Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:51 PM GMT

PDB ID	:	1MDT
Title	:	THE REFINED STRUCTURE OF MONOMERIC DIPHTHERIA TOXIN AT 2.3 ANGSTROMS RESOLUTION
Authors	:	Bennett, M.J.; Eisenberg, D.
Deposited on	:	1994-03-21
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

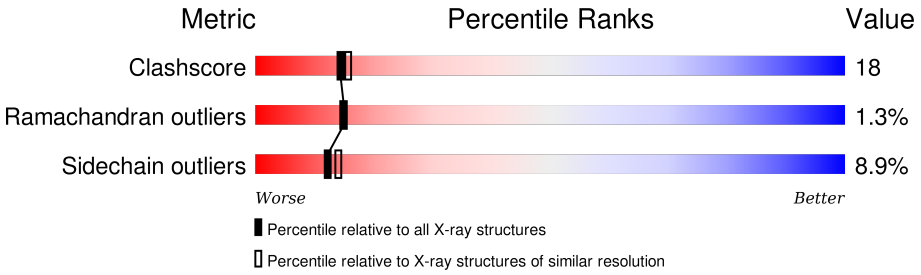
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	535	61% 31%
1	B	535	63% 31%

2 Entry composition

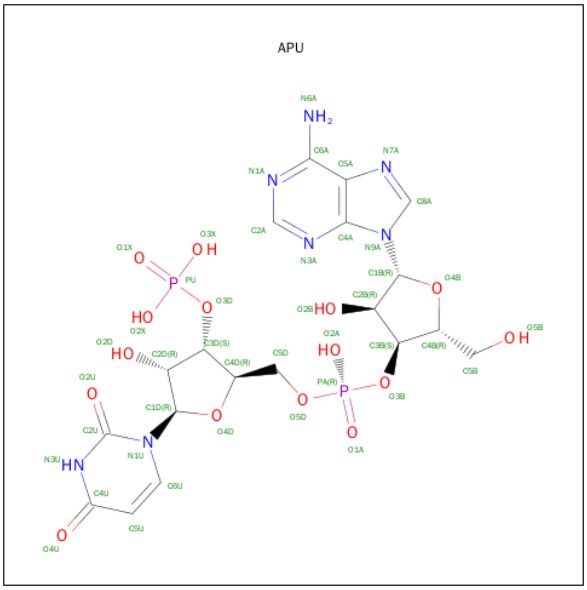
There are 3 unique types of molecules in this entry. The entry contains 8524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			
1	B	523	Total	C	N	O	S	0	0	0
			4021	2531	683	795	12			

- Molecule 2 is ADENYLYL-3'-5'-PHOSPHO-URIDINE-3'-MONOPHOSPHATE (three-letter code: APU) (formula: $C_{19}H_{25}N_7O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			43	19	7	15	2		
2	B	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	192	Total O 192 192	0	0
3	B	204	Total O 204 204	0	0

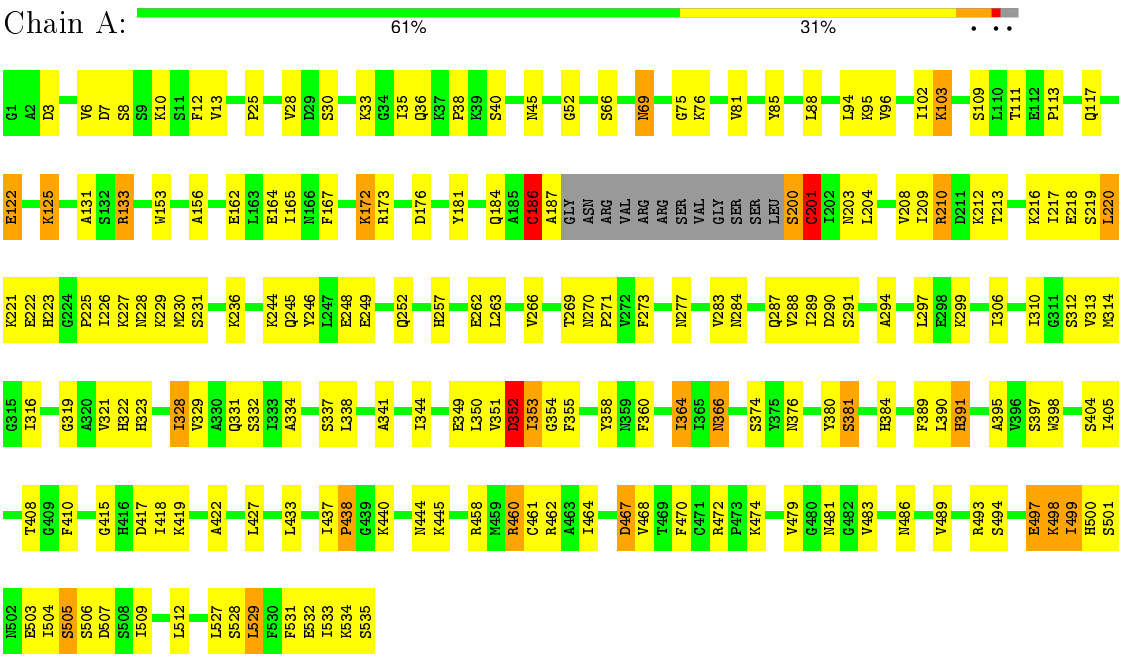
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

