



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:18 PM UTC

PDB ID : 1F0L / pdb_00001f0l
Title : 1.55 ANGSTROM CRYSTAL STRUCTURE OF WILD TYPE DIPHTHERIA TOXIN
Authors : Steere, B.; Eisenberg, D.
Deposited on : 2000-05-16
Resolution : 1.55 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

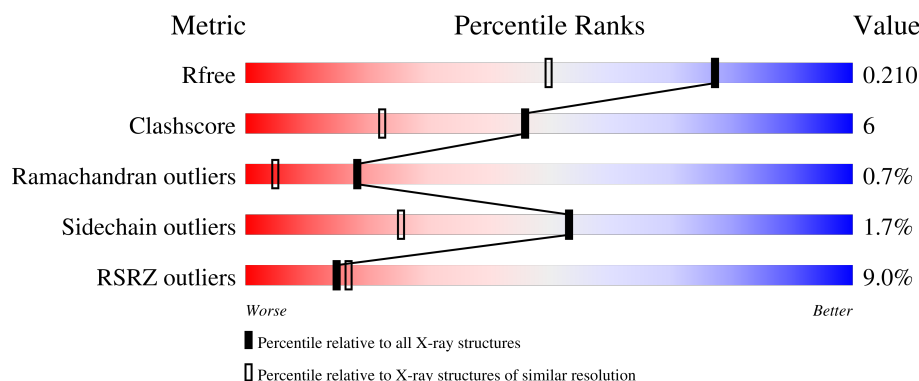
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	535	10% 83% 13% ..
1	B	535	8% 85% 12% ..

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.

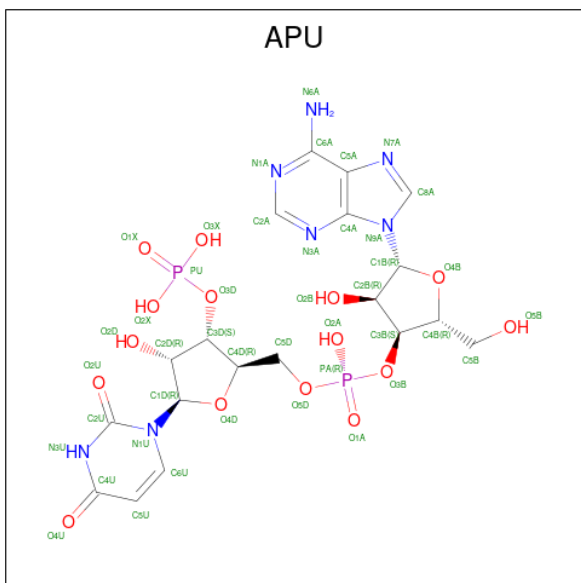
- Molecule 1 is a protein called DIPHTHERIA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total 4112	C 2596	N 692	O 808	S 16	0	35	0
1	B	522	Total 4188	C 2636	N 707	O 830	S 15	0	43	0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cl 4 4	0	0
2	B	5	Total Cl 5 5	0	0

- Molecule 3 is ADENYLYL-3'-5'-PHOSPHO-URIDINE-3'-MONOPHOSPHATE (CCD ID: APU) (formula: $\text{C}_{19}\text{H}_{25}\text{N}_7\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 19	N 7	O 15	P 2	0	0
3	B	1	Total 43	C 19	N 7	O 15	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	910	Total 910	O 910	0	0
4	B	899	Total 899	O 899	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.77Å 134.88Å 46.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.55 40.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-1.55) 94.6 (40.00-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.55Å)	Xtriage
Refinement program	SHELXL, SHELXL-97	Depositor
R, R_{free}	0.188 , 0.238 0.190 , 0.210	Depositor DCC
R_{free} test set	7212 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10204	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1698e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: APU, CL

