



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:19 AM UTC

PDB ID : 1Q84 / pdb_00001q84
Title : Crystal structure of the mouse acetylcholinesterase-TZ2PA6 anti complex
Authors : Bourne, Y.; Kolb, H.C.; Radic, Z.; Sharpless, K.B.; Taylor, P.; Marchot, P.
Deposited on : 2003-08-20
Resolution : 2.45 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

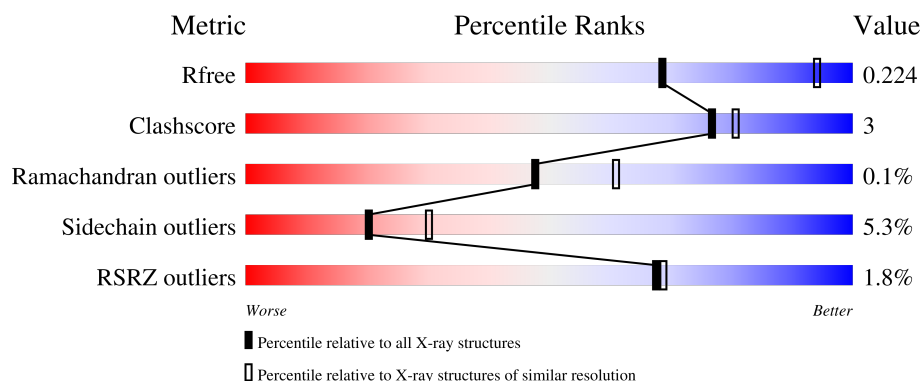
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	580	
1	B	580	

2 Entry composition [i](#)

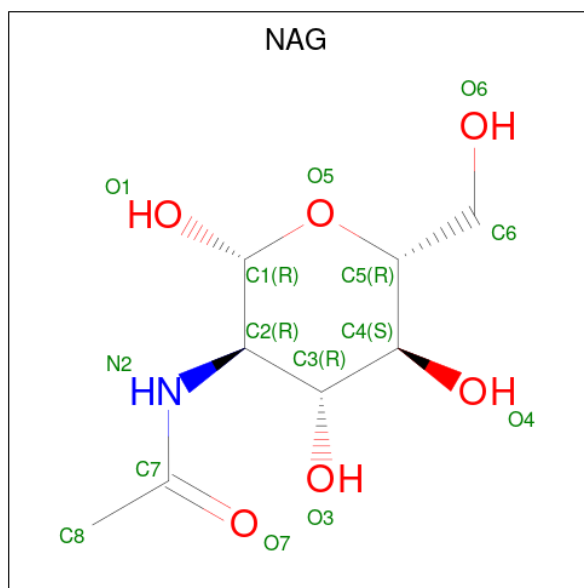
There are 5 unique types of molecules in this entry. The entry contains 8799 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

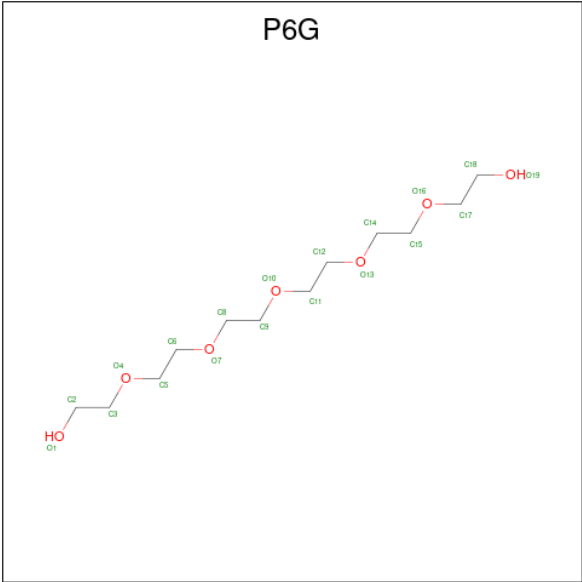
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4172	2678	723	757	14			
1	B	531	Total	C	N	O	S	0	0	0
			4142	2662	715	751	14			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



