



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:31 PM UTC

PDB ID : 1DDT / pdb_00001ddt
Title : THE REFINED STRUCTURE OF DIMERIC DIPHTHERIA TOXIN AT 2.0
ANGSTROMS RESOLUTION
Authors : Bennett, M.J.; Eisenberg, D.
Deposited on : 1994-03-01
Resolution : 2.00 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

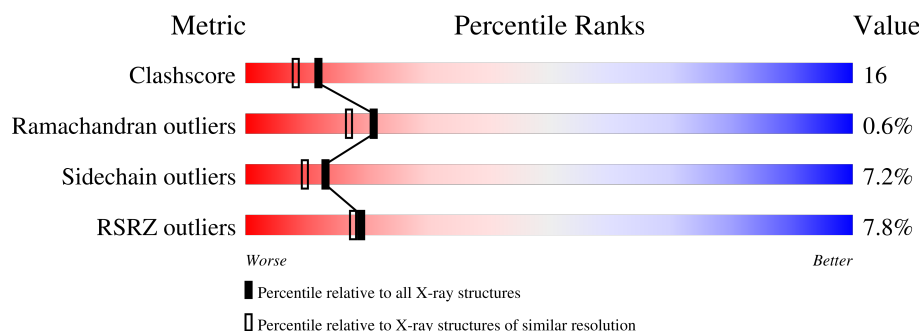
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	

2 Entry composition [i](#)

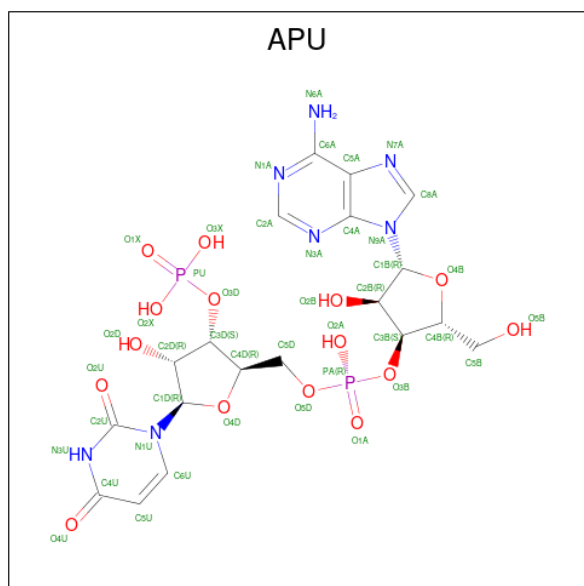
There are 3 unique types of molecules in this entry. The entry contains 4469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIPHTHERIA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4021	2531	683	795	12			

- Molecule 2 is ADENYLYL-3'-5'-PHOSPHO-URIDINE-3'-MONOPHOSPHATE (CCD ID: APU) (formula: C₁₉H₂₅N₇O₁₅P₂).



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

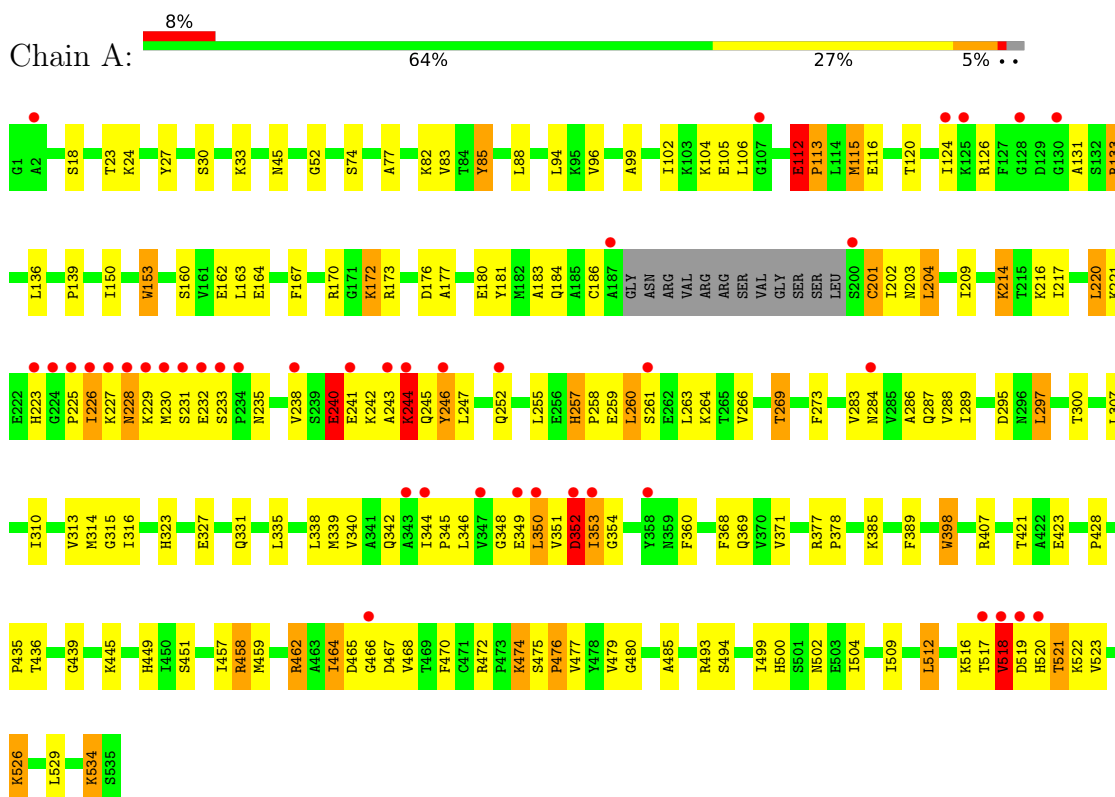
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	405	Total	O	0	0
			405	405		