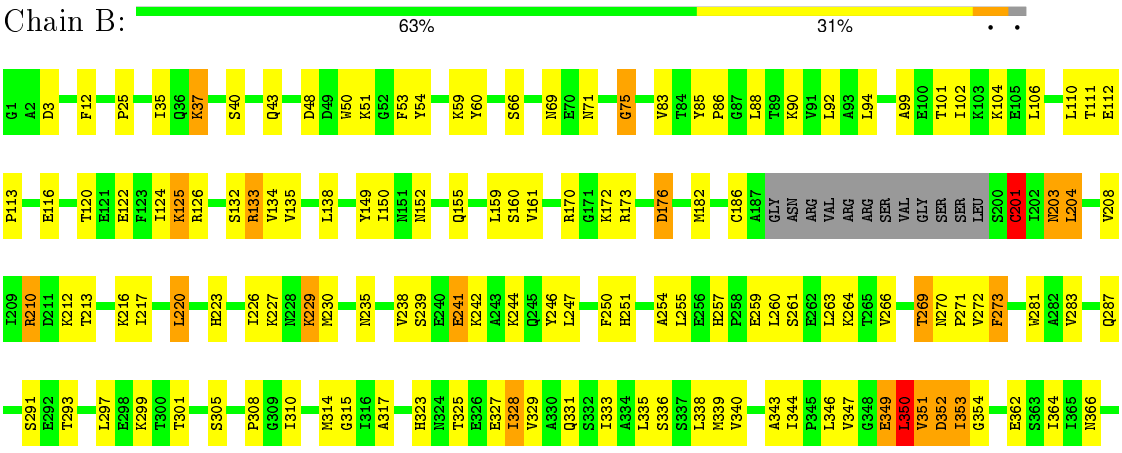
- Molecule 1: DIPHTHERIA TOXIN

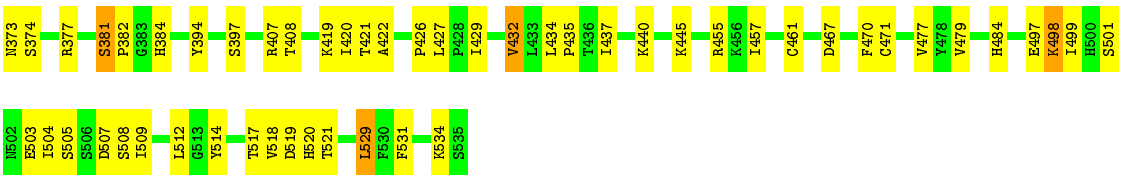
Chain A:



- Molecule 1: DIPHTHERIA TOXIN

Chain B:




N373
S374
R377
S381
P382
G383
H384
Y394
S397
R407
T408
K419
I420
T421
A422
P426
L427
P428
I429
V432
L433
L434
P435
T436
I437
K440
K445
R455
K456
I457
C461
D467
F470
C471
V477
Y478
V479
H484
E497
K498
I499
H500
S501
N502
E503
I504
S505
S506
D507
S508
I509
L512
G513
Y514
T517
V518
D519
H520
T521
L529
F530
F531
K534
S535

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	168.50Å 135.50Å 47.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.8 (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8524	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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	1.01	2/4102 (0.0%)	1.13	11/5556 (0.2%)
1	B	1.04	2/4102 (0.0%)	1.13	9/5556 (0.2%)
All	All	1.02	4/8204 (0.0%)	1.13	20/11112 (0.2%)

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
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	TRP	CB-CG	6.98	1.62	1.50
1	B	241	GLU	CG-CD	6.12	1.61	1.51
1	A	210	ARG	CZ-NH2	-5.62	1.25	1.33
1	A	156	ALA	CA-CB	5.50	1.64	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	210	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	458	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	201	CYS	N-CA-C	7.75	131.92	111.00
1	B	201	CYS	CA-CB-SG	-7.55	100.41	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	ILE	N-CA-C	-7.40	91.02	111.00
1	A	186	CYS	CA-CB-SG	6.84	126.31	114.00
1	B	176	ASP	CB-CG-OD1	6.67	124.31	118.30
1	B	210	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	467	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	103	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	A	438	PRO	N-CA-C	5.72	126.98	112.10
1	B	201	CYS	N-CA-C	5.52	125.91	111.00
1	A	460	ARG	N-CA-C	-5.38	96.47	111.00
1	B	186	CYS	CA-CB-SG	5.36	123.65	114.00
1	B	437	ILE	N-CA-C	-5.30	96.68	111.00
1	B	92	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	220	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	176	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	B	455	ARG	NE-CZ-NH2	-5.19	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	TYR	Sidechain
1	B	246	TYR	Sidechain

5.2 Too-close contacts (i)

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	145	0
1	B	4021	0	3951	144	0
2	A	43	0	22	3	0
2	B	43	0	22	1	0
3	A	192	0	0	1	0
3	B	204	0	0	9	0
All	All	8524	0	7946	290	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 18.