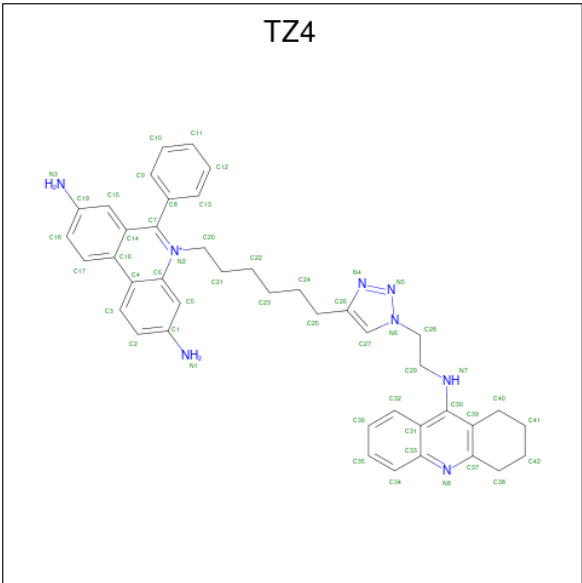
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is 3,8-DIAMINO-6-PHENYL-5-[6-[1-[2-[(1,2,3,4-TETRAHYDRO-9-ACRIDINY L)AMINO]ETHYL]-1H-1,2,3-TRIAZOL-4-YL]HEXYL]-PHENANTHRIDINIUM (CCD ID: TZ4) (formula: C₄₂H₄₅N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			50	42	8		
4	B	1	Total	C	N	0	0
			50	42	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total 214	O 214	0	0
5	B	124	Total 124	O 124	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.27Å 111.77Å 227.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.45) 99.5 (20.00-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.214 0.199 , 0.224	Depositor DCC
R_{free} test set	1508 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: P6G, TZ4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	0/4296	0.93	0/5872
1	B	0.85	2/4266 (0.0%)	0.91	1/5833 (0.0%)
All	All	0.87	2/8562 (0.0%)	0.92	1/11705 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	MET	SD-CE	8.28	2.00	1.79
1	B	497	SER	CA-C	7.42	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	PRO	N-CA-C	-5.74	97.17	112.10

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 ⓘ

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	4172	0	4050	28	0
1	B	4142	0	4023	19	0
2	A	28	0	26	0	0
3	A	19	0	26	3	0
4	A	50	0	45	1	0
4	B	50	0	45	1	0
5	A	214	0	0	6	0
5	B	124	0	0	2	0
All	All	8799	0	8215	48	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 3.

All (48) 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	1.36	0.72
1:B:30:SER:HB2	1:B:103:THR:HG22	1.71	0.71
1:B:245:ARG:O	1:B:249:THR:HG23	1.94	0.67
1:B:112:THR:HG21	1:B:143:GLY:O	1.96	0.65
4:A:951:TZ4:H291	5:A:1755:HOH:O	1.96	0.65
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.99	0.61
1:A:197:VAL:H	1:A:223:HIS:HD2	1.48	0.61
1:A:527:GLN:HG3	3:A:901:P6G:H22	1.83	0.59
1:B:534:ARG:HD3	5:B:1075:HOH:O	2.02	0.58
1:A:325:GLN:HE21	1:A:487:GLY:HA3	1.68	0.58
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.86	0.57
1:A:112:THR:HG21	1:A:143:GLY:O	2.05	0.56
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.90	0.54
1:A:369:GLN:HB2	5:A:1726:HOH:O	2.09	0.52
1:A:13:ARG:NH2	5:A:1722:HOH:O	2.43	0.51
1:A:245:ARG:O	1:A:249:THR:HG23	2.11	0.50
1:A:328:VAL:O	1:A:427:ALA:HA	2.12	0.49
1:A:274:ARG:HD3	5:A:1794:HOH:O	2.12	0.48
1:A:433:ARG:HD3	5:A:1810:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.95	0.48
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.96	0.48
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.50	0.47
1:A:381:HIS:HA	3:A:901:P6G:H172	1.96	0.46
1:B:328:VAL:O	1:B:427:ALA:HA	2.15	0.46
1:A:393:HIS:HB2	5:A:1780:HOH:O	2.14	0.46
1:A:437:LEU:HD11	1:A:449:TYR:CD2	2.50	0.46
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.51	0.46
1:B:369:GLN:HB3	5:B:1024:HOH:O	2.16	0.46
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.31	0.45
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.98	0.44
1:B:497:SER:HB2	1:B:498:PRO:HA	2.00	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.18	0.43
1:B:497:SER:CB	1:B:498:PRO:HA	2.49	0.43
1:A:200:PHE:CB	1:A:226:VAL:HB	2.48	0.43
1:A:245:ARG:O	1:A:249:THR:CG2	2.67	0.42
1:A:224:ARG:HG2	1:A:325:GLN:HB2	2.01	0.42
1:B:294:ILE:HD11	1:B:402:VAL:HG21	2.02	0.42
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.55	0.42
1:B:337:TYR:CD1	1:B:337:TYR:C	2.98	0.42
1:B:439:TRP:CZ2	4:B:952:TZ4:H36	2.55	0.41
1:B:161:LEU:HD11	1:B:269:LEU:HD22	2.03	0.41
1:A:531:PHE:HB2	3:A:901:P6G:H62	2.02	0.41
1:A:99:LEU:HD12	1:A:99:LEU:C	2.46	0.41
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.56	0.41
1:B:195:MET:HA	1:B:195:MET:HE2	2.03	0.41
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.94	0.41
1:A:291:GLN:HE22	1:A:369:GLN:NE2	2.19	0.40
1:B:295:PHE:CE2	1:B:338:PHE:CE1	3.09	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	532/580 (92%)	517 (97%)	15 (3%)	0	100	100
1	B	527/580 (91%)	511 (97%)	15 (3%)	1 (0%)	43	54
All	All	1059/1160 (91%)	1028 (97%)	30 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER