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: DIPHTHERIA TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.64Å 92.56Å 65.58Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 91.8 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available) 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 118.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4469	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: APU

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	1.03	2/4102 (0.0%)	1.62	48/5556 (0.9%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	MET	SD-CE	-8.98	1.57	1.79
1	A	459	MET	SD-CE	-5.02	1.67	1.79

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLU	CA-C-N	10.45	131.11	119.83
1	A	112	GLU	C-N-CA	10.45	131.11	119.83
1	A	423	GLU	N-CA-C	9.81	122.99	111.71
1	A	288	VAL	N-CA-C	-8.12	105.22	113.10
1	A	348	GLY	N-CA-C	7.78	122.13	112.79
1	A	113	PRO	N-CA-C	-7.71	99.16	111.03
1	A	466	GLY	N-CA-C	-7.11	105.03	115.63
1	A	474	LYS	N-CA-C	-7.04	103.53	111.07
1	A	266	VAL	N-CA-C	6.95	121.89	111.89
1	A	244	LYS	N-CA-C	-6.88	103.71	111.14
1	A	226	ILE	N-CA-C	-6.72	104.11	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	VAL	N-CA-C	-6.71	99.98	108.84
1	A	340	VAL	N-CA-C	-6.67	103.98	110.72
1	A	126	ARG	N-CA-C	6.54	118.41	111.28
1	A	247	LEU	N-CA-C	6.50	118.37	111.28
1	A	77	ALA	N-CA-C	-6.45	99.20	109.59
1	A	458	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	A	389	PHE	N-CA-C	-6.22	98.38	108.52
1	A	257	HIS	CA-C-N	6.17	127.55	119.84
1	A	257	HIS	C-N-CA	6.17	127.55	119.84
1	A	368	PHE	N-CA-C	-6.03	104.63	111.14
1	A	499	ILE	N-CA-C	-5.82	101.24	109.63
1	A	327	GLU	N-CA-C	5.82	117.29	111.07
1	A	164	GLU	N-CA-C	-5.77	102.73	111.56
1	A	371	VAL	N-CA-C	5.73	118.25	111.09
1	A	476	PRO	N-CA-C	5.72	119.85	111.03
1	A	260	LEU	N-CA-C	-5.72	103.13	111.30
1	A	99	ALA	N-CA-C	5.55	118.26	111.82
1	A	240	GLU	N-CA-C	-5.54	104.66	111.75
1	A	464	ILE	N-CA-C	-5.54	97.81	109.34
1	A	520	HIS	CA-C-N	5.47	131.06	123.07
1	A	520	HIS	C-N-CA	5.47	131.06	123.07
1	A	85	TYR	CB-CA-C	-5.39	102.68	109.31
1	A	131	ALA	N-CA-C	-5.29	102.69	110.52
1	A	526	LYS	CD-CE-NZ	5.29	128.82	111.90
1	A	24	LYS	N-CA-C	5.25	118.27	110.39
1	A	480	GLY	CA-C-O	-5.22	115.87	121.35
1	A	534	LYS	CA-C-N	5.20	131.06	121.70
1	A	534	LYS	C-N-CA	5.20	131.06	121.70
1	A	186	CYS	CA-C-N	5.17	131.01	121.70
1	A	186	CYS	C-N-CA	5.17	131.01	121.70
1	A	153	TRP	N-CA-C	5.12	117.53	111.33
1	A	385	LYS	CA-C-N	-5.11	114.50	122.73
1	A	385	LYS	C-N-CA	-5.11	114.50	122.73
1	A	360	PHE	N-CA-C	-5.03	105.88	111.36
1	A	398	TRP	N-CA-C	-5.02	102.43	109.96
1	A	295	ASP	N-CA-C	5.01	119.25	113.18
1	A	24	LYS	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain

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	4021	0	3951	126	0
2	A	43	0	22	0	0
3	A	405	0	0	9	0
All	All	4469	0	3973	126	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 16.

All (126) 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:353:ILE:HG13	1:A:354:GLY:N	1.90	0.85
1:A:436:THR:O	1:A:467:ASP:HB3	1.78	0.84
1:A:283:VAL:O	1:A:287:GLN:HG3	1.78	0.83
1:A:216:LYS:O	1:A:220:LEU:HD22	1.82	0.79
1:A:344:ILE:HB	1:A:352:ASP:HB3	1.66	0.77
1:A:351:VAL:HG22	1:A:353:ILE:HG12	1.69	0.75
1:A:30:SER:HA	1:A:33:LYS:HE2	1.69	0.74
1:A:470:PHE:HE1	1:A:512:LEU:HD22	1.53	0.72
1:A:104:LYS:HE3	1:A:105:GLU:OE2	1.90	0.72
1:A:85:TYR:CE1	1:A:133:ARG:HD2	2.25	0.71
1:A:240:GLU:OE1	1:A:283:VAL:HG21	1.89	0.71
1:A:238:VAL:HG12	1:A:346:LEU:HB3	1.73	0.70
1:A:18:SER:HB2	3:A:822:HOH:O	1.92	0.70
1:A:223:HIS:CD2	1:A:225:PRO:HD2	2.28	0.69
1:A:344:ILE:HD13	1:A:352:ASP:HA	1.75	0.69
1:A:94:LEU:HD11	1:A:136:LEU:HD13	1.75	0.67
1:A:344:ILE:CD1	1:A:352:ASP:HA	2.26	0.66
1:A:240:GLU:HA	1:A:243:ALA:HB3	1.78	0.65
1:A:263:LEU:H	1:A:331:GLN:HE22	1.43	0.65
1:A:133:ARG:HD3	3:A:677:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PHE:O	1:A:170:ARG:HB2	1.99	0.62
1:A:518:VAL:HB	1:A:523:VAL:CG1	2.31	0.61
1:A:315:GLY:HA3	1:A:323:HIS:CD2	2.37	0.60
1:A:183:ALA:HB1	1:A:203:ASN:HD22	1.67	0.59
1:A:351:VAL:O	1:A:351:VAL:HG13	2.03	0.59
1:A:349:GLU:O	1:A:350:LEU:HB3	2.01	0.59
1:A:220:LEU:O	1:A:226:ILE:HG21	2.02	0.58
1:A:269:THR:HG23	3:A:916:HOH:O	2.03	0.58
1:A:238:VAL:HG22	1:A:242:LYS:HB3	1.85	0.58
1:A:344:ILE:CB	1:A:352:ASP:HB3	2.34	0.58
1:A:398:TRP:HH2	1:A:509:ILE:HD12	1.67	0.58
1:A:85:TYR:CD1	1:A:133:ARG:HD2	2.41	0.55
1:A:230:MET:O	1:A:233:SER:HB3	2.06	0.55
1:A:518:VAL:HB	1:A:523:VAL:HG12	1.87	0.55
1:A:470:PHE:CE1	1:A:512:LEU:HD22	2.37	0.55
1:A:435:PRO:HB2	1:A:504:ILE:HD11	1.88	0.55
1:A:216:LYS:NZ	1:A:259:GLU:O	2.40	0.55
1:A:260:LEU:HA	1:A:331:GLN:NE2	2.21	0.55
1:A:120:THR:O	1:A:124:ILE:HG13	2.07	0.54