All (290) 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:221:LYS:NZ	1:A:353:ILE:HD11	1.72	1.03
1:B:122:GLU:HA	1:B:125:LYS:HD3	1.43	1.01
1:A:283:VAL:O	1:A:287:GLN:HG3	1.61	1.01
1:A:499:ILE:HD11	1:A:533:ILE:HD13	1.46	0.97
1:A:221:LYS:HZ2	1:A:353:ILE:HD11	1.28	0.95
1:A:220:LEU:HD23	1:A:338:LEU:HD22	1.46	0.95
1:B:125:LYS:HG2	1:B:126:ARG:N	1.89	0.87
1:A:344:ILE:HG21	1:A:352:ASP:HA	1.58	0.86
1:A:212:LYS:O	1:A:216:LYS:HG3	1.75	0.85
1:A:263:LEU:H	1:A:331:GLN:HE22	1.24	0.85
1:A:493:ARG:NH2	1:A:498:LYS:HA	1.93	0.84
1:A:493:ARG:HH22	1:A:498:LYS:HA	1.42	0.82
1:B:283:VAL:O	1:B:287:GLN:HG3	1.80	0.81
1:B:261:SER:HA	1:B:264:LYS:HE3	1.65	0.79
1:A:384:HIS:HD2	1:A:397:SER:OG	1.65	0.79
1:B:83:VAL:HG12	1:B:161:VAL:HG22	1.64	0.79
1:A:341:ALA:HB1	1:A:353:ILE:HB	1.65	0.79
1:A:223:HIS:O	1:A:227:LYS:HG3	1.83	0.79
1:B:509:ILE:HG13	1:B:531:PHE:HE2	1.50	0.76
1:B:310:ILE:HD13	1:B:314:MET:HE3	1.66	0.75
1:B:94:LEU:HD22	1:B:102:ILE:HD13	1.69	0.74
1:A:433:LEU:CD1	1:A:512:LEU:HD21	2.19	0.73
1:B:498:LYS:H	1:B:498:LYS:HD2	1.53	0.73
1:A:433:LEU:HD11	1:A:512:LEU:HD21	1.70	0.73
1:B:407:ARG:HA	1:B:534:LYS:O	1.89	0.72
1:A:221:LYS:HZ1	1:A:353:ILE:HD11	1.53	0.72
1:B:229:LYS:HA	1:B:229:LYS:HE3	1.70	0.72
1:A:266:VAL:O	1:A:269:THR:HG22	1.87	0.72
1:B:349:GLU:HG3	1:B:350:LEU:N	2.04	0.72
1:B:170:ARG:HB3	1:B:172:LYS:HG3	1.71	0.71
1:A:226:ILE:O	1:A:230:MET:HG3	1.90	0.71
1:B:125:LYS:HE2	1:B:126:ARG:HG3	1.74	0.70
1:B:497:GLU:HA	1:B:498:LYS:HE3	1.75	0.69
1:B:263:LEU:H	1:B:331:GLN:HE22	1.41	0.68
1:A:6:VAL:O	1:A:95:LYS:HE3	1.94	0.68
1:B:247:LEU:HD12	1:B:283:VAL:HG23	1.76	0.68
1:A:460:ARG:HD3	1:A:474:LYS:NZ	2.09	0.68
1:A:418:ILE:HD13	1:A:529:LEU:HD23	1.77	0.67
1:B:509:ILE:HG13	1:B:531:PHE:CE2	2.30	0.67
1:B:435:PRO:HB2	1:B:504:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:O	1:B:124:ILE:HG13	1.95	0.66
1:B:498:LYS:H	1:B:498:LYS:CD	2.08	0.66
1:B:323:HIS:HA	1:B:328:ILE:HD13	1.74	0.66
1:B:251:HIS:CE1	1:B:255:LEU:HD22	2.30	0.66
1:A:460:ARG:HD3	1:A:474:LYS:HZ3	1.61	0.65
1:B:173:ARG:HB2	1:B:210:ARG:NH2	2.10	0.65
1:A:223:HIS:HD2	1:A:226:ILE:HG13	1.61	0.64
1:A:460:ARG:HG2	1:A:474:LYS:HE2	1.80	0.64
1:A:176:ASP:OD2	1:A:210:ARG:NH2	2.31	0.64
1:A:351:VAL:HG23	1:A:351:VAL:O	1.98	0.64
1:A:7:ASP:OD2	1:A:10:LYS:HD2	1.97	0.64
1:A:263:LEU:N	1:A:331:GLN:HE22	1.92	0.64
1:B:247:LEU:HD11	1:B:343:ALA:HB2	1.80	0.63
1:A:263:LEU:H	1:A:331:GLN:NE2	1.94	0.63
1:A:223:HIS:HB3	1:A:226:ILE:HD12	1.80	0.63
1:B:467:ASP:HB2	1:B:505:SER:OG	1.98	0.63
1:A:216:LYS:O	1:A:220:LEU:HB2	1.98	0.62
1:A:291:SER:HA	1:A:351:VAL:CG1	2.30	0.62
1:A:389:PHE:CD2	1:A:527:LEU:HD23	2.35	0.62