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	437/473 (92%)	412 (94%)	25 (6%)	18	27
1	B	435/473 (92%)	414 (95%)	21 (5%)	23	34
All	All	872/946 (92%)	826 (95%)	46 (5%)	20	30

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

Mol	Chain	Res	Type
1	A	4	GLU
1	A	13	ARG
1	A	23	LYS
1	A	45	ARG
1	A	70	TYR
1	A	195	MET
1	A	216	LEU
1	A	246	ARG
1	A	249	THR
1	A	251	LEU
1	A	291	GLN
1	A	313	GLU
1	A	322	GLN
1	A	325	GLN
1	A	337	TYR

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Mol	Chain	Res	Type
1	A	389	GLU
1	A	413	GLN
1	A	424	ARG
1	A	468	GLU
1	A	478	LYS
1	A	497	SER
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	A	540	LEU
1	B	11	ARG
1	B	21	ARG
1	B	61	ASP
1	B	115	LEU
1	B	136	ARG
1	B	166	GLU
1	B	195	MET
1	B	246	ARG
1	B	249	THR
1	B	281	LEU
1	B	291	GLN
1	B	337	TYR
1	B	360	LEU
1	B	369	GLN
1	B	389	GLU
1	B	413	GLN
1	B	424	ARG
1	B	470	ARG
1	B	525	ARG
1	B	536	LEU
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	223	HIS
1	A	265	ASN
1	A	291	GLN
1	A	317	ASN
1	A	325	GLN
1	A	393	HIS

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Mol	Chain	Res	Type
1	A	405	HIS
1	B	184	GLN
1	B	291	GLN
1	B	474	GLN
1	B	499	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](#)

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](#)

5 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	$\# Z > 2$
4	TZ4	B	952	-	55,57,57	1.72	10 (18%)	72,80,80	2.44	27 (37%)
2	NAG	A	1701	1	14,14,15	0.78	1 (7%)	17,19,21	1.62	4 (23%)
2	NAG	A	1501	1	14,14,15	1.22	1 (7%)	17,19,21	1.88	5 (29%)
3	P6G	A	901	-	18,18,18	2.12	6 (33%)	17,17,17	1.29	1 (5%)
4	TZ4	A	951	-	55,57,57	1.58	9 (16%)	72,80,80	2.39	25 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TZ4	B	952	-	-	9/19/26/26	0/8/8/8
2	NAG	A	1701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
3	P6G	A	901	-	-	7/16/16/16	-
4	TZ4	A	951	-	-	6/19/26/26	0/8/8/8