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	0.54	0/4328	1.36	28/5853 (0.5%)
1	B	0.55	0/4425	1.35	27/5983 (0.5%)
All	All	0.54	0/8753	1.36	55/11836 (0.5%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ARG	NE-CZ-NH2	9.28	127.55	119.20
1	A	344	ILE	O-C-N	8.01	125.55	120.42
1	B	460	ARG	CD-NE-CZ	7.87	135.42	124.40
1	B	530	PHE	CA-CB-CG	-7.51	106.29	113.80
1	B	368	PHE	CA-CB-CG	6.91	120.71	113.80
1	B	258	PRO	CA-C-N	6.88	131.70	120.63
1	B	258	PRO	C-N-CA	6.88	131.70	120.63
1	B	455	ARG	NH1-CZ-NH2	6.87	128.22	119.30
1	B	515	GLN	OE1-CD-NE2	6.58	129.19	122.60
1	B	145[A]	SER	CA-C-O	6.56	127.33	119.59
1	B	145[B]	SER	CA-C-O	6.56	127.33	119.59
1	A	344	ILE	CA-C-O	-6.55	114.30	118.69
1	A	122[A]	GLU	CA-C-N	6.50	128.88	120.44
1	A	122[A]	GLU	C-N-CA	6.50	128.88	120.44
1	A	122[B]	GLU	CA-C-N	6.50	128.88	120.44
1	A	122[B]	GLU	C-N-CA	6.50	128.88	120.44
1	A	274	ALA	CA-C-O	6.46	128.61	121.56
1	A	358	TYR	CA-C-O	-6.25	115.24	119.68
1	A	368	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	380	TYR	CA-C-O	-6.14	114.43	121.19
1	A	176	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	251	HIS	CA-CB-CG	5.99	119.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	A	145[A]	SER	CA-C-N	5.96	131.82	120.97
1	A	145[A]	SER	C-N-CA	5.96	131.82	120.97
1	A	145[B]	SER	CA-C-N	5.96	131.82	120.97
1	A	145[B]	SER	C-N-CA	5.96	131.82	120.97
1	A	145[C]	SER	CA-C-N	5.96	131.82	120.97
1	A	145[C]	SER	C-N-CA	5.96	131.82	120.97
1	B	257	HIS	CB-CG-CD2	5.91	138.88	131.20
1	A	268	GLY	CA-C-N	5.90	128.78	120.28
1	A	268	GLY	C-N-CA	5.90	128.78	120.28
1	B	239	SER	CA-C-O	-5.90	115.38	121.87
1	A	355	PHE	O-C-N	-5.86	115.91	122.12
1	A	126	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	94	LEU	O-C-N	5.52	130.22	123.21
1	B	207	ASP	CA-CB-CG	-5.47	107.13	112.60
1	B	380	TYR	CA-C-O	-5.46	115.05	121.16
1	A	495	SER	CA-C-N	5.44	127.57	120.28
1	A	495	SER	C-N-CA	5.44	127.57	120.28
1	B	123	PHE	O-C-N	5.39	127.91	122.09
1	B	270	ASN	CA-CB-CG	5.29	117.89	112.60
1	B	122[A]	GLU	CA-C-N	5.28	127.63	120.44
1	B	122[A]	GLU	C-N-CA	5.28	127.63	120.44
1	B	122[B]	GLU	CA-C-N	5.28	127.63	120.44
1	B	122[B]	GLU	C-N-CA	5.28	127.63	120.44
1	B	294	ALA	O-C-N	5.26	128.37	122.22
1	B	171	GLY	O-C-N	-5.25	118.26	122.51
1	B	330	ALA	O-C-N	5.22	128.10	122.15
1	A	163	LEU	CA-C-O	5.16	126.57	120.69
1	B	505	SER	CA-C-N	-5.12	115.51	122.93
1	B	505	SER	C-N-CA	-5.12	115.51	122.93
1	A	81	VAL	O-C-N	5.11	128.39	123.03
1	B	336	SER	CA-C-O	5.05	125.78	120.42
1	A	505	SER	CA-C-O	5.03	125.88	120.70

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	4112	0	4023	49	0
1	B	4188	0	4086	47	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	43	0	22	0	0
3	B	43	0	22	0	0
4	A	910	0	0	26	0
4	B	899	0	0	22	0
All	All	10204	0	8153	96	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 6.