1:A:263:LEU:H	1:A:331:GLN:NE2	2.05	0.54
1:A:500:HIS:HD2	1:A:502:ASN:H	1.56	0.54
1:A:516:LYS:HG3	1:A:523:VAL:HG13	1.90	0.54
1:A:462:ARG:HG3	1:A:470:PHE:O	2.08	0.54
1:A:289:ILE:O	1:A:350:LEU:HD22	2.08	0.53
1:A:504:ILE:HD12	3:A:684:HOH:O	2.09	0.53
1:A:204:LEU:HG	1:A:209:ILE:HD11	1.90	0.53
1:A:286:ALA:HB1	1:A:344:ILE:HA	1.89	0.53
1:A:102:ILE:O	1:A:106:LEU:HB2	2.08	0.52
1:A:233:SER:HB2	1:A:246:TYR:CZ	2.45	0.52
1:A:220:LEU:HD12	1:A:257:HIS:CD2	2.45	0.52
1:A:18:SER:OG	1:A:82:LYS:HE2	2.10	0.52
1:A:475:SER:HB2	1:A:476:PRO:CD	2.40	0.51
1:A:500:HIS:CD2	1:A:502:ASN:H	2.28	0.51
1:A:240:GLU:O	1:A:244:LYS:HB3	2.10	0.51
1:A:240:GLU:O	1:A:244:LYS:N	2.36	0.51
1:A:261:SER:O	1:A:264:LYS:HB3	2.10	0.51
1:A:472:ARG:HD3	3:A:750:HOH:O	2.10	0.51
1:A:217:ILE:O	1:A:221:LYS:HG3	2.11	0.50
1:A:398:TRP:CH2	1:A:509:ILE:HD12	2.47	0.50
1:A:223:HIS:HB3	1:A:226:ILE:HD12	1.94	0.49
1:A:310:ILE:HD13	1:A:314:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:HA	1:A:479:VAL:HB	1.95	0.49
1:A:201:CYS:SG	1:A:203:ASN:ND2	2.83	0.49
1:A:445:LYS:HB3	1:A:445:LYS:HE2	1.47	0.48
1:A:238:VAL:CG1	1:A:346:LEU:HB3	2.43	0.48
1:A:230:MET:HA	1:A:246:TYR:OH	2.14	0.48
1:A:344:ILE:HB	1:A:345:PRO:HD3	1.95	0.48
1:A:314:MET:HB3	1:A:316:ILE:HG13	1.96	0.48
1:A:344:ILE:CG2	1:A:352:ASP:HB3	2.43	0.48
1:A:451:SER:O	1:A:485:ALA:HA	2.14	0.48
1:A:517:THR:HG22	1:A:522:LYS:HG2	1.96	0.47
1:A:177:ALA:HA	1:A:180:GLU:HG2	1.97	0.47
1:A:345:PRO:HD3	1:A:352:ASP:HB3	1.96	0.47
1:A:342:GLN:HG2	3:A:718:HOH:O	2.14	0.47
1:A:229:LYS:HA	1:A:229:LYS:HD2	1.44	0.47
1:A:172:LYS:NZ	1:A:176:ASP:HB3	2.30	0.46
1:A:202:ILE:HG22	1:A:204:LEU:HD22	1.96	0.46
1:A:516:LYS:HG3	1:A:523:VAL:O	2.16	0.46
1:A:315:GLY:HA3	1:A:323:HIS:CG	2.50	0.46
1:A:335:LEU:O	1:A:339:MET:HG3	2.15	0.46
1:A:353:ILE:CG1	1:A:354:GLY:N	2.73	0.46
1:A:398:TRP:CE2	1:A:529:LEU:HB3	2.51	0.46
1:A:349:GLU:O	1:A:350:LEU:CB	2.64	0.46
1:A:74:SER:HB2	1:A:297:LEU:HD13	1.98	0.46
1:A:104:LYS:HB3	1:A:104:LYS:HE2	1.52	0.46