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	952	TZ4	C40-C39	-5.51	1.43	1.51
4	A	951	TZ4	C40-C39	-4.70	1.44	1.51
4	B	952	TZ4	C41-C40	-4.03	1.37	1.51
3	A	901	P6G	O10-C9	4.02	1.59	1.42
4	B	952	TZ4	C42-C38	-3.99	1.37	1.51
4	A	951	TZ4	C41-C40	-3.96	1.37	1.51
4	B	952	TZ4	C38-C37	-3.87	1.45	1.50
4	A	951	TZ4	C42-C38	-3.78	1.38	1.51
3	A	901	P6G	O13-C12	3.77	1.58	1.42
2	A	1501	NAG	C1-C2	3.63	1.57	1.52
4	A	951	TZ4	C38-C37	-3.53	1.45	1.50
3	A	901	P6G	O16-C15	3.50	1.57	1.42
3	A	901	P6G	O4-C3	3.33	1.56	1.42
3	A	901	P6G	O19-C18	3.31	1.59	1.42
3	A	901	P6G	O7-C6	2.81	1.54	1.42
4	A	951	TZ4	C39-C37	2.65	1.44	1.40
4	B	952	TZ4	C39-C37	2.60	1.44	1.40
4	B	952	TZ4	C42-C41	-2.52	1.42	1.51
4	A	951	TZ4	C42-C41	-2.44	1.42	1.51
4	B	952	TZ4	C15-C14	2.34	1.46	1.42
4	B	952	TZ4	C37-N8	2.32	1.35	1.32
4	B	952	TZ4	C30-C39	2.29	1.43	1.39
4	B	952	TZ4	C6-N2	2.27	1.43	1.40
4	A	951	TZ4	C3-C4	2.16	1.45	1.41
4	A	951	TZ4	C26-N4	-2.07	1.32	1.36
2	A	1701	NAG	C1-C2	2.04	1.55	1.52
4	A	951	TZ4	C37-N8	2.00	1.34	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	952	TZ4	C40-C39-C37	-9.08	112.36	120.90
4	A	951	TZ4	C40-C39-C37	-6.98	114.34	120.90
4	B	952	TZ4	C42-C38-C37	5.77	122.47	113.48
4	A	951	TZ4	C28-N6-N5	5.58	131.99	120.78
4	B	952	TZ4	C41-C40-C39	5.40	123.82	112.84
4	A	951	TZ4	C24-C25-C26	-5.39	102.67	113.56
4	A	951	TZ4	C13-C8-C7	5.23	127.49	120.25
2	A	1501	NAG	C1-O5-C5	4.96	118.84	112.19
4	B	952	TZ4	C28-N6-N5	4.72	130.25	120.78
4	A	951	TZ4	C21-C20-N2	4.47	121.85	111.83
4	A	951	TZ4	C41-C40-C39	4.46	121.90	112.84
4	B	952	TZ4	N6-N5-N4	4.41	110.99	107.02
4	A	951	TZ4	C28-N6-C27	-4.41	120.61	128.83
4	A	951	TZ4	C1-C5-C6	4.29	125.59	119.93
4	B	952	TZ4	C24-C25-C26	-4.28	104.92	113.56
4	B	952	TZ4	C1-C5-C6	4.14	125.40	119.93
4	A	951	TZ4	C42-C38-C37	4.08	119.84	113.48
4	A	951	TZ4	C9-C8-C7	-3.92	114.82	120.25
4	B	952	TZ4	C13-C8-C7	3.84	125.56	120.25
4	B	952	TZ4	C27-N6-N5	-3.74	107.11	110.75
4	B	952	TZ4	C8-C7-N2	3.72	123.14	119.30
4	B	952	TZ4	C9-C8-C7	-3.69	115.14	120.25
4	A	951	TZ4	N6-N5-N4	3.63	110.29	107.02
4	A	951	TZ4	C27-N6-N5	-3.44	107.40	110.75
4	B	952	TZ4	C31-C30-N7	-3.33	111.51	121.86
