS:HE3	1.59	1.03
1:B:197:VAL:H	1:B:223:HIS:HD2	1.13	0.92
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.33	0.91
1:A:197:VAL:H	1:A:223:HIS:HD2	1.25	0.83
1:B:369:GLN:HB2	4:B:2065:HOH:O	1.80	0.80
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.65	0.78
1:A:219:ARG:HA	1:A:219:ARG:HE	1.51	0.76
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.03	0.72
1:B:197:VAL:H	1:B:223:HIS:CD2	2.04	0.69
1:B:48:MET:HE3	1:B:166:GLU:HA	1.74	0.68
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.09	0.68
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:O	1:B:494:ASP:HB2	1.92	0.68
1:A:291:GLN:HE22	1:A:369:GLN:NE2	1.92	0.66
1:A:219:ARG:HA	1:A:219:ARG:NE	2.09	0.66
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.78	0.66
1:A:54:ARG:HH11	1:A:54:ARG:HG2	1.59	0.65
1:B:291:GLN:HE22	1:B:369:GLN:NE2	1.95	0.65
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.80	0.64
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.79	0.63
1:A:369:GLN:HB2	4:A:2104:HOH:O	1.99	0.62
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.82	0.62
1:B:424:ARG:HB2	1:B:424:ARG:HH11	1.64	0.62
1:B:320:ASP:OD1	1:B:322:GLN:HG2	2.00	0.61
1:A:54:ARG:HH11	1:A:54:ARG:CB	2.13	0.61
1:A:527:GLN:HE21	3:B:1545:P6G:H171	1.66	0.61
1:A:493:ARG:HB2	4:A:2122:HOH:O	2.01	0.60
1:A:381:HIS:HA	3:B:1545:P6G:H31	1.84	0.59
1:A:211:MET:HE3	1:A:301:PRO:HG2	1.84	0.59
1:A:424:ARG:HD2	4:A:2112:HOH:O	2.03	0.59
1:A:380:LEU:HB3	3:B:1545:P6G:H51	1.84	0.58
1:A:197:VAL:H	1:A:223:HIS:CD2	2.14	0.58
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.86	0.58
1:A:380:LEU:HB3	3:B:1545:P6G:C5	2.34	0.57
1:A:122:GLY:HA2	2:A:1543:NTJ:H2C3	1.86	0.57
1:A:207:ALA:O	1:A:211:MET:HG2	2.06	0.56
1:B:107:ARG:HB3	4:B:2020:HOH:O	2.04	0.56
1:A:319:GLY:O	1:A:421:GLN:HG2	2.07	0.55
1:B:245:ARG:O	1:B:249:THR:HG23	2.06	0.55
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.89	0.54
1:B:112:THR:HG21	1:B:143:GLY:O	2.07	0.54
1:A:219:ARG:HE	1:A:219:ARG:CA	2.20	0.53
1:A:54:ARG:HG2	1:A:54:ARG:NH1	2.25	0.52
1:A:313:GLU:HB2	4:A:2067:HOH:O	2.09	0.52
1:B:477:MET:O	1:B:481:THR:OG1	2.24	0.51
1:B:48:MET:HE1	1:B:165:ARG:O	2.10	0.51
1:A:245:ARG:O	1:A:249:THR:CG2	2.59	0.51
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.93	0.50
1:A:352:SER:O	1:A:395:ARG:HG3	2.11	0.50
1:B:493:ARG:O	1:B:494:ASP:CB	2.59	0.50
1:A:112:THR:HG21	1:A:143:GLY:O	2.12	0.49
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.93	0.48
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH12	1:A:51:GLU:CD	2.21	0.48
1:B:45:ARG:NH2	1:B:48:MET:SD	2.87	0.48