1:A:226:ILE:HG22	1:A:230:MET:CE	2.30	0.62
1:B:210:ARG:HD3	1:B:362:GLU:OE2	1.99	0.62
1:B:94:LEU:HD12	1:B:138:LEU:HG	1.82	0.62
1:B:37:LYS:HD3	1:B:43:GLN:NE2	2.14	0.61
1:A:176:ASP:CG	1:A:210:ARG:HH22	2.04	0.61
1:A:352:ASP:O	1:A:354:GLY:N	2.34	0.61
1:B:308:PRO:HB3	1:B:514:TYR:CG	2.36	0.61
1:A:464:ILE:HD13	1:A:470:PHE:HB2	1.83	0.60
1:A:208:VAL:CG1	1:A:212:LYS:HE2	2.31	0.60
1:A:226:ILE:HG22	1:A:230:MET:HE3	1.82	0.60
1:A:390:LEU:O	1:A:391:HIS:HB2	2.00	0.60
1:B:264:LYS:HD2	3:B:1071:HOH:O	2.01	0.60
1:A:384:HIS:CD2	1:A:397:SER:OG	2.51	0.59
1:A:113:PRO:O	1:A:117:GLN:HG3	2.03	0.59
1:A:223:HIS:CD2	1:A:226:ILE:HG13	2.37	0.58
1:B:263:LEU:H	1:B:331:GLN:NE2	2.00	0.58
1:A:410:PHE:CZ	1:A:493:ARG:HB2	2.40	0.57
1:B:251:HIS:CD2	1:B:335:LEU:HD21	2.40	0.57
1:B:152:ASN:HB3	1:B:155:GLN:HB2	1.87	0.57
1:A:497:GLU:OE1	1:A:498:LYS:N	2.37	0.57
1:A:208:VAL:HG12	1:A:212:LYS:HE2	1.86	0.56
1:B:220:LEU:HD23	1:B:338:LEU:HD22	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:OE1	1:A:125:LYS:HE3	2.06	0.56
1:A:266:VAL:O	1:A:273:PHE:HD2	1.87	0.56
2:B:901:APU:O2A	2:B:901:APU:H4B	2.04	0.56
1:B:351:VAL:HG13	1:B:353:ILE:HG13	1.88	0.56
1:B:349:GLU:HG3	1:B:350:LEU:HD23	1.86	0.56
1:B:315:GLY:HA3	1:B:323:HIS:CG	2.41	0.56
1:B:327:GLU:O	1:B:331:GLN:HG3	2.05	0.55
1:B:266:VAL:O	1:B:269:THR:HB	2.06	0.55
1:A:381:SER:O	1:A:419:LYS:NZ	2.35	0.55
1:A:415:GLY:HA2	1:A:489:VAL:O	2.07	0.54
1:A:460:ARG:HG3	1:A:474:LYS:HD2	1.90	0.54
1:B:86:PRO:O	1:B:133:ARG:NH2	2.38	0.54
1:B:366:ASN:ND2	3:B:959:HOH:O	2.39	0.54
1:A:310:ILE:HD13	1:A:314:MET:HE3	1.89	0.54
1:B:325:THR:H	1:B:328:ILE:HD12	1.72	0.53
1:A:284:ASN:O	1:A:288:VAL:HG13	2.09	0.53
1:B:54:TYR:CZ	1:B:150:ILE:HG23	2.43	0.53
1:B:229:LYS:HG2	1:B:250:PHE:HA	1.91	0.53
1:B:293:THR:HG23	1:B:299:LYS:HB3	1.90	0.53
1:A:498:LYS:HE3	1:A:498:LYS:H	1.74	0.52
1:A:69:ASN:ND2	1:A:474:LYS:HZ2	2.07	0.52
1:A:103:LYS:HD2	1:A:109:SER:O	2.10	0.52
1:A:244:LYS:O	1:A:248:GLU:HG3	2.09	0.52
1:B:263:LEU:O	1:B:266:VAL:HG22	2.09	0.52
1:A:418:ILE:HD13	1:A:529:LEU:CD2	2.39	0.52
1:A:440:LYS:NZ	1:A:498:LYS:O	2.40	0.52
1:B:384:HIS:HD2	1:B:397:SER:OG	1.92	0.52
1:A:291:SER:HA	1:A:351:VAL:HG12	1.92	0.52
1:B:251:HIS:HB2	1:B:339:MET:CE	2.39	0.51
1:B:497:GLU:HA	1:B:498:LYS:CE	2.40	0.51
1:A:218:GLU:O	1:A:222:GLU:HG2	2.10	0.51
1:B:352:ASP:O	1:B:353:ILE:O	2.28	0.51
1:A:509:ILE:HG13	1:A:531:PHE:CE2	2.46	0.51
1:A:405:ILE:CG2	1:A:534:LYS:HB2	2.41	0.51
1:B:518:VAL:O	1:B:519:ASP:HB3	2.10	0.51
1:A:500:HIS:O	1:A:503:GLU:HB2	2.11	0.51
1:B:254:ALA:O	1:B:260:LEU:HD12	2.11	0.51
1:B:467:ASP:OD2	1:B:505:SER:HB3	2.11	0.51
1:A:25:PRO:HD3	1:A:66:SER:O	2.11	0.50