All (96) 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:36[B]:GLN:HG2	4:B:1719:HOH:O	1.81	0.79
1:B:212:LYS:HE2	4:B:1756:HOH:O	1.84	0.76
1:B:408[A]:THR:HG21	4:B:2531:HOH:O	1.91	0.70
1:B:164[A]:GLU:OE2	4:B:2303:HOH:O	2.10	0.69
1:B:460:ARG:NH1	1:B:474[A]:LYS:HA	2.09	0.67
1:A:104:LYS:NZ	4:A:1649:HOH:O	2.25	0.67
1:B:357:ALA:HB3	4:B:2537:HOH:O	1.97	0.64
1:B:408[B]:THR:HG23	4:B:2227:HOH:O	1.96	0.63
1:A:266:VAL:O	1:A:269:THR:HB	1.99	0.63
1:A:438[A]:PRO:HB2	4:A:1624:HOH:O	1.98	0.62
1:A:104:LYS:HE3	1:A:411:GLN:OE1	1.99	0.62
1:A:220:LEU:HD23	1:A:257:HIS:CD2	2.35	0.61
1:B:460:ARG:NH1	1:B:474[B]:LYS:HA	2.16	0.61
1:B:76:LYS:HE2	4:B:2518:HOH:O	2.02	0.59
1:A:223:HIS:CD2	1:A:226:ILE:HD12	2.38	0.58
1:A:251:HIS:CE1	1:A:255:LEU:HD22	2.39	0.58
1:A:408[A]:THR:HG22	4:A:1594:HOH:O	2.03	0.58
1:B:498:LYS:HA	4:B:2162:HOH:O	2.04	0.57
1:A:121:GLU:HG3	4:A:1339:HOH:O	2.03	0.56
1:B:442[B]:ASP:OD1	1:B:492:HIS:HB3	2.05	0.56
1:B:522:LYS:HE3	4:B:2151:HOH:O	2.05	0.56
1:B:251:HIS:CE1	1:B:255:LEU:HD22	2.41	0.55
1:A:40:SER:HA	4:A:1442:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125[A]:LYS:CD	4:A:846:HOH:O	2.54	0.54
1:B:33[B]:LYS:NZ	4:B:2128:HOH:O	2.40	0.54
1:A:408[A]:THR:HG23	1:A:499:ILE:O	2.08	0.54
1:A:385:LYS:NZ	4:A:1660:HOH:O	2.38	0.53
1:B:310:ILE:O	1:B:313[B]:VAL:HG12	2.08	0.53
1:B:408[B]:THR:OG1	1:B:499:ILE:O	2.29	0.50
1:B:442[B]:ASP:OD1	1:B:492:HIS:O	2.29	0.50
1:B:504:ILE:HG12	1:B:506:SER:O	2.12	0.50
1:A:439[B]:GLY:O	1:A:494:SER:OG	2.30	0.49
1:B:439[A]:GLY:O	1:B:495:SER:HB2	2.12	0.49
1:B:216:LYS:O	1:B:220:LEU:HG	2.11	0.49
1:A:408[B]:THR:OG1	1:A:499:ILE:O	2.29	0.49
1:A:125[A]:LYS:HD2	4:A:846:HOH:O	2.12	0.48
1:A:125[A]:LYS:HD3	4:A:846:HOH:O	2.14	0.48
1:B:437[B]:ILE:HD12	1:B:499:ILE:HD13	1.95	0.48
1:A:233:SER:HB2	1:A:246:TYR:CZ	2.49	0.48
1:A:121:GLU:HG2	4:A:1240:HOH:O	2.13	0.47
1:A:172[A]:LYS:HE2	4:A:1426:HOH:O	2.15	0.47
1:A:186[A]:CYS:O	1:A:187[A]:ALA:HB2	2.15	0.47
1:A:297:LEU:HD21	4:A:1663:HOH:O	2.14	0.47
1:B:214:LYS:HE2	4:B:2319:HOH:O	2.14	0.47
1:B:522:LYS:HE2	4:B:2500:HOH:O	2.14	0.46
1:A:172[A]:LYS:NZ	4:A:1547:HOH:O	2.45	0.46
1:B:244[A]:LYS:NZ	4:B:2237:HOH:O	2.49	0.46
1:A:348:GLY:HA3	4:A:1406:HOH:O	2.15	0.46
1:B:437[A]:ILE:HD12	1:B:499:ILE:HD13	1.96	0.46
1:B:442[A]:ASP:HB2	4:B:2348:HOH:O	2.15	0.46
1:B:494:SER:HB3	4:B:2348:HOH:O	2.16	0.46
1:A:184:GLN:NE2	4:A:1316:HOH:O	2.49	0.46
1:B:470:PHE:CZ	1:B:472[B]:ARG:HG3	2.51	0.45
1:A:64:GLY:HA2	4:A:1465:HOH:O	2.15	0.45
1:A:187[A]:ALA:HB3	1:A:201[A]:CYS:SG	2.56	0.45
1:A:223:HIS:CD2	1:A:225:PRO:HD2	2.50	0.45
1:B:46:TYR:OH	1:B:442[B]:ASP:OD2	2.30	0.45
1:B:495:SER:OG	1:B:497:GLU:HG3	2.17	0.45
1:A:82[A]:LYS:NZ	4:A:1325:HOH:O	2.49	0.45
1:A:411:GLN:HG2	4:A:1646:HOH:O	2.16	0.45
1:A:16:ASN:ND2	4:A:1255:HOH:O	2.49	0.45
1:A:236:LYS:HE3	4:A:1679:HOH:O	2.16	0.44
1:B:59:LYS:NZ	4:B:2303:HOH:O	2.49	0.44
1:A:262:GLU:OE1	1:A:262:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASN:ND2	4:B:1932:HOH:O	2.50	0.44
1:B:236:LYS:NZ	4:B:2475:HOH:O	2.50	0.44
1:A:252:GLN:NE2	4:A:1713:HOH:O	2.50	0.44
1:A:411:GLN:NE2	4:A:1645:HOH:O	2.50	0.44
1:B:36[B]:GLN:NE2	4:B:1720:HOH:O	2.50	0.44
1:B:284[B]:ASN:ND2	4:B:1973:HOH:O	2.49	0.43
1:B:508:SER:HB3	1:B:530:PHE:CD1	2.53	0.43
1:B:387:GLN:HB3	4:B:2535:HOH:O	2.18	0.43
1:A:264:LYS:HE2	4:A:910:HOH:O	2.17	0.43
1:B:167:PHE:O	1:B:170:ARG:HB2	2.19	0.42
1:A:257:HIS:ND1	1:A:258[B]:PRO:HD2	2.34	0.42
1:A:492:HIS:HE1	4:A:1120:HOH:O	2.02	0.42
1:A:315:GLY:HA3	1:A:323:HIS:CD2	2.56	0.41
1:B:292:GLU:OE2	1:B:299:LYS:HE2	2.20	0.41
1:B:408[A]:THR:HG23	1:B:534:LYS:C	2.45	0.41
1:A:508:SER:HB3	1:A:530:PHE:CD1	2.56	0.41
1:B:401:VAL:HB	4:B:2377:HOH:O	2.20	0.41
1:A:328:ILE:HG23	4:A:1682:HOH:O	2.21	0.41
1:A:504:ILE:HG12	1:A:506:SER:O	2.21	0.41
1:A:52:GLY:HA2	1:A:153:TRP:CD1	2.56	0.40
1:A:472:ARG:HD3	4:A:1261:HOH:O	2.22	0.40
1:B:504:ILE:O	1:B:504:ILE:HG23	2.21	0.40
1:A:73:LEU:HD23	1:A:474[B]:LYS:O	2.21	0.40
1:A:325:THR:OG1	1:A:328:ILE:HD13	2.21	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	550/535 (103%)	534 (97%)	12 (2%)	4 (1%)	18 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	559/535 (104%)	543 (97%)	11 (2%)	5 (1%)	14	3
All	All	1109/1070 (104%)	1077 (97%)	23 (2%)	9 (1%)	18	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	SER
1	B	381	SER
1	B	438[A]	PRO
1	B	438[B]	PRO
1	B	501	SER
1	A	424	ASN
1	A	438[A]	PRO
1	A	438[B]	PRO
1	B	424	ASN