4	B	952	TZ4	C28-N6-C27	-3.33	122.62	128.83
4	A	951	TZ4	C31-C30-N7	-3.26	111.73	121.86
4	B	952	TZ4	C26-N4-N5	-3.18	105.57	109.01
3	A	901	P6G	O1-C2-C3	3.14	130.28	111.82
4	A	951	TZ4	C26-N4-N5	-3.10	105.66	109.01
2	A	1501	NAG	O5-C5-C6	3.09	113.69	107.66
4	B	952	TZ4	C4-C6-N2	-3.00	116.52	118.46
4	B	952	TZ4	C17-C16-C14	-2.94	114.10	117.72
4	A	951	TZ4	C17-C16-C14	-2.92	114.12	117.72
4	A	951	TZ4	C4-C6-N2	-2.88	116.59	118.46
2	A	1701	NAG	C3-C4-C5	-2.88	105.01	110.23
4	A	951	TZ4	C29-C28-N6	-2.85	106.95	111.61
4	B	952	TZ4	C39-C37-N8	-2.83	121.66	123.66
2	A	1701	NAG	O5-C5-C6	2.76	113.03	107.66
4	A	951	TZ4	C40-C39-C30	2.70	127.49	121.23
4	B	952	TZ4	C40-C39-C30	2.68	127.43	121.23
2	A	1701	NAG	O4-C4-C5	2.59	115.70	109.32
4	A	951	TZ4	C18-C19-C15	-2.59	114.66	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	951	TZ4	C37-N8-C33	2.39	120.50	117.67
4	B	952	TZ4	C18-C19-C15	-2.37	115.06	119.48
4	B	952	TZ4	C2-C1-C5	-2.35	115.11	119.48
4	A	951	TZ4	C39-C37-N8	-2.34	122.00	123.66
4	A	951	TZ4	C2-C1-C5	-2.28	115.23	119.48
4	A	951	TZ4	C35-C34-C33	2.28	123.21	120.09
4	B	952	TZ4	C3-C4-C6	-2.25	114.87	117.78
4	A	951	TZ4	C3-C4-C6	-2.22	114.91	117.78
4	B	952	TZ4	C28-C29-N7	-2.21	103.97	110.29
4	B	952	TZ4	C42-C41-C40	2.21	121.87	112.39
4	B	952	TZ4	C2-C3-C4	2.19	124.99	121.62
2	A	1501	NAG	C2-N2-C7	2.18	125.82	122.90
4	B	952	TZ4	C35-C34-C33	2.12	122.99	120.09
2	A	1501	NAG	O7-C7-C8	-2.11	118.29	122.05
4	B	952	TZ4	C8-C7-C14	-2.08	116.94	121.05
4	A	951	TZ4	C38-C37-C39	-2.03	119.32	121.40
4	B	952	TZ4	C36-C32-C31	2.03	123.65	120.91
2	A	1501	NAG	C1-C2-N2	2.02	113.61	110.43
2	A	1701	NAG	O5-C5-C4	-2.02	105.92	110.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	951	TZ4	C29-C28-N6-N5
4	B	952	TZ4	C29-C28-N6-N5
4	B	952	TZ4	C29-C28-N6-C27
4	A	951	TZ4	N6-C28-C29-N7
4	B	952	TZ4	N6-C28-C29-N7
2	A	1501	NAG	C4-C5-C6-O6
3	A	901	P6G	O1-C2-C3-O4
2	A	1501	NAG	O5-C5-C6-O6
4	B	952	TZ4	C22-C23-C24-C25
4	A	951	TZ4	C29-C28-N6-C27
4	B	952	TZ4	C23-C24-C25-C26
2	A	1501	NAG	C8-C7-N2-C2
3	A	901	P6G	C18-C17-O16-C15
3	A	901	P6G	C11-C12-O13-C14
2	A	1501	NAG	O7-C7-N2-C2
4	A	951	TZ4	C22-C23-C24-C25
3	A	901	P6G	C2-C3-O4-C5
2	A	1701	NAG	C8-C7-N2-C2