1:B:461:CYS:HA	1:B:470:PHE:O	2.11	0.50
1:B:111:THR:HG22	1:B:112:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HB	1:A:162:GLU:O	2.11	0.50
1:B:498:LYS:N	1:B:498:LYS:CD	2.74	0.50
1:B:349:GLU:CG	1:B:350:LEU:HD23	2.42	0.50
1:A:380:TYR:O	1:A:381:SER:C	2.49	0.50
1:A:35:ILE:HG23	2:A:901:APU:H2A	1.94	0.50
1:B:213:THR:O	1:B:217:ILE:HG13	2.11	0.49
1:A:445:LYS:HG2	1:A:461:CYS:HB2	1.94	0.49
1:A:181:TYR:O	1:A:184:GLN:HB2	2.12	0.49
1:B:421:THR:HG22	1:B:484:HIS:HB3	1.93	0.49
1:A:313:VAL:HG11	1:A:364:ILE:HD11	1.93	0.49
1:B:125:LYS:HG2	1:B:126:ARG:H	1.72	0.49
1:A:263:LEU:HB2	1:A:331:GLN:HE21	1.78	0.49
1:A:374:SER:HB3	1:A:483:VAL:HG13	1.94	0.49
1:B:270:ASN:OD1	1:B:272:VAL:HG23	2.12	0.49
1:B:90:LYS:O	1:B:134:VAL:HA	2.12	0.49
1:B:122:GLU:CA	1:B:125:LYS:HD3	2.28	0.49
1:B:315:GLY:HA3	1:B:323:HIS:CD2	2.47	0.49
1:B:373:ASN:HB3	3:B:987:HOH:O	2.12	0.49
1:A:200:SER:HB2	1:A:376:ASN:HA	1.95	0.49
1:B:170:ARG:HD2	1:B:170:ARG:N	2.28	0.49
1:B:325:THR:OG1	1:B:328:ILE:HG13	2.13	0.49
1:A:316:ILE:HG12	1:A:321:VAL:HA	1.94	0.49
1:B:351:VAL:HG13	1:B:353:ILE:CG1	2.42	0.49
1:A:422:ALA:HB1	1:A:427:LEU:HD12	1.95	0.49
1:B:432:VAL:HG12	1:B:471:CYS:HB2	1.94	0.49
1:B:220:LEU:O	1:B:226:ILE:HD12	2.13	0.48
1:B:133:ARG:HD2	3:B:914:HOH:O	2.13	0.48
1:B:101:THR:HA	1:B:104:LYS:HE2	1.96	0.48
1:A:349:GLU:C	1:A:351:VAL:H	2.16	0.48
1:B:35:ILE:HD12	1:B:53:PHE:CZ	2.49	0.48
1:B:176:ASP:CG	1:B:210:ARG:HH22	2.15	0.48
1:B:244:LYS:HE3	3:B:918:HOH:O	2.13	0.48
1:B:227:LYS:O	1:B:230:MET:HB2	2.14	0.48
1:A:334:ALA:O	1:A:337:SER:HB3	2.14	0.48
1:B:273:PHE:CD1	1:B:273:PHE:N	2.78	0.48
1:B:251:HIS:HB2	1:B:339:MET:HE1	1.97	0.47
1:B:517:THR:HA	1:B:521:THR:O	2.14	0.47
1:B:270:ASN:HB3	1:B:273:PHE:CE2	2.49	0.47
1:A:422:ALA:HB2	1:A:479:VAL:HG23	1.95	0.47
1:B:85:TYR:CE2	1:B:159:LEU:HD21	2.49	0.47
1:B:381:SER:HA	1:B:382:PRO:HD3	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:HE3	1:B:331:GLN:CG	2.45	0.47
1:B:239:SER:OG	1:B:242:LYS:HG2	2.15	0.47
1:A:512:LEU:HD22	1:A:512:LEU:N	2.29	0.46
1:B:216:LYS:HE3	1:B:331:GLN:HG2	1.97	0.46
1:B:113:PRO:HG2	1:B:116:GLU:OE2	2.15	0.46
1:A:263:LEU:CB	1:A:331:GLN:HE21	2.28	0.46
1:B:220:LEU:HD12	1:B:257:HIS:CD2	2.50	0.46
1:A:229:LYS:NZ	1:A:249:GLU:HB2	2.31	0.46
1:A:52:GLY:HA2	1:A:153:TRP:CD1	2.50	0.46
1:A:289:ILE:CG2	1:A:294:ALA:HB2	2.45	0.46
1:B:519:ASP:O	1:B:520:HIS:HB2	2.15	0.46
1:B:394:TYR:HA	1:B:422:ALA:HA	1.97	0.46
1:A:460:ARG:CD	1:A:474:LYS:HZ3	2.28	0.46
1:A:220:LEU:HD12	1:A:257:HIS:CD2	2.50	0.46
1:B:223:HIS:HB3	1:B:226:ILE:HD12	1.97	0.46
1:B:208:VAL:O	1:B:212:LYS:HG3	2.15	0.45
1:B:432:VAL:HG13	1:B:434:LEU:HD21	1.97	0.45