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	464/452 (103%)	454 (98%)	10 (2%)	45	18
1	B	480/452 (106%)	474 (99%)	6 (1%)	61	36
All	All	944/904 (104%)	928 (98%)	16 (2%)	53	25

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	42	THR
1	A	45	ASN
1	A	226	ILE
1	A	235	ASN
1	A	236	LYS
1	A	291	SER

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Mol	Chain	Res	Type
1	A	328	ILE
1	A	408[A]	THR
1	A	408[B]	THR
1	B	42	THR
1	B	45	ASN
1	B	170	ARG
1	B	495	SER
1	B	499	ILE
1	B	533	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	184	GLN
1	A	203	ASN
1	A	223	HIS
1	A	492	HIS
1	A	524	ASN
1	B	16	ASN
1	B	151	ASN
1	B	203	ASN
1	B	223	HIS
1	B	251	HIS
1	B	257	HIS
1	B	342	GLN
1	B	387	GLN
1	B	502	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	APU	A	601	-	47,47,47	0.99	1 (2%)	70,72,72	1.28	6 (8%)
3	APU	B	602	-	47,47,47	1.01	1 (2%)	70,72,72	1.46	9 (12%)

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
3	APU	A	601	-	-	4/26/58/58	0/5/5/5
3	APU	B	602	-	-	4/26/58/58	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	APU	O2U-C2U	2.76	1.28	1.23
3	A	601	APU	PU-O3D	2.05	1.63	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	APU	N3U-C2U-N1U	4.90	121.27	114.89
3	B	602	APU	C4U-N3U-C2U	-4.35	121.21	126.61
3	B	602	APU	C6U-C5U-C4U	4.10	124.77	119.53
3	A	601	APU	N3U-C2U-N1U	3.86	119.92	114.89
3	A	601	APU	O4B-C4B-C5B	3.43	116.47	109.22
3	A	601	APU	O2B-C2B-C3B	2.99	119.56	111.19
3	B	602	APU	O2B-C2B-C3B	2.94	119.42	111.19
3	B	602	APU	O4B-C4B-C5B	2.84	115.23	109.22
3	A	601	APU	C4U-N3U-C2U	-2.81	123.12	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	APU	O3B-C3B-C2B	-2.76	101.78	111.68
3	A	601	APU	O2U-C2U-N1U	-2.71	119.27	122.80
3	B	602	APU	O3B-C3B-C2B	-2.42	103.00	111.68
3	B	602	APU	O4B-C1B-N9A	-2.27	103.74	108.09
3	B	602	APU	O4D-C1D-C2D	-2.10	102.12	106.62
3	B	602	APU	O3X-PU-O1X	2.09	118.99	110.83

There are no chirality outliers.

