



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:28 PM GMT

PDB ID : 1DNK
Title : THE X-RAY STRUCTURE OF THE DNASE I-D(GGTATACC)2 COM-
PLEX AT 2.3 ANGSTROMS RESOLUTION
Authors : Weston, S.A.; Lahm, A.; Suck, D.
Deposited on : 1992-08-10
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

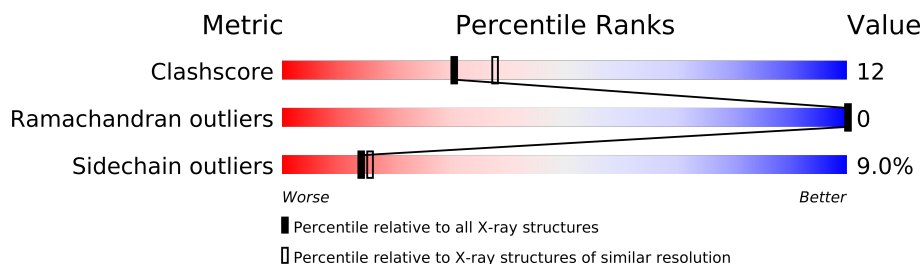
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	7	
2	C	8	
3	A	260	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2390 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called DNA (5'-D(*GP*GP*TP*AP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	7	Total	C	N	O	P	0	0	0
			142	69	27	40	6			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*TP*AP*TP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 3 is a protein called PROTEIN (DEOXYRIBONUCLEASE I (DNASE I) (E.C.3.1.21.1)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	250	Total	C	N	O	S	0	0	0
			1982	1264	330	382	6			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	3	Total	O	0	0
			3	3		
5	C	4	Total	O	0	0
			4	4		

3 Residue-property plots

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: DNA (5'-D(*GP*GP*TP*AP*TP*AP*C)-3')

Chain B: 



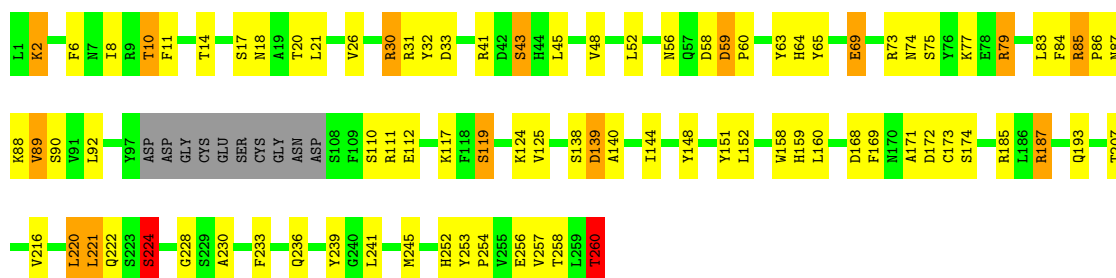
- Molecule 2: DNA (5'-D(*GP*GP*TP*AP*TP*AP*CP*C)-3')

Chain C: 



- Molecule 3: PROTEIN (DEOXYRIBONUCLEASE I (DNASE I) (E.C.3.1.21.1))

Chain A: 



4 Data and refinement statistics

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	51.10Å 108.40Å 62.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2390	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: 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	B	2.21	7/159 (4.4%)	3.33	29/244 (11.9%)
2	C	2.54	13/180 (7.2%)	3.71	51/276 (18.5%)
3	A	3.83	1/2027 (0.0%)	1.84	31/2760 (1.1%)
All	All	3.66	21/2366 (0.9%)	2.20	111/3280 (3.4%)