1:A:516:LYS:HB2	1:A:518:VAL:HG23	1.97	0.45
1:A:428:PRO:HA	1:A:477:VAL:O	2.16	0.45
1:A:257:HIS:HA	1:A:258:PRO:HD2	1.70	0.45
1:A:407:ARG:O	1:A:493:ARG:NH2	2.48	0.45
1:A:264:LYS:HB3	1:A:264:LYS:NZ	2.32	0.44
1:A:349:GLU:O	1:A:350:LEU:HD23	2.17	0.44
1:A:310:ILE:CD1	1:A:314:MET:HE3	2.47	0.44
1:A:255:LEU:O	3:A:739:HOH:O	2.21	0.44
1:A:439:GLY:HA2	1:A:494:SER:OG	2.17	0.44
1:A:351:VAL:O	1:A:352:ASP:C	2.61	0.43
1:A:526:LYS:HE3	3:A:806:HOH:O	2.17	0.43
1:A:83:VAL:HA	1:A:160:SER:O	2.19	0.43
1:A:269:THR:HG23	3:A:753:HOH:O	2.17	0.43
1:A:115:MET:HE2	1:A:150:ILE:HG22	2.00	0.43
1:A:181:TYR:O	1:A:184:GLN:HB2	2.19	0.43
1:A:214:LYS:HD2	1:A:214:LYS:HA	1.65	0.42
1:A:183:ALA:HB1	1:A:203:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:HA	1:A:113:PRO:HD3	1.83	0.42
1:A:344:ILE:HD12	1:A:352:ASP:HA	2.02	0.42
1:A:353:ILE:HG13	1:A:354:GLY:H	1.78	0.42
1:A:241:GLU:O	1:A:244:LYS:HD2	2.20	0.42
1:A:407:ARG:HA	1:A:534:LYS:O	2.19	0.41
1:A:273:PHE:CD1	1:A:273:PHE:N	2.84	0.41
1:A:449:HIS:HB2	1:A:457:ILE:O	2.20	0.41
1:A:23:THR:HG22	1:A:27:TYR:HB2	2.02	0.41
1:A:113:PRO:HB2	1:A:116:GLU:HG3	2.02	0.41
1:A:315:GLY:CA	1:A:323:HIS:CD2	3.04	0.41
1:A:349:GLU:O	1:A:350:LEU:CD2	2.69	0.41
1:A:464:ILE:HB	1:A:468:VAL:O	2.21	0.41
1:A:228:ASN:O	1:A:231:SER:HB2	2.21	0.41
1:A:235:ASN:C	1:A:235:ASN:HD22	2.28	0.41
1:A:349:GLU:O	1:A:349:GLU:HG3	2.20	0.41
1:A:227:LYS:HE2	1:A:227:LYS:HB3	1.81	0.40
1:A:284:ASN:CG	1:A:307:LEU:HD22	2.47	0.40
1:A:240:GLU:CD	1:A:283:VAL:HG11	2.46	0.40
1:A:377:ARG:HA	1:A:378:PRO:HD3	1.91	0.40
1:A:518:VAL:O	1:A:521:THR:O	2.39	0.40
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.75	0.40
1:A:369:GLN:HE21	1:A:369:GLN:HB2	1.66	0.40
1:A:52:GLY:HA2	1:A:153:TRP:CD1	2.57	0.40
1:A:458:ARG:HH11	1:A:458:ARG:HD2	1.67	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	519/535 (97%)	498 (96%)	18 (4%)	3 (1%)	21 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	LEU
1	A	201	CYS
1	A	352	ASP