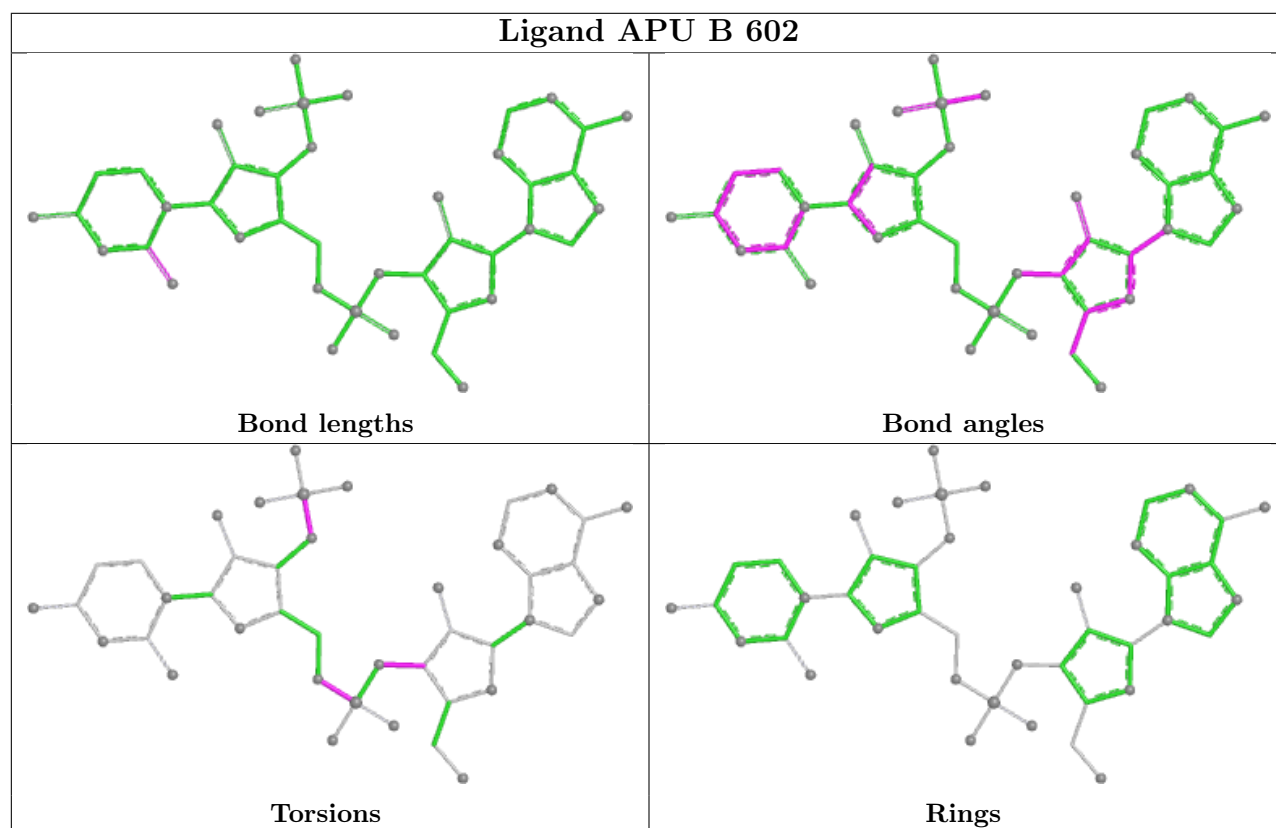
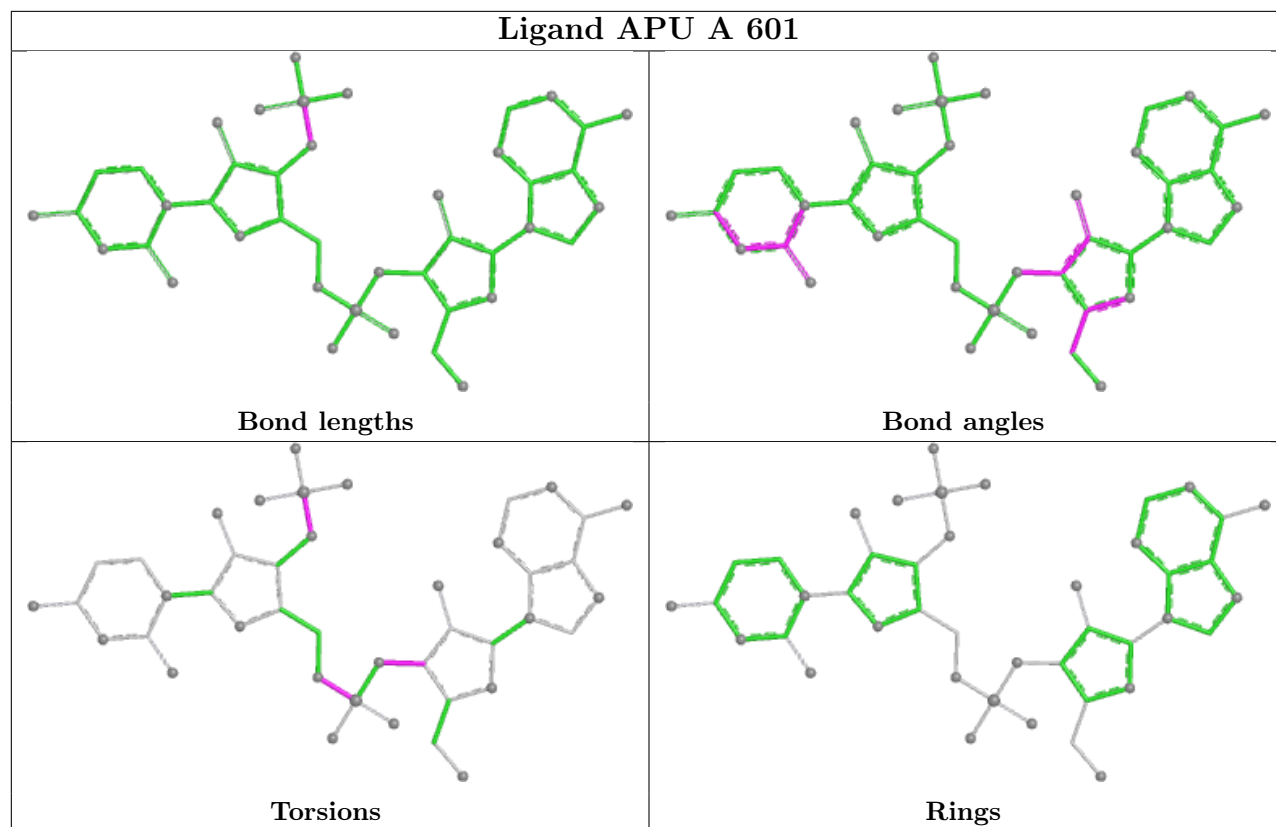
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	APU	C4B-C3B-O3B-PA
3	B	602	APU	C4B-C3B-O3B-PA
3	A	601	APU	C2B-C3B-O3B-PA
3	B	602	APU	C2B-C3B-O3B-PA
3	A	601	APU	C5D-O5D-PA-O1A
3	B	602	APU	C5D-O5D-PA-O1A
3	B	602	APU	C3D-O3D-PU-O1X
3	A	601	APU	C3D-O3D-PU-O1X