1:B:498:PRO:HD2	1:B:518:LEU:HB2	1.94	0.48
1:A:245:ARG:O	1:A:249:THR:HG23	2.13	0.48
1:A:80:PHE:O	1:A:84:GLU:HG2	2.14	0.48
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.14	0.47
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.44	0.47
1:B:528:THR:O	1:B:531:PHE:HB3	2.14	0.47
1:A:219:ARG:NE	1:A:219:ARG:CA	2.69	0.47
1:B:393:HIS:HB3	4:B:2069:HOH:O	2.13	0.47
1:B:20:ILE:HB	1:B:63:THR:HB	1.95	0.47
1:B:381:HIS:CE1	3:B:1545:P6G:H181	2.50	0.47
1:B:328:VAL:O	1:B:427:ALA:HA	2.15	0.47
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.50	0.47
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.96	0.47
1:B:233:ASN:HD22	1:B:413:GLN:HE21	1.61	0.47
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.97	0.47
1:A:493:ARG:O	1:A:495:SER:N	2.48	0.46
1:A:23:LYS:HG2	4:A:2002:HOH:O	2.14	0.46
1:A:511:VAL:HG11	1:A:518:LEU:HD13	1.96	0.46
1:B:122:GLY:HA2	2:B:1544:NTJ:H2C3	1.97	0.46
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.97	0.46
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.81	0.46
1:A:238:THR:HA	1:A:301:PRO:O	2.16	0.46
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.51	0.46
1:A:393:HIS:HD2	4:A:2107:HOH:O	2.00	0.45
1:B:36:PRO:HB3	1:B:98:TYR:CE1	2.51	0.45
1:B:233:ASN:ND2	1:B:413:GLN:HE21	2.15	0.45
1:A:463:LEU:O	1:A:464:ASN:HB2	2.17	0.45
1:A:507:ALA:O	1:A:522:ARG:NH1	2.49	0.45
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.97	0.45
1:B:134:ASP:OD2	1:B:136:ARG:HD2	2.17	0.44
1:B:162:PRO:O	1:B:245:ARG:NH1	2.46	0.44
1:A:111:PRO:HB2	1:A:193:ASP:HB2	2.00	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.52	0.44
1:B:13:ARG:HD2	4:B:2037:HOH:O	2.17	0.44
1:B:300:VAL:O	1:B:301:PRO:C	2.60	0.44
1:A:200:PHE:CB	1:A:226:VAL:HB	2.47	0.44
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.48	0.44
1:B:243:GLU:O	1:B:247:ARG:HG3	2.18	0.44
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.53	0.44
1:B:424:ARG:HH11	1:B:424:ARG:CB	2.29	0.44
1:A:227:LEU:HD12	1:A:227:LEU:N	2.32	0.43
1:B:136:ARG:HG2	1:B:137:PHE:N	2.33	0.43
1:A:291:GLN:HE22	1:A:369:GLN:HE22	1.67	0.43
1:A:141:VAL:HG21	1:A:459:LEU:HD23	2.01	0.43
1:B:179:ALA:O	1:B:183:VAL:HG23	2.18	0.43
1:A:473:ALA:O	1:A:477:MET:HG3	2.19	0.42
1:A:524:LEU:O	1:A:525:ARG:C	2.62	0.42
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.51	0.42
1:A:321:PHE:CD2	1:A:418:LEU:HD12	2.54	0.42
1:B:353:LEU:HB3	1:B:391:PRO:HB2	2.01	0.42
1:B:424:ARG:HH11	1:B:424:ARG:CG	2.32	0.42
1:A:479:TYR:OH	1:A:518:LEU:HG	2.18	0.42
1:A:48:MET:HE2	1:A:49:PRO:HD2	2.02	0.42
1:B:407:VAL:C	1:B:410:PRO:HD2	2.45	0.42