1:A:405:ILE:HG23	1:A:534:LYS:HB2	1.99	0.45
1:A:504:ILE:HG12	1:A:506:SER:O	2.17	0.45
1:A:85:TYR:CE1	1:A:133:ARG:HD2	2.50	0.45
1:B:421:THR:HG22	1:B:484:HIS:CD2	2.51	0.45
1:A:398:TRP:CG	1:A:404:SER:HB3	2.52	0.45
1:B:48:ASP:OD1	1:B:51:LYS:HE2	2.16	0.45
1:A:165:ILE:HD13	1:A:167:PHE:CE1	2.52	0.45
1:A:353:ILE:O	1:A:353:ILE:CG1	2.65	0.45
1:A:319:GLY:HA2	1:A:481:ASN:O	2.17	0.45
1:A:467:ASP:HB2	1:A:505:SER:HB2	1.99	0.45
1:B:247:LEU:CD1	1:B:283:VAL:HG23	2.45	0.45
1:B:272:VAL:HG21	1:B:317:ALA:CB	2.46	0.45
1:A:498:LYS:H	1:A:498:LYS:CE	2.30	0.45
1:A:366:ASN:C	1:A:366:ASN:ND2	2.70	0.45
1:A:35:ILE:HA	2:A:901:APU:N1A	2.32	0.45
1:B:270:ASN:HA	1:B:271:PRO:HD2	1.51	0.45
1:B:422:ALA:HB2	1:B:479:VAL:HG23	1.99	0.45
1:B:60:TYR:CD1	1:B:182:MET:HA	2.53	0.44
1:B:347:VAL:HG22	3:B:1026:HOH:O	2.16	0.44
1:B:445:LYS:HD3	1:B:461:CYS:HB2	1.98	0.44
1:B:85:TYR:CD2	1:B:159:LEU:HD21	2.51	0.44
1:A:30:SER:O	1:A:33:LYS:HB2	2.17	0.44
1:A:262:GLU:HB2	1:A:331:GLN:OE1	2.16	0.44
1:A:217:ILE:HG22	1:A:221:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:APU:H4B	2:A:901:APU:O2A	2.16	0.44
1:B:48:ASP:HA	1:B:51:LYS:HG3	1.99	0.44
1:A:245:GLN:NE2	1:A:249:GLU:OE2	2.50	0.44
1:A:94:LEU:HD13	1:A:102:ILE:HD13	1.99	0.44
1:A:390:LEU:HD23	1:A:395:ALA:CB	2.47	0.44
1:B:132:SER:HB2	1:B:133:ARG:CZ	2.48	0.44
1:A:33:LYS:HE2	1:A:33:LYS:HB3	1.91	0.44
1:A:433:LEU:HD22	1:A:464:ILE:HD11	1.98	0.44
1:A:186:CYS:SG	1:A:201:CYS:N	2.91	0.44
1:B:204:LEU:HA	1:B:204:LEU:HD12	1.68	0.44
1:B:176:ASP:OD2	1:B:210:ARG:NH2	2.51	0.43
1:A:291:SER:HA	1:A:351:VAL:HG11	2.00	0.43
1:A:360:PHE:CZ	1:A:364:ILE:HD12	2.53	0.43
1:A:12:PHE:HB2	1:B:12:PHE:HB2	2.00	0.43
1:A:353:ILE:HG12	1:A:353:ILE:O	2.18	0.43
1:A:226:ILE:HG22	1:A:230:MET:HE2	2.00	0.43
1:B:220:LEU:HD23	1:B:338:LEU:CD2	2.47	0.43
1:B:172:LYS:HE3	3:B:1083:HOH:O	2.18	0.43
1:A:470:PHE:HE2	1:A:472:ARG:NH1	2.16	0.43
1:A:389:PHE:O	1:A:395:ALA:HA	2.19	0.43
1:A:366:ASN:C	1:A:366:ASN:HD22	2.21	0.43
1:A:323:HIS:HA	1:A:328:ILE:HD12	2.00	0.43
1:A:172:LYS:NZ	1:A:172:LYS:HA	2.34	0.43
1:B:220:LEU:HB3	1:B:338:LEU:HD21	2.00	0.43
1:A:213:THR:O	1:A:217:ILE:HG13	2.19	0.43
1:A:433:LEU:CD2	1:A:464:ILE:HD11	2.49	0.43
1:B:340:VAL:O	1:B:344:ILE:HG13	2.17	0.43
1:A:186:CYS:O	1:A:187:ALA:HB2	2.19	0.43
1:B:308:PRO:HB3	1:B:514:TYR:CD2	2.54	0.43
1:A:289:ILE:HG22	1:A:294:ALA:HB2	2.01	0.43
1:A:96:VAL:O	1:A:102:ILE:HD11	2.18	0.43
1:A:417:ASP:HB3	1:A:486:ASN:OD1	2.19	0.43
1:B:407:ARG:HD3	1:B:407:ARG:HA	1.83	0.43
1:A:273:PHE:N	1:A:273:PHE:CD1	2.86	0.43
1:A:534:LYS:HB3	1:A:535:SER:H	1.72	0.43
1:B:508:SER:HB2	1:B:529:LEU:O	2.19	0.42