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	520/535 (97%)	0.75	53 (10%)	12 14	10, 23, 45, 66	35 (6%)
1	B	522/535 (97%)	0.49	41 (7%)	18 22	10, 21, 38, 60	41 (7%)
All	All	1042/1070 (97%)	0.62	94 (9%)	15 17	10, 22, 43, 66	76 (7%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	9.7
1	A	439[A]	GLY	7.0
1	A	353	ILE	6.0
1	A	348	GLY	5.9
1	B	499	ILE	5.2
1	A	187[A]	ALA	4.9
1	A	499	ILE	4.9
1	B	353[A]	ILE	4.7
1	A	531	PHE	4.5
1	B	187[A]	ALA	4.4
1	B	186[A]	CYS	4.1
1	B	350	LEU	4.0
1	A	266	VAL	4.0
1	A	328	ILE	3.8
1	A	497	GLU	3.7
1	A	438[A]	PRO	3.7
1	A	338	LEU	3.6
1	B	531	PHE	3.6
1	B	202[A]	ILE	3.6
1	A	269	THR	3.5
1	A	3	ASP	3.4
1	B	533	ILE	3.4
1	B	501	SER	3.4
1	A	292	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	349	GLU	3.3
1	A	40	SER	3.3
1	B	502	ASN	3.3
1	A	202[A]	ILE	3.3
1	A	254	ALA	3.1
1	A	231	SER	3.1
1	A	170	ARG	3.1
1	A	217	ILE	3.0
1	B	460	ARG	3.0
1	A	500	HIS	2.9
1	A	498	LYS	2.8
1	B	171	GLY	2.8
1	A	263	LEU	2.8
1	B	69	ASN	2.8
1	B	351[A]	VAL	2.8
1	B	504	ILE	2.8
1	B	507	ASP	2.7
1	B	3	ASP	2.7
1	B	268	GLY	2.7
1	B	4	ASP	2.7
1	B	170	ARG	2.7
1	A	228	ASN	2.6
1	B	474[A]	LYS	2.6
1	A	389	PHE	2.6
1	B	389	PHE	2.6
1	A	502	ASN	2.6
1	B	201[A]	CYS	2.5
1	A	268	GLY	2.5
1	A	203	ASN	2.5
1	B	110	LEU	2.5
1	A	507	ASP	2.5
1	B	500	HIS	2.4
1	A	255	LEU	2.4
1	B	40	SER	2.4
1	A	185	ALA	2.3
1	A	220	LEU	2.3
1	B	520	HIS	2.3
1	A	382	PRO	2.3
1	B	6	VAL	2.3
1	A	215	THR	2.3
1	A	265	THR	2.3
1	A	504	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	357	ALA	2.2
1	A	234	PRO	2.2
1	A	213	THR	2.2
1	A	257	HIS	2.2
1	B	349	GLU	2.2
1	A	474[A]	LYS	2.2
1	B	348	GLY	2.2
1	A	501	SER	2.2
1	A	347	VAL	2.2
1	A	267	THR	2.2
1	B	439[A]	GLY	2.2
1	A	219	SER	2.2
1	A	5	VAL	2.2
1	B	338	LEU	2.1
1	B	269	THR	2.1
1	A	494	SER	2.1
1	B	352[A]	ASP	2.1
1	A	496	SER	2.1
1	A	4	ASP	2.1
1	B	169	THR	2.1
1	B	521	THR	2.1
1	A	533	ILE	2.1
1	B	382	PRO	2.1
1	A	154	GLU	2.0
1	B	438[A]	PRO	2.0
1	B	2	ALA	2.0
1	B	266	VAL	2.0
1	B	273	PHE	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.