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
4	A	1	0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	260	THR	C-OXT	166.98	4.40	1.23
2	C	310	DG	P-O5'	9.03	1.68	1.59
1	B	307	DC	C2'-C1'	8.16	1.60	1.52
2	C	310	DG	C2'-C1'	7.51	1.59	1.52
1	B	301	DG	C3'-C2'	7.28	1.60	1.52
2	C	314	DA	C6-N1	-6.94	1.30	1.35
2	C	309	DG	C3'-C2'	6.80	1.60	1.52
2	C	309	DG	C2'-C1'	6.70	1.59	1.52
2	C	311	DT	P-O5'	6.58	1.66	1.59
1	B	305	DT	P-O5'	6.46	1.66	1.59
2	C	316	DC	P-O5'	6.15	1.66	1.59
2	C	312	DA	C2'-C1'	6.09	1.58	1.52
2	C	311	DT	C2'-C1'	5.99	1.58	1.52
1	B	302	DG	C3'-C2'	5.76	1.59	1.52
2	C	314	DA	C2'-C1'	5.60	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	DA	C2'-C1'	5.57	1.57	1.52
1	B	303	DT	C3'-C2'	5.54	1.58	1.52
2	C	314	DA	C5-C4	-5.50	1.34	1.38
1	B	302	DG	P-O5'	5.38	1.65	1.59
2	C	315	DC	C3'-C2'	5.38	1.58	1.52
2	C	315	DC	C2'-C1'	5.22	1.57	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	185	ARG	NE-CZ-NH1	17.64	129.12	120.30
3	A	30	ARG	NE-CZ-NH1	17.26	128.93	120.30
3	A	85	ARG	NE-CZ-NH2	15.28	127.94	120.30
3	A	111	ARG	NE-CZ-NH1	14.45	127.52	120.30
3	A	79	ARG	NE-CZ-NH1	13.07	126.83	120.30
3	A	185	ARG	NE-CZ-NH2	-12.32	114.14	120.30
3	A	30	ARG	CD-NE-CZ	12.20	140.68	123.60
1	B	301	DG	O4'-C4'-C3'	-11.88	98.87	106.00
3	A	85	ARG	NE-CZ-NH1	-11.57	114.51	120.30
3	A	187	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	B	307	DC	C4-C5-C6	11.24	123.02	117.40
1	B	307	DC	C5-C6-N1	-10.66	115.67	121.00
2	C	311	DT	C5-C6-N1	-10.53	117.38	123.70
2	C	314	DA	N1-C6-N6	10.39	124.83	118.60
1	B	307	DC	C2-N3-C4	-10.33	114.73	119.90
2	C	310	DG	N3-C4-C5	-10.06	123.57	128.60
2	C	315	DC	N1-C2-O2	9.95	124.87	118.90
2	C	309	DG	P-O3'-C3'	9.74	131.39	119.70
2	C	309	DG	C3'-C2'-C1'	-9.42	91.19	102.50
2	C	310	DG	C6-N1-C2	-9.29	119.53	125.10
3	A	73	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	B	301	DG	C3'-C2'-C1'	-9.02	91.68	102.50
1	B	307	DC	O4'-C1'-N1	8.66	114.06	108.00
1	B	306	DA	O4'-C1'-N9	-8.62	101.97	108.00
2	C	311	DT	C6-N1-C2	8.60	125.60	121.30
1	B	303	DT	C6-C5-C7	-8.51	117.80	122.90
2	C	312	DA	C5-C6-N1	-8.48	113.46	117.70
2	C	315	DC	OP1-P-OP2	-8.40	107.00	119.60
2	C	311	DT	C6-C5-C7	-8.28	117.94	122.90
1	B	304	DA	O4'-C1'-C2'	8.23	112.48	105.90
2	C	311	DT	C2-N3-C4	-8.05	122.37	127.20
3	A	168	ASP	CB-CG-OD2	8.04	125.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	316	DC	O4'-C1'-C2'	8.02	112.31	105.90
2	C	314	DA	O4'-C4'-C3'	7.98	110.79	106.00
1	B	306	DA	C2-N3-C4	7.84	114.52	110.60
2	C	313	DT	N3-C2-O2	-7.80	117.62	122.30
3	A	79	ARG	NE-CZ-NH2	-7.69	116.46	120.30
3	A	89	VAL	N-CA-CB	-7.67	94.63	111.50
1	B	304	DA	O4'-C4'-C3'	-7.62	101.43	106.00
2	C	311	DT	C3'-C2'-C1'	-7.59	93.39	102.50
2	C	315	DC	P-O3'-C3'	7.53	128.73	119.70
2	C	316	DC	C4-C5-C6	7.49	121.15	117.40
1	B	307	DC	N1-C2-N3	7.44	124.41	119.20
1	B	307	DC	C1'-O4'-C4'	-7.36	102.74	110.10
1	B	303	DT	O4'-C1'-C2'	7.35	111.78	105.90
3	A	18	ASN	OD1-CG-ND2	7.32	138.73	121.90