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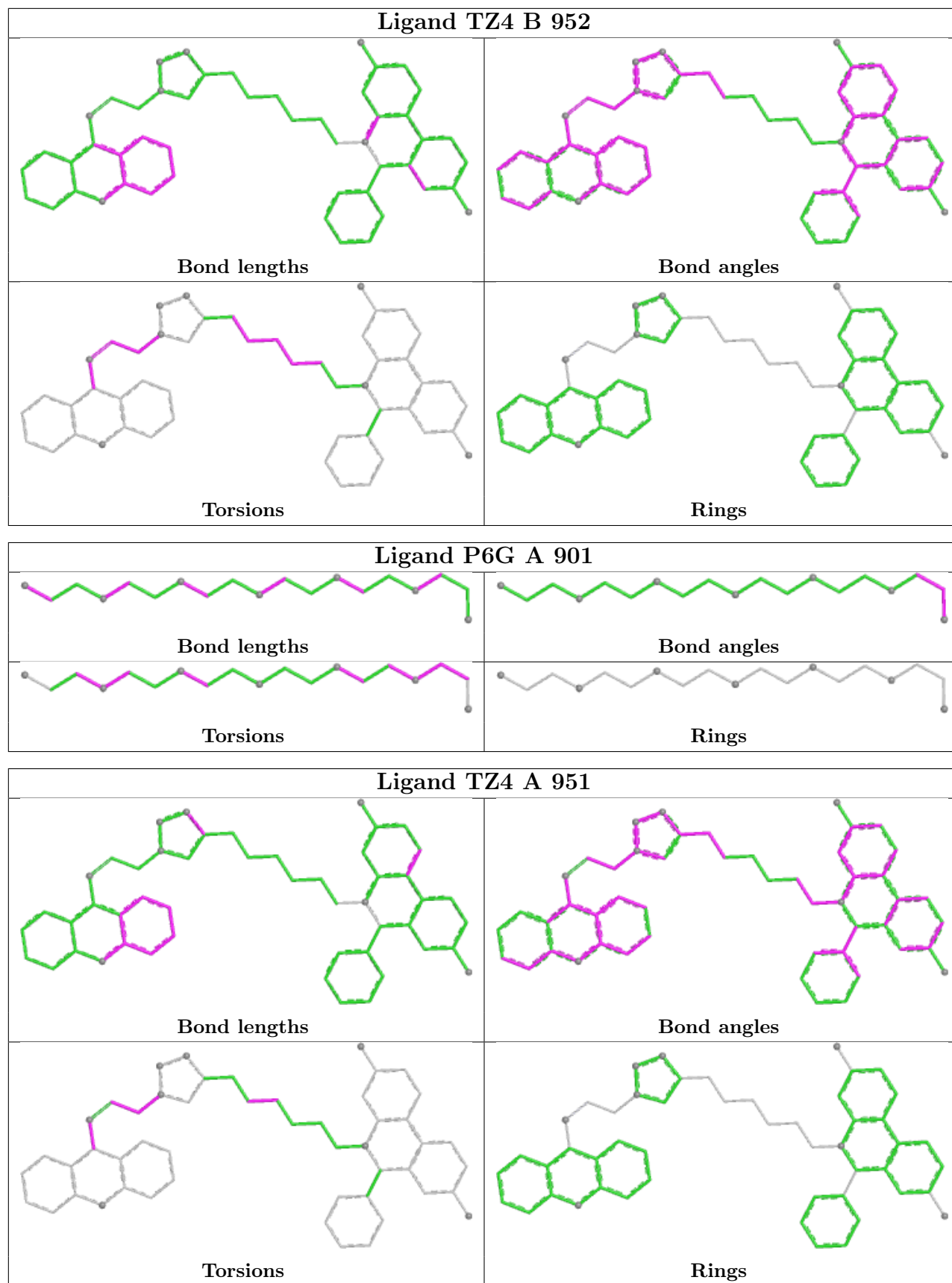
Mol	Chain	Res	Type	Atoms
4	A	951	TZ4	C31-C30-N7-C29
4	B	952	TZ4	C20-C21-C22-C23
4	B	952	TZ4	C21-C22-C23-C24
3	A	901	P6G	C6-C5-O4-C3
2	A	1701	NAG	O7-C7-N2-C2
4	B	952	TZ4	C39-C30-N7-C29
4	A	951	TZ4	C39-C30-N7-C29
4	B	952	TZ4	C28-C29-N7-C30
3	A	901	P6G	C14-C15-O16-C17
3	A	901	P6G	C5-C6-O7-C8