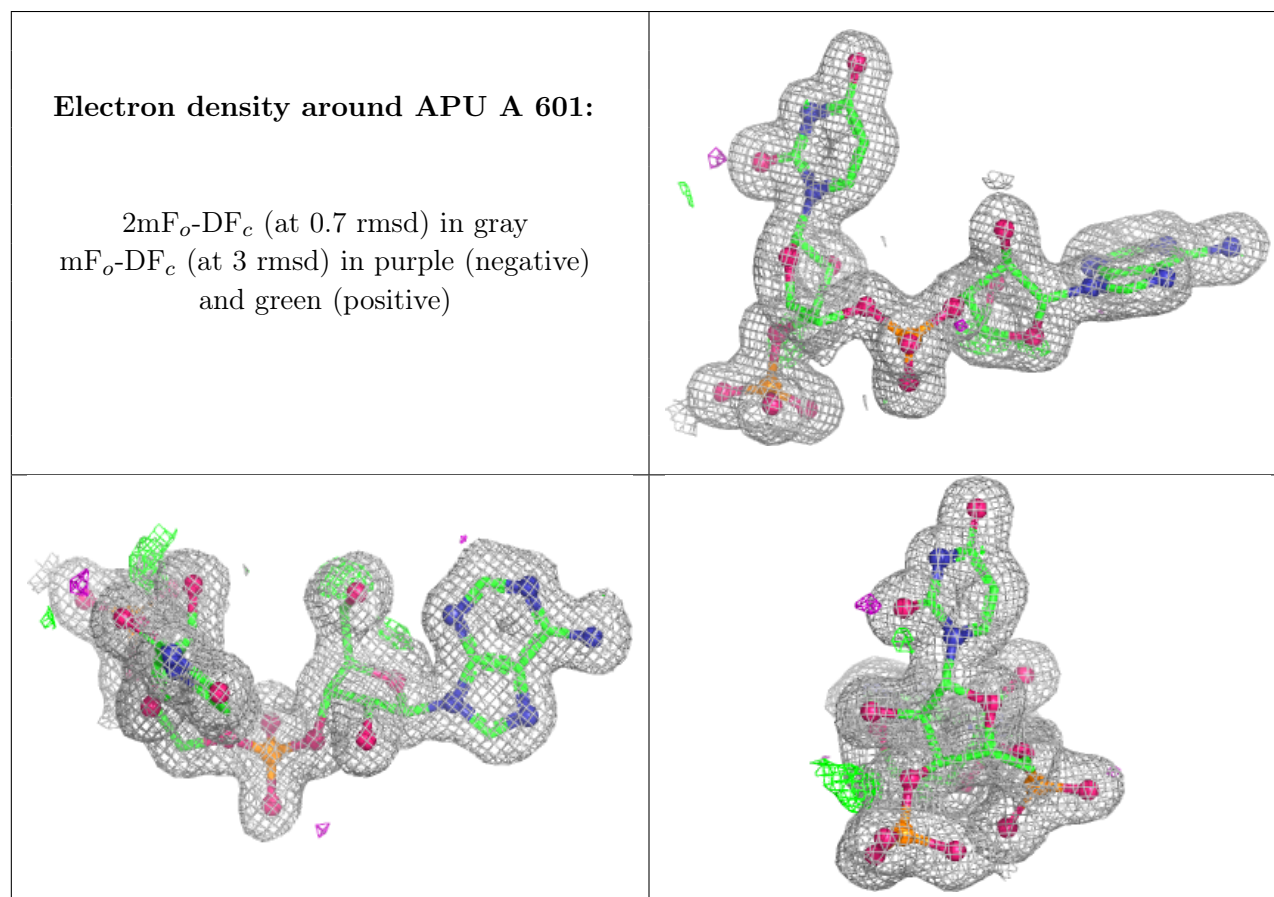
6.4 Ligands [i](#)