3	A	69	GLU	CG-CD-OE2	-7.14	104.01	118.30
3	A	69	GLU	CG-CD-OE1	7.10	132.49	118.30
3	A	31	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	302	DG	O4'-C1'-C2'	7.04	111.53	105.90
2	C	316	DC	C4'-C3'-C2'	6.97	109.37	103.10
3	A	187	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	C	311	DT	O4'-C1'-N1	-6.87	103.19	108.00
2	C	314	DA	C5-C6-N6	-6.87	118.20	123.70
2	C	313	DT	C6-C5-C7	-6.86	118.79	122.90
3	A	224	SER	CB-CA-C	6.83	123.09	110.10
1	B	306	DA	C4'-C3'-C2'	6.81	109.23	103.10
2	C	315	DC	N3-C2-O2	-6.79	117.14	121.90
1	B	302	DG	C3'-C2'-C1'	-6.76	94.39	102.50
2	C	311	DT	C4'-C3'-C2'	6.70	109.13	103.10
2	C	313	DT	C4-C5-C6	6.60	121.96	118.00
3	A	111	ARG	NE-CZ-NH2	-6.58	117.01	120.30
3	A	169	PHE	CA-CB-CG	6.55	129.63	113.90
2	C	313	DT	O4'-C1'-C2'	6.54	111.13	105.90
2	C	314	DA	C4-C5-C6	6.47	120.24	117.00
2	C	316	DC	C5-C6-N1	-6.42	117.79	121.00
2	C	312	DA	C4-C5-C6	6.38	120.19	117.00
2	C	315	DC	O4'-C4'-C3'	-6.37	101.95	104.50
2	C	309	DG	N3-C2-N2	6.34	124.34	119.90
2	C	312	DA	P-O3'-C3'	6.21	127.15	119.70
2	C	309	DG	C6-C5-N7	-6.20	126.68	130.40
2	C	312	DA	C1'-O4'-C4'	-6.04	104.06	110.10
2	C	314	DA	C6-C5-N7	-5.99	128.10	132.30
2	C	315	DC	C3'-C2'-C1'	-5.96	95.35	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	193	GLN	CA-CB-CG	5.92	126.42	113.40
1	B	307	DC	C4'-C3'-C2'	5.86	108.37	103.10
1	B	307	DC	C3'-C2'-C1'	-5.85	95.48	102.50
3	A	59	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	304	DA	C3'-C2'-C1'	-5.79	95.55	102.50
3	A	30	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	301	DG	O4'-C1'-C2'	5.72	110.48	105.90
1	B	307	DC	N3-C2-O2	-5.70	117.91	121.90
2	C	311	DT	C4-C5-C6	5.70	121.42	118.00
2	C	314	DA	O4'-C1'-C2'	5.67	110.44	105.90
2	C	310	DG	C4-C5-C6	5.55	122.13	118.80
2	C	310	DG	C3'-C2'-C1'	-5.55	95.84	102.50
1	B	301	DG	C6-N1-C2	-5.52	121.79	125.10
2	C	309	DG	O4'-C4'-C3'	-5.52	102.29	104.50
1	B	301	DG	N1-C6-O6	-5.44	116.64	119.90
1	B	301	DG	C4-C5-N7	-5.40	108.64	110.80
3	A	169	PHE	CB-CG-CD1	5.40	124.58	120.80
2	C	310	DG	N3-C4-N9	5.35	129.21	126.00
1	B	303	DT	C5-C6-N1	-5.33	120.50	123.70
1	B	304	DA	C1'-O4'-C4'	-5.30	104.80	110.10
2	C	313	DT	C5-C6-N1	-5.28	120.53	123.70
3	A	30	ARG	NH1-CZ-NH2	-5.26	113.62	119.40
2	C	309	DG	O4'-C1'-C2'	5.21	110.07	105.90
1	B	302	DG	C4-C5-N7	-5.17	108.73	110.80
2	C	313	DT	C2-N3-C4	-5.16	124.10	127.20
2	C	309	DG	N1-C6-O6	5.16	123.00	119.90
3	A	139	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	C	309	DG	C4-C5-N7	5.13	112.85	110.80
2	C	314	DA	OP1-P-O3'	5.09	116.41	105.20
1	B	305	DT	N3-C2-O2	-5.08	119.25	122.30
3	A	160	LEU	CB-CA-C	5.06	119.81	110.20
2	C	312	DA	N1-C6-N6	5.05	121.63	118.60
2	C	313	DT	C4'-C3'-C2'	5.04	107.64	103.10
3	A	112	GLU	N-CA-CB	5.02	119.64	110.60
3	A	173	CYS	CA-CB-SG	-5.02	104.96	114.00
2	C	312	DA	C2-N3-C4	-5.02	108.09	110.60
3	A	187	ARG	CD-NE-CZ	5.01	130.61	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	261	NAG	C2