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	952	TZ4	1	0
3	A	901	P6G	3	0
4	A	951	TZ4	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 [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	536/580 (92%)	-0.15	11 (2%) 63 65	36, 50, 72, 99	0
1	B	531/580 (91%)	0.04	8 (1%) 72 74	39, 55, 77, 97	0
All	All	1067/1160 (91%)	-0.06	19 (1%) 67 69	36, 52, 75, 99	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	LEU	4.9
1	A	540	LEU	4.2
1	A	1	GLU	4.1
1	B	497	SER	3.9
1	A	258	PRO	3.9
1	B	258	PRO	3.8
1	A	264	GLY	3.5
1	B	286	TRP	2.9
1	A	323	ASP	2.9
1	A	541	SER	2.7
1	A	2	GLY	2.3
1	A	493	ARG	2.3
1	B	495	SER	2.3
1	B	265	ASN	2.2
1	A	495	SER	2.2
1	A	492	PRO	2.2
1	B	492	PRO	2.2
1	B	496	LYS	2.1
1	A	109	ALA	2.1

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](#)

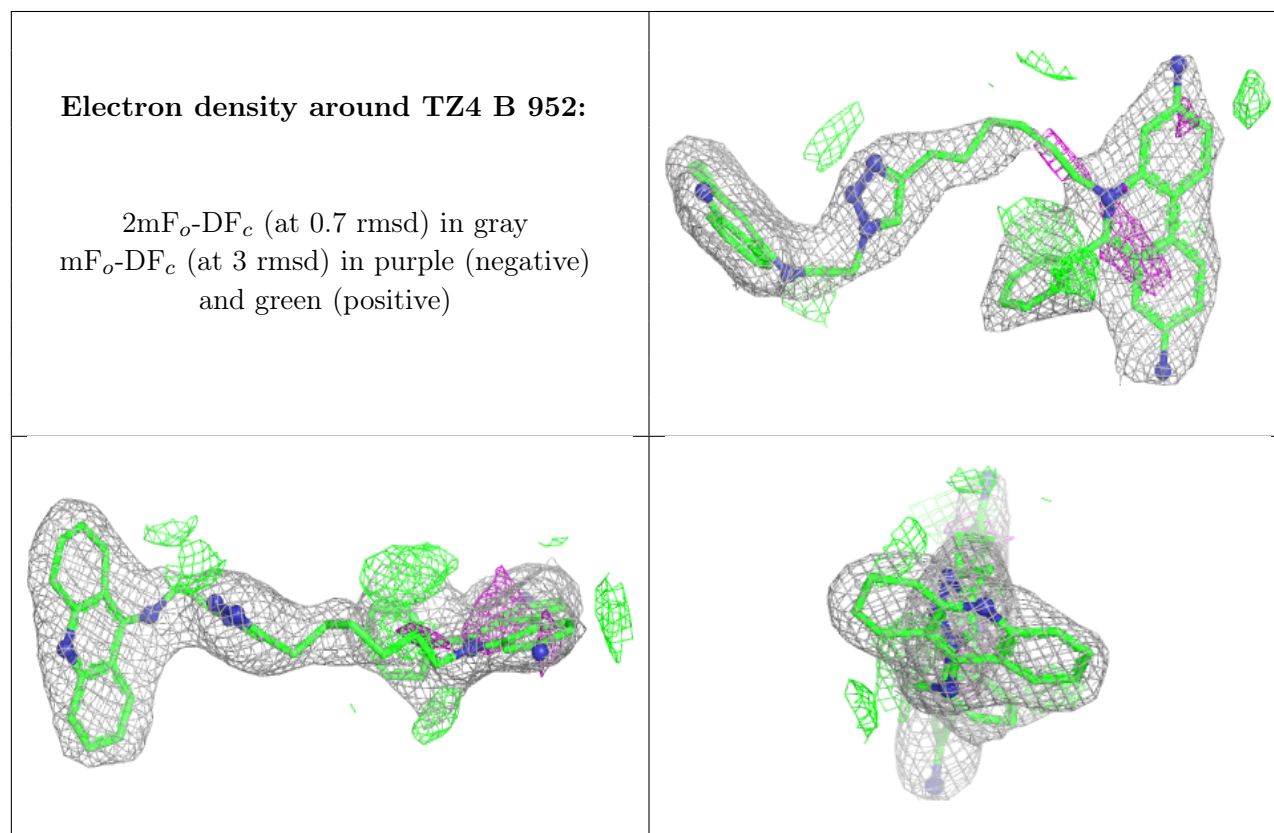
There are no oligosaccharides in this entry.

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.