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.01	0.42
1:B:417:ARG:HA	1:B:417:ARG:HE	1.85	0.42
1:B:76:LEU:HD23	1:B:77:TYR:CE2	2.55	0.42
1:A:160:ALA:HB2	1:A:169:GLY:HA3	2.01	0.41
1:A:183:VAL:HG13	1:A:187:ILE:HB	2.02	0.41
1:B:384:ASP:C	1:B:384:ASP:OD1	2.63	0.41
1:B:539:LEU:HD12	1:B:539:LEU:HA	1.80	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.56	0.41
1:B:428:TYR:CD1	1:B:428:TYR:C	2.97	0.41
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.82	0.41
1:B:277:PRO:O	1:B:278:ALA:C	2.63	0.41
1:B:252:ALA:HB2	1:B:269:LEU:HD21	2.02	0.41
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.55	0.41
1:B:5:ASP:HA	1:B:6:PRO:HD3	1.96	0.41
1:B:36:PRO:HB2	1:B:53:LYS:HD3	2.01	0.41
1:B:172:GLY:O	1:B:175:ASP:HB2	2.20	0.41
1:A:16:GLN:HB2	1:A:59:VAL:HA	2.03	0.41
1:A:122:GLY:O	1:A:123:PHE:HB2	2.20	0.41
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.03	0.41
1:A:524:LEU:HD13	1:A:524:LEU:HA	1.97	0.40
1:B:48:MET:CE	1:B:166:GLU:HA	2.48	0.40
1:A:319:GLY:O	1:A:421:GLN:CG	2.69	0.40
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.03	0.40
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.55	0.40
1:A:460:ASP:HB3	1:A:463:LEU:HD12	2.04	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	531/548 (97%)	508 (96%)	20 (4%)	3 (1%)	21	38
1	B	530/548 (97%)	503 (95%)	22 (4%)	5 (1%)	14	27
All	All	1061/1096 (97%)	1011 (95%)	42 (4%)	8 (1%)	16	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	ASP
1	B	494	ASP
1	B	542	ALA
1	B	543	THR
1	A	342	GLY
1	A	523	GLY
1	B	108	PRO
1	B	342	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	439/446 (98%)	410 (93%)	29 (7%)	15	32
1	B	438/446 (98%)	415 (95%)	23 (5%)	20	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	877/892 (98%)	825 (94%)	52 (6%)	18	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
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
1	A	249	THR
1	A	280	ASP
1	A	291	GLN
1	A	295	PHE
1	A	323	ASP
1	A	325	GLN
1	A	332	LYS
1	A	376	GLU
1	A	380	LEU
1	A	386	LEU
1	A	418	LEU
1	A	421	GLN
1	A	436	THR
1	A	441	LEU
1	A	468	GLU
1	A	493	ARG
1	A	518	LEU
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	9	LEU
1	B	23	LYS
1	B	48	MET
1	B	136	ARG
1	B	146	LEU
1	B	166	GLU
1	B	180	LEU
1	B	181	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	200	PHE
1	B	216	LEU
1	B	281	LEU
1	B	291	GLN
1	B	296	ARG
1	B	332	LYS
1	B	352	SER
1	B	372	ASP
1	B	386	LEU
1	B	424	ARG
1	B	463	LEU
1	B	467	THR
1	B	478	LYS
1	B	524	LEU
1	B	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	284	HIS
1	A	287	HIS
1	A	291	GLN
1	A	387	HIS
1	A	447	HIS
1	A	509	GLN
1	B	16	GLN