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	442/452 (98%)	410 (93%)	32 (7%)	13	10

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	88	LEU
1	A	96	VAL
1	A	112	GLU
1	A	133	ARG
1	A	139	PRO
1	A	162	GLU
1	A	172	LYS
1	A	173	ARG
1	A	204	LEU
1	A	214	LYS
1	A	220	LEU
1	A	228	ASN
1	A	232	GLU
1	A	240	GLU
1	A	244	LYS
1	A	245	GLN
1	A	252	GLN
1	A	269	THR
1	A	297	LEU
1	A	300	THR
1	A	313	VAL

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	352	ASP
1	A	353	ILE
1	A	462	ARG
1	A	465	ASP
1	A	474	LYS
1	A	512	LEU
1	A	518	VAL
1	A	519	ASP
1	A	521	THR

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	151	ASN
1	A	203	ASN
1	A	228	ASN
1	A	235	ASN
1	A	245	GLN
1	A	331	GLN
1	A	369	GLN
1	A	373	ASN
1	A	449	HIS
1	A	500	HIS
1	A	515	GLN
1	A	524	ASN

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

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APU	A	950	-	47,47,47	1.04	2 (4%)	70,72,72	1.54	13 (18%)

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	APU	A	950	-	-	5/26/58/58	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	APU	O2B-C2B	2.49	1.49	1.43
2	A	950	APU	O2D-C2D	2.19	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	APU	C4U-N3U-C2U	-3.95	121.70	126.61
2	A	950	APU	N3U-C2U-N1U	3.71	119.72	114.89
2	A	950	APU	O3X-PU-O2X	3.16	119.67	107.80
2	A	950	APU	N6A-C6A-N1A	3.16	125.41	118.38
2	A	950	APU	PU-O3D-C3D	3.09	131.69	123.43
2	A	950	APU	O4B-C4B-C5B	3.00	115.55	109.22
2	A	950	APU	C5A-C6A-N6A	-2.83	116.27	123.29
2	A	950	APU	O2U-C2U-N1U	-2.69	119.30	122.80
2	A	950	APU	C5B-C4B-C3B	-2.65	106.50	114.84
2	A	950	APU	O3B-C3B-C2B	-2.49	102.75	111.68
2	A	950	APU	O4U-C4U-N3U	2.38	122.73	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	APU	C6U-C5U-C4U	2.33	122.51	119.53
2	A	950	APU	O3B-PA-O1A	-2.05	103.24	109.81

There are no chirality outliers.

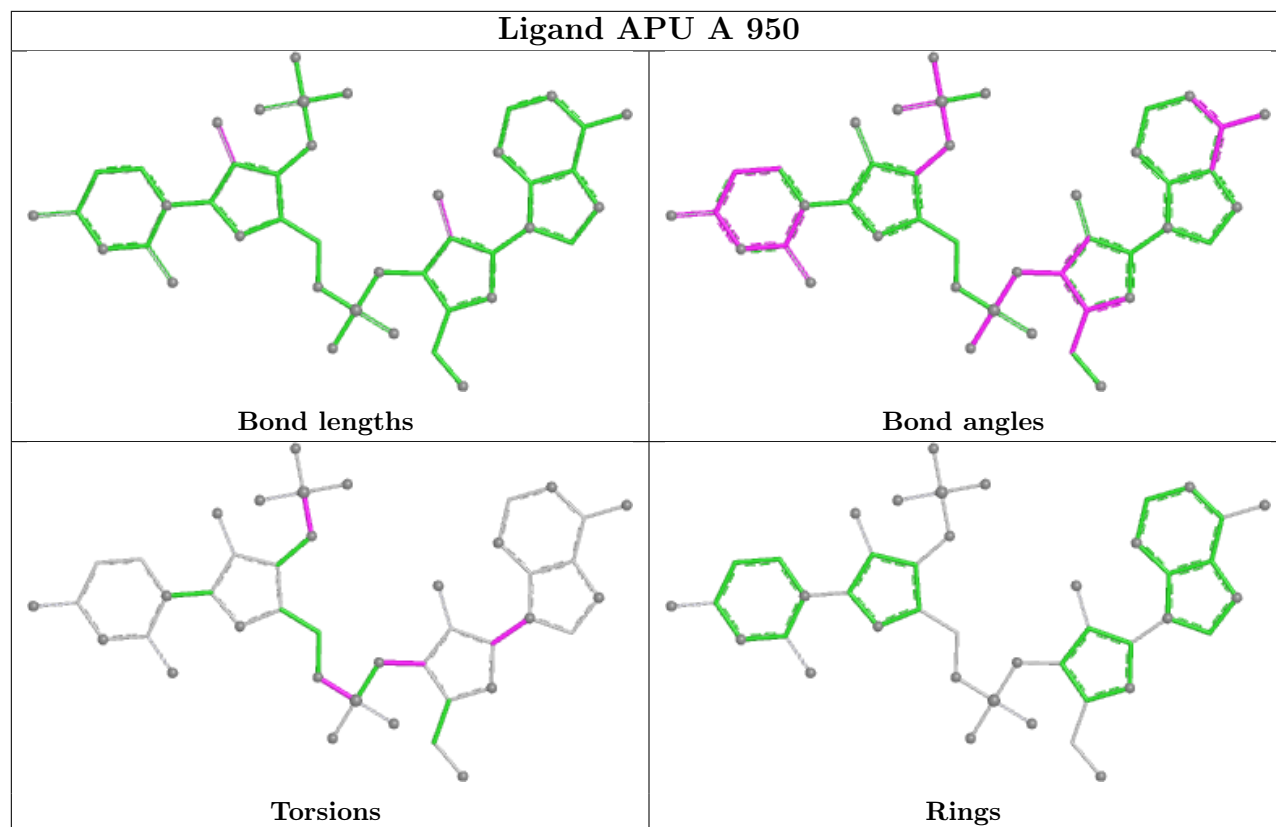
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	950	APU	C4B-C3B-O3B-PA
2	A	950	APU	C2B-C3B-O3B-PA
2	A	950	APU	C5D-O5D-PA-O1A
2	A	950	APU	C3D-O3D-PU-O2X
2	A	950	APU	O4B-C1B-N9A-C4A