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.

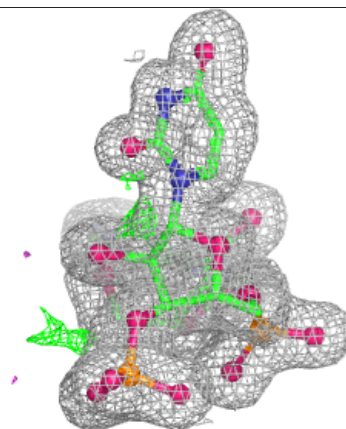
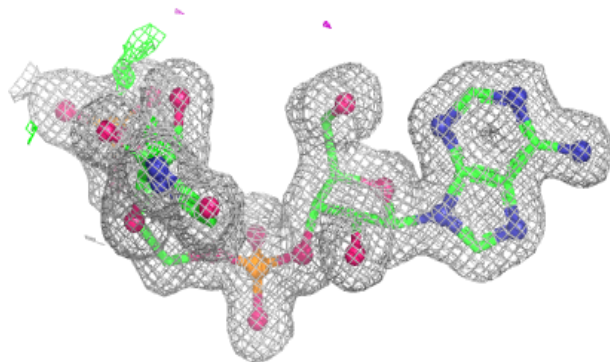
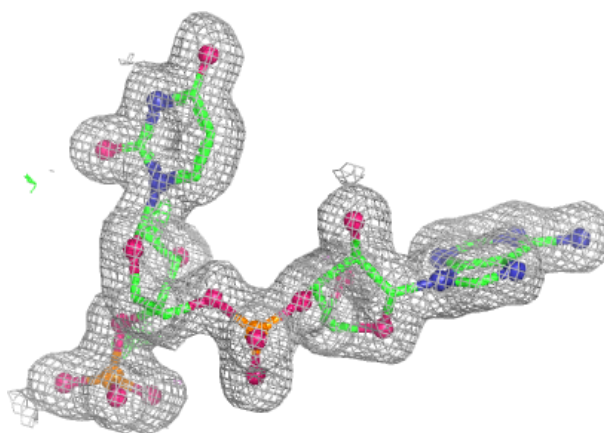
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	B	708	1/1	0.93	0.18	34,34,34,34	0
2	CL	A	703	1/1	0.94	0.10	38,38,38,38	0
2	CL	B	706	1/1	0.97	0.09	28,28,28,28	0
2	CL	A	702	1/1	0.97	0.07	24,24,24,24	0
3	APU	A	601	43/43	0.97	0.06	15,18,21,21	0
3	APU	B	602	43/43	0.97	0.06	14,17,21,22	0
2	CL	B	709	1/1	0.98	0.09	28,28,28,28	0
2	CL	B	707	1/1	0.98	0.07	27,27,27,27	0
2	CL	A	704	1/1	0.98	0.08	31,31,31,31	0
2	CL	A	701	1/1	0.99	0.06	20,20,20,20	0
2	CL	B	705	1/1	0.99	0.07	19,19,19,19	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 APU B 602:

$2mF_o-DF_c$ (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.