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	142	0	81	2	0
2	C	161	0	92	5	0
3	A	1982	0	1937	47	1
4	A	28	0	22	0	1
5	A	70	0	0	4	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
All	All	2390	0	2132	52	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:125:VAL:HA	3:A:220:LEU:HD13	1.52	0.91
3:A:84:PHE:O	3:A:86:PRO:HD3	1.79	0.81
3:A:252:HIS:HB3	5:A:468:HOH:O	1.81	0.78
3:A:63:TYR:OH	3:A:85:ARG:NH1	2.20	0.73
3:A:10:THR:HG23	3:A:41:ARG:HD3	1.76	0.68
3:A:125:VAL:HA	3:A:220:LEU:CD1	2.22	0.68
3:A:124:LYS:HE3	3:A:260:THR:CG2	2.27	0.64
2:C:314:DA:H2"	2:C:315:DC:O4'	1.98	0.64
3:A:239:TYR:HB2	3:A:241:LEU:HG	1.79	0.64
3:A:58:ASP:HB2	5:A:444:HOH:O	1.98	0.63
3:A:10:THR:HG23	3:A:41:ARG:HH11	1.66	0.60
3:A:230:ALA:HA	3:A:256:GLU:O	2.02	0.59
3:A:20:THR:HG22	3:A:245:MET:HE1	1.84	0.58
3:A:216:VAL:HG23	3:A:222:GLN:HG2	1.87	0.56
3:A:74:ASN:O	3:A:77:LYS:NZ	2.36	0.55
3:A:14:THR:O	3:A:17:SER:HB2	2.05	0.55
2:C:313:DT:OP2	3:A:74:ASN:ND2	2.39	0.55
3:A:125:VAL:CA	3:A:220:LEU:HD13	2.32	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:DT:H2'	1:B:306:DA:C8	2.42	0.54
3:A:20:THR:HG22	3:A:245:MET:CE	2.37	0.54
3:A:65:TYR:HB3	3:A:83:LEU:HD23	1.90	0.53
3:A:56:ASN:HB3	3:A:60:PRO:HA	1.95	0.49
3:A:48:VAL:O	3:A:52:LEU:HD12	2.13	0.49
3:A:125:VAL:HG12	3:A:224:SER:OG	2.13	0.49
3:A:59:ASP:OD1	3:A:60:PRO:HD2	2.13	0.49
3:A:253:TYR:N	5:A:468:HOH:O	2.46	0.48
3:A:158:TRP:O	3:A:159:HIS:HB2	2.13	0.48
3:A:33:ASP:OD1	3:A:85:ARG:HD2	2.14	0.48
3:A:124:LYS:HB2	3:A:224:SER:HB2	1.95	0.48
3:A:26:VAL:O	3:A:30:ARG:HG3	2.14	0.47
2:C:316:DC:H5''	3:A:207:THR:HG21	1.96	0.47
3:A:87:ASN:HD21	3:A:88:LYS:NZ	2.14	0.46
3:A:216:VAL:HB	3:A:221:LEU:HD13	1.97	0.46
3:A:140:ALA:O	3:A:144:ILE:HG13	2.16	0.46
2:C:313:DT:H4'	2:C:313:DT:OP1	2.16	0.45
3:A:2:LYS:HB2	3:A:2:LYS:HE3	1.50	0.45
3:A:32:TYR:O	3:A:85:ARG:NH1	2.51	0.43
3:A:6:PHE:CD2	3:A:8:ILE:HD11	2.54	0.43
3:A:92:LEU:HD11	3:A:119:SER:HB2	1.99	0.43
3:A:233:PHE:O	3:A:253:TYR:HB3	2.19	0.42
1:B:305:DT:H2''	1:B:306:DA:O5'	2.18	0.42
2:C:313:DT:H2'	2:C:314:DA:C8	2.55	0.42
3:A:64:HIS:CG	3:A:86:PRO:HG3	2.54	0.42
3:A:69:GLU:OE1	3:A:69:GLU:HA	2.20	0.42
3:A:221:LEU:O	3:A:224:SER:N	2.38	0.42
3:A:92:LEU:HD12	3:A:117:LYS:HD2	2.02	0.41
3:A:171:ALA:O	3:A:172:ASP:HB2	2.20	0.41
3:A:148:TYR:O	3:A:151:TYR:HB3	2.20	0.41
3:A:43:SER:O	3:A:79:ARG:NH2	2.53	0.41
3:A:236:GLN:NE2	5:A:406:HOH:O	2.53	0.41
3:A:257:VAL:HG22	3:A:258:THR:N	2.36	0.40
3:A:233:PHE:O	3:A:254:PRO:HD2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:228:GLY:CA	4:A:262:NAG:O7[4_455]	2.18	0.02