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	523/535 (97%)	0.21	41 (7%) 19 18	10, 24, 59, 75	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	VAL	5.0
1	A	238	VAL	4.4
1	A	353	ILE	3.7
1	A	187	ALA	3.4
1	A	223	HIS	3.1
1	A	224	GLY	3.0
1	A	232	GLU	3.0
1	A	261	SER	3.0
1	A	230	MET	2.9
1	A	229	LYS	2.9
1	A	466	GLY	2.9
1	A	234	PRO	2.8
1	A	225	PRO	2.8
1	A	200	SER	2.8
1	A	124	ILE	2.8
1	A	2	ALA	2.7
1	A	352	ASP	2.7
1	A	350	LEU	2.7
1	A	520	HIS	2.6
1	A	227	LYS	2.6
1	A	246	TYR	2.5
1	A	128	GLY	2.5
1	A	130	GLY	2.4
1	A	226	ILE	2.4
1	A	347	VAL	2.4
1	A	243	ALA	2.4
1	A	244	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	231	SER	2.3
1	A	125	LYS	2.3
1	A	343	ALA	2.3
1	A	517	THR	2.2
1	A	107	GLY	2.2
1	A	252	GLN	2.2
1	A	284	ASN	2.2
1	A	228	ASN	2.2
1	A	241	GLU	2.1
1	A	344	ILE	2.1
1	A	233	SER	2.1
1	A	358	TYR	2.1
1	A	519	ASP	2.1
1	A	349	GLU	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](#)

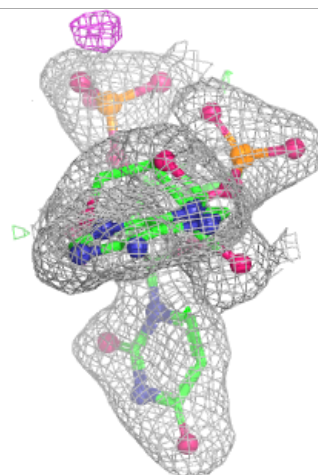
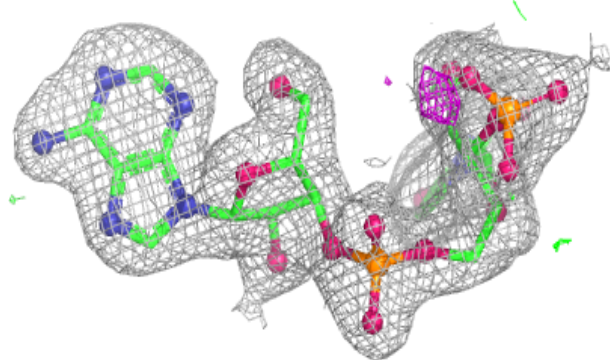
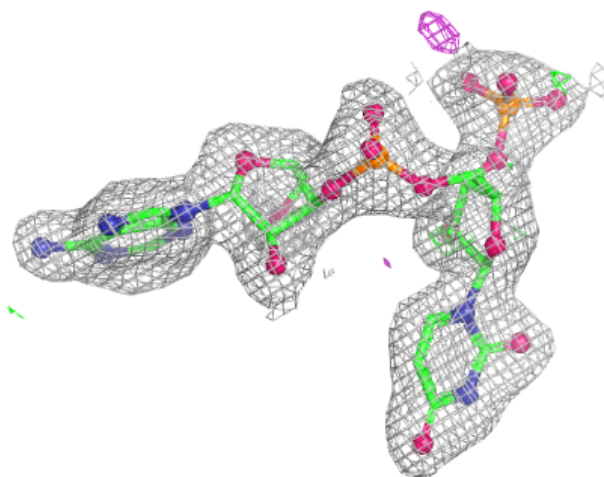
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	APU	A	950	43/43	0.96	0.06	8,17,21,22	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 A 950:

$2mF_o-DF_c$ (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.