1:B:420:ILE:HG21	1:B:429:ILE:HD11	2.01	0.42
1:A:125:LYS:C	1:A:125:LYS:HD2	2.40	0.42
1:A:355:PHE:CE2	1:A:360:PHE:HB2	2.54	0.42
1:A:408:THR:HA	1:A:499:ILE:HG23	2.01	0.42
1:A:352:ASP:C	1:A:354:GLY:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:CG1	1:A:468:VAL:HB	2.49	0.42
1:A:405:ILE:HA	1:A:532:GLU:O	2.19	0.42
1:A:444:ASN:OD1	1:A:444:ASN:C	2.56	0.42
1:A:13:VAL:HG13	1:A:131:ALA:HB2	2.01	0.42
1:A:277:ASN:HB3	1:A:312:SER:OG	2.20	0.42
1:B:440:LYS:HD2	1:B:499:ILE:HG12	2.02	0.42
1:A:164:GLU:HG3	3:A:701:HOH:O	2.19	0.42
1:B:25:PRO:HD3	1:B:66:SER:O	2.20	0.42
1:B:270:ASN:CB	1:B:273:PHE:CE2	3.03	0.42
1:B:135:VAL:CG1	1:B:149:TYR:HB3	2.50	0.42
1:A:270:ASN:HA	1:A:271:PRO:HD2	1.77	0.42
1:B:203:ASN:HA	1:B:203:ASN:HD22	1.66	0.42
1:B:301:THR:O	1:B:305:SER:HB3	2.19	0.42
1:A:223:HIS:CB	1:A:226:ILE:HD12	2.47	0.41
1:B:497:GLU:CA	1:B:498:LYS:HE3	2.47	0.41
1:B:264:LYS:HE3	1:B:264:LYS:HB3	1.85	0.41
1:A:273:PHE:HZ	1:A:322:HIS:CD2	2.38	0.41
1:A:69:ASN:HD22	1:A:474:LYS:HZ2	1.67	0.41
1:B:384:HIS:HD2	1:B:397:SER:CB	2.33	0.41
1:B:329:VAL:O	1:B:333:ILE:HG13	2.21	0.41
1:B:71:ASN:O	1:B:75:GLY:HA3	2.21	0.41
1:A:230:MET:HA	1:A:246:TYR:OH	2.20	0.41
1:B:133:ARG:CD	3:B:914:HOH:O	2.69	0.41
1:A:228:ASN:O	1:A:231:SER:HB2	2.21	0.41
1:B:122:GLU:HB3	1:B:125:LYS:NZ	2.35	0.41
1:B:263:LEU:HB2	1:B:331:GLN:HE21	1.85	0.41
1:B:518:VAL:O	1:B:519:ASP:CB	2.65	0.41
1:B:217:ILE:HD12	3:B:1022:HOH:O	2.20	0.41
1:B:310:ILE:HG22	1:B:426:PRO:HB2	2.03	0.41
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.86	0.41
1:B:50:TRP:NE1	1:B:99:ALA:HB2	2.36	0.41
1:A:349:GLU:C	1:A:351:VAL:N	2.74	0.41
1:B:71:ASN:O	1:B:75:GLY:N	2.50	0.41
1:B:419:LYS:HE3	1:B:419:LYS:HB2	1.71	0.41
1:B:503:GLU:O	1:B:503:GLU:HG2	2.20	0.41
1:B:238:VAL:HG22	1:B:346:LEU:HB3	2.03	0.41
1:A:290:ASP:C	1:A:351:VAL:HG11	2.42	0.41
1:B:421:THR:CG2	1:B:484:HIS:CD2	3.04	0.41
1:B:272:VAL:HG21	1:B:317:ALA:HB2	2.01	0.40
1:B:422:ALA:HB1	1:B:427:LEU:HD12	2.03	0.40
1:B:374:SER:O	1:B:377:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ILE:HD13	1:B:477:VAL:HG22	2.04	0.40
1:A:209:ILE:HD13	1:A:329:VAL:HG11	2.04	0.40
1:B:220:LEU:HB3	1:B:338:LEU:CD2	2.51	0.40
1:A:306:ILE:HG21	1:A:306:ILE:HD13	1.83	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	519/535 (97%)	496 (96%)	16 (3%)	7 (1%)	15	15
1	B	519/535 (97%)	492 (95%)	21 (4%)	6 (1%)	16	16
All	All	1038/1070 (97%)	988 (95%)	37 (4%)	13 (1%)	15	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	ILE
1	B	350	LEU
1	B	353	ILE
1	B	354	GLY
1	A	201	CYS
1	A	391	HIS
1	B	201	CYS
1	A	352	ASP
1	A	381	SER
1	A	438	PRO
1	B	75	GLY
1	A	75	GLY
1	B	381	SER