1	B	223	HIS
1	B	265	ASN
1	B	291	GLN
1	B	322	GLN
1	B	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	NTJ	B	1544	1	4,7,7	0.44	0	4,8,8	0.77	0
2	NTJ	A	1543	1	4,7,7	0.47	0	4,8,8	1.02	0
3	P6G	B	1545	-	18,18,18	1.76	5 (27%)	17,17,17	2.35	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	NTJ	B	1544	1	-	0/1/7/7	-
2	NTJ	A	1543	1	-	1/1/7/7	-
3	P6G	B	1545	-	-	8/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1545	P6G	C9-C8	-2.94	1.34	1.49
3	B	1545	P6G	C15-C14	-2.88	1.34	1.49
3	B	1545	P6G	C17-C18	-2.85	1.34	1.49
3	B	1545	P6G	C3-C2	-2.81	1.34	1.49
3	B	1545	P6G	C6-C5	-2.64	1.35	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1545	P6G	O7-C8-C9	3.61	126.81	110.35
3	B	1545	P6G	O7-C6-C5	3.56	126.56	110.35
3	B	1545	P6G	O4-C5-C6	3.01	124.08	110.35
3	B	1545	P6G	O10-C9-C8	2.95	123.79	110.35
3	B	1545	P6G	O16-C15-C14	2.89	123.54	110.35
3	B	1545	P6G	O4-C3-C2	2.85	122.68	110.11
3	B	1545	P6G	O13-C14-C15	2.77	122.98	110.35
3	B	1545	P6G	C5-O4-C3	2.32	123.42	113.26
3	B	1545	P6G	O16-C17-C18	2.26	120.09	110.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1545	P6G	O13-C14-C15-O16
3	B	1545	P6G	O4-C5-C6-O7
3	B	1545	P6G	O7-C8-C9-O10
3	B	1545	P6G	O10-C11-C12-O13
3	B	1545	P6G	C14-C15-O16-C17
3	B	1545	P6G	C2-C3-O4-C5
2	A	1543	NTJ	C4-C3-O2-P1
3	B	1545	P6G	C12-C11-O10-C9
3	B	1545	P6G	C6-C5-O4-C3

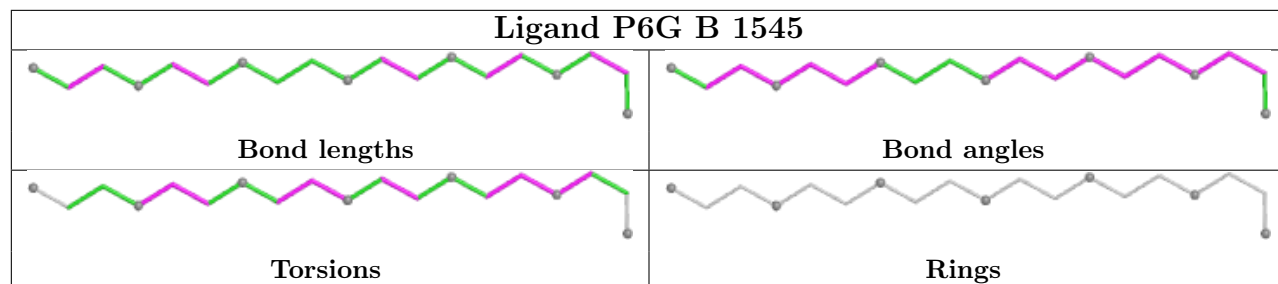
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1544	NTJ	1	0
2	A	1543	NTJ	1	0
3	B	1545	P6G	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/548 (97%)	-0.36	8 (1%) 72 68	29, 43, 62, 86	0
1	B	534/548 (97%)	-0.16	11 (2%) 63 59	31, 48, 68, 88	0
All	All	1069/1096 (97%)	-0.26	19 (1%) 67 64	29, 45, 67, 88	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	5.3
1	B	544	ALA	4.1
1	B	496	LYS	3.9
1	B	543	THR	3.9
1	A	540	LEU	3.6
1	A	542	ALA	3.5
1	B	257	CYS	3.4
1	B	542	ALA	3.3
1	A	496	LYS	2.7
1	B	492	PRO	2.7
1	A	541	SER	2.6
1	B	493	ARG	2.6
1	A	492	PRO	2.4
1	A	338	PHE	2.3
1	A	539	LEU	2.2
1	B	338	PHE	2.2
1	B	540	LEU	2.2
1	A	323	ASP	2.1
1	B	495	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

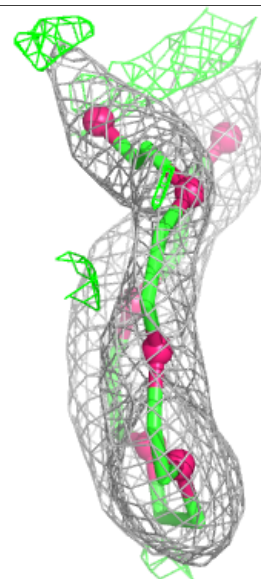
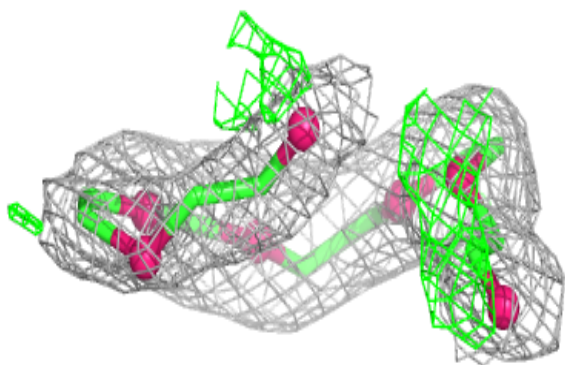
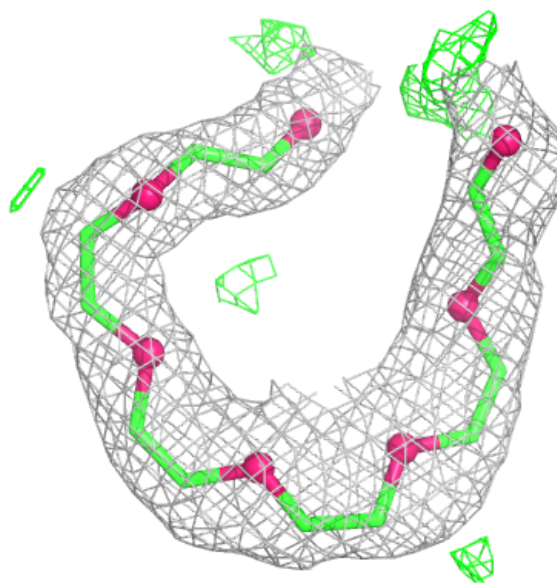
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P6G	B	1545	19/19	0.92	0.15	64,70,75,75	0
2	NTJ	B	1544	8/8	0.98	0.09	45,49,54,57	0
2	NTJ	A	1543	8/8	0.98	0.07	39,43,46,47	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.

Electron density around P6G B 1545:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.