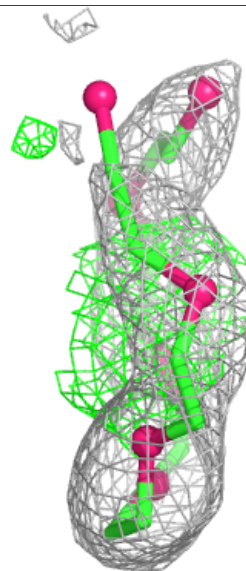
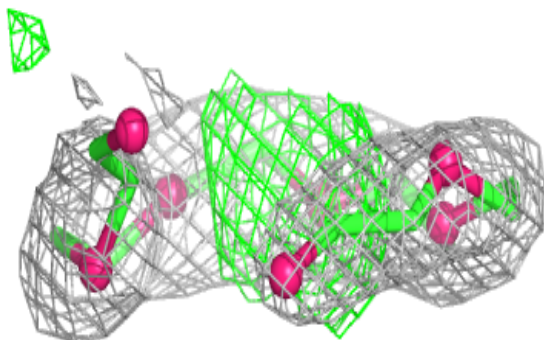
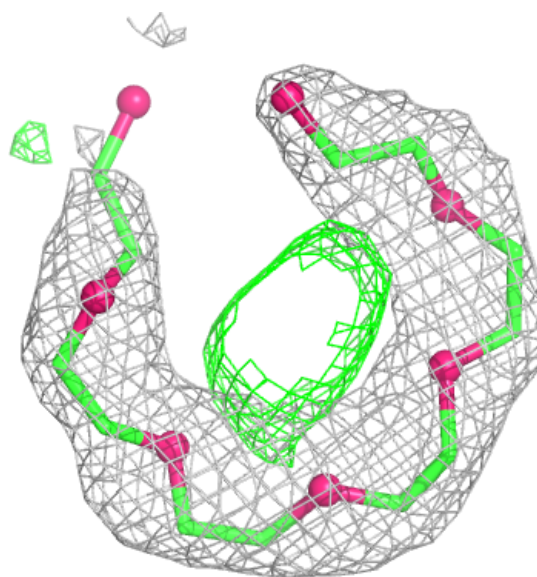
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1501	14/15	0.57	0.19	79,87,94,94	0
2	NAG	A	1701	14/15	0.66	0.13	86,95,98,99	0
4	TZ4	B	952	50/50	0.86	0.14	53,71,77,78	0
3	P6G	A	901	19/19	0.90	0.15	61,72,83,86	0
4	TZ4	A	951	50/50	0.91	0.10	44,62,66,67	0

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.



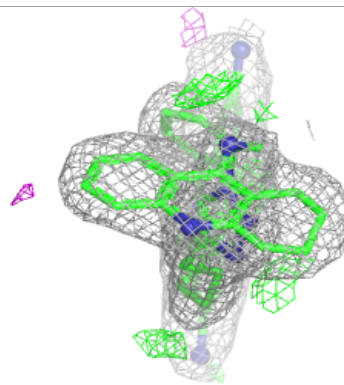
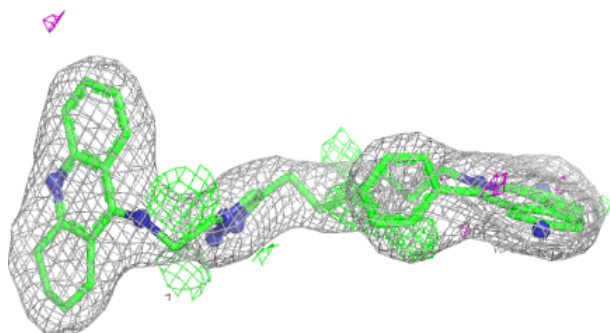
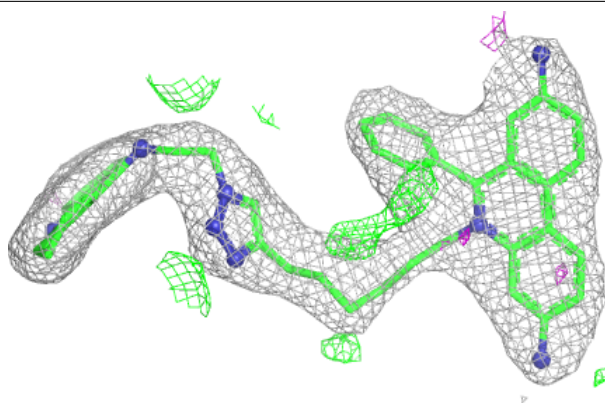
Electron density around P6G A 901:

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



Electron density around TZ4 A 951:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.