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	442/452 (98%)	400 (90%)	42 (10%)	11	12
1	B	442/452 (98%)	405 (92%)	37 (8%)	14	16
All	All	884/904 (98%)	805 (91%)	79 (9%)	12	14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	8	SER
1	A	28	VAL
1	A	36	GLN
1	A	38	PRO
1	A	40	SER
1	A	45	ASN
1	A	69	ASN
1	A	76	LYS
1	A	88	LEU
1	A	111	THR
1	A	122	GLU
1	A	125	LYS
1	A	133	ARG
1	A	172	LYS
1	A	173	ARG
1	A	186	CYS
1	A	200	SER
1	A	203	ASN
1	A	204	LEU
1	A	219	SER
1	A	225	PRO
1	A	236	LYS
1	A	252	GLN
1	A	297	LEU
1	A	299	LYS
1	A	328	ILE

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Mol	Chain	Res	Type
1	A	332	SER
1	A	350	LEU
1	A	352	ASP
1	A	364	ILE
1	A	366	ASN
1	A	462	ARG
1	A	494	SER
1	A	497	GLU
1	A	498	LYS
1	A	499	ILE
1	A	501	SER
1	A	505	SER
1	A	507	ASP
1	A	528	SER
1	A	529	LEU
1	B	3	ASP
1	B	37	LYS
1	B	40	SER
1	B	59	LYS
1	B	69	ASN
1	B	88	LEU
1	B	106	LEU
1	B	110	LEU
1	B	125	LYS
1	B	133	ARG
1	B	160	SER
1	B	201	CYS
1	B	203	ASN
1	B	204	LEU
1	B	220	LEU
1	B	229	LYS
1	B	235	ASN
1	B	241	GLU
1	B	259	GLU
1	B	269	THR
1	B	273	PHE
1	B	291	SER
1	B	297	LEU
1	B	328	ILE
1	B	336	SER
1	B	349	GLU
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	351	VAL
1	B	352	ASP
1	B	364	ILE
1	B	408	THR
1	B	432	VAL
1	B	498	LYS
1	B	501	SER
1	B	507	ASP
1	B	512	LEU
1	B	529	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	151	ASN
1	A	223	HIS
1	A	235	ASN
1	A	251	HIS
1	A	331	GLN
1	A	366	ASN
1	A	369	GLN
1	A	384	HIS
1	A	515	GLN
1	B	203	ASN
1	B	223	HIS
1	B	323	HIS
1	B	331	GLN
1	B	366	ASN
1	B	369	GLN
1	B	384	HIS
1	B	502	ASN
1	B	515	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	APU	A	901	-	36,47,47	1.64	8 (22%)	43,72,72	2.63	8 (18%)
2	APU	B	901	-	36,47,47	1.41	5 (13%)	43,72,72	2.40	8 (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	901	-	-	0/18/58/58	0/5/5/5
2	APU	B	901	-	-	0/18/58/58	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	APU	C8A-N7A	-2.76	1.29	1.34
2	A	901	APU	C5A-C4A	-2.30	1.35	1.40
2	B	901	APU	C8A-N7A	-2.23	1.30	1.34
2	A	901	APU	PU-O2X	-2.18	1.46	1.54
2	A	901	APU	O4D-C1D	2.05	1.43	1.41
2	B	901	APU	C4A-N3A	2.22	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	APU	PA-O3B	2.62	1.67	1.60
2	A	901	APU	C5D-C4D	2.85	1.60	1.51
2	A	901	APU	PU-O1X	3.06	1.61	1.51
2	B	901	APU	C6U-N1U	3.22	1.40	1.35
2	A	901	APU	C6U-N1U	3.57	1.40	1.35
2	B	901	APU	C4U-N3U	3.62	1.39	1.33
2	A	901	APU	O4B-C1B	4.54	1.46	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	APU	N3A-C2A-N1A	-4.51	125.44	128.89
2	B	901	APU	C5U-C4U-N3U	-4.36	111.93	123.12
2	B	901	APU	O2X-PU-O1X	-3.35	99.80	110.58
2	A	901	APU	C5U-C4U-N3U	-3.34	114.56	123.12
2	A	901	APU	O3D-PU-O1X	-3.29	98.90	107.11
2	B	901	APU	C2B-C3B-C4B	-2.55	98.50	103.29
2	A	901	APU	O3B-C3B-C2B	-2.20	102.96	111.51
2	B	901	APU	O3X-PU-O1X	2.09	117.30	110.58
2	B	901	APU	C3D-C2D-C1D	2.24	105.35	99.98
2	B	901	APU	C6U-C5U-C4U	2.67	122.27	117.28
2	A	901	APU	C4D-O4D-C1D	3.01	113.03	109.72
2	A	901	APU	O3X-PU-O2X	3.10	119.19	107.38
2	A	901	APU	O4B-C1B-N9A	3.23	114.86	108.10
2	B	901	APU	O3X-PU-O2X	3.24	119.70	107.38
2	B	901	APU	C4U-N3U-C2U	12.57	126.59	114.14
2	A	901	APU	C4U-N3U-C2U	13.05	127.07	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	APU	3	0
2	B	901	APU	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.