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	
3	A	246/260 (95%)	229 (93%)	17 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	A	221/229 (96%)	201 (91%)	20 (9%)	14	15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	LYS
3	A	10	THR
3	A	11	PHE
3	A	21	LEU
3	A	43	SER
3	A	45	LEU
3	A	75	SER
3	A	89	VAL
3	A	90	SER
3	A	110	SER
3	A	119	SER
3	A	138	SER
3	A	139	ASP
3	A	152	LEU
3	A	174	SER
3	A	187	ARG

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Mol	Chain	Res	Type
3	A	220	LEU
3	A	221	LEU
3	A	224	SER
3	A	260	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	ASN
3	A	155	GLN
3	A	161	ASN
3	A	236	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 carbohydrates 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	NAG	A	261	3,4	12,14,15	0.89	1 (8%)	15,19,21	8.07	10 (66%)
4	NAG	A	262	4	12,14,15	2.30	3 (25%)	15,19,21	4.84	10 (66%)

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	NAG	A	261	3,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	262	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	262	NAG	C2-N2	-4.62	1.40	1.46
4	A	262	NAG	O7-C7	4.55	1.33	1.23
4	A	262	NAG	C8-C7	3.85	1.58	1.50
4	A	261	NAG	C4-C5	-2.04	1.48	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	261	NAG	C2-N2-C7	26.19	167.07	123.09
4	A	261	NAG	O7-C7-C8	-11.88	98.86	122.04
4	A	262	NAG	C3-C2-N2	9.09	125.61	111.76
4	A	262	NAG	C2-N2-C7	8.08	136.66	123.09
4	A	261	NAG	C3-C2-N2	6.82	122.15	111.76
4	A	261	NAG	O5-C5-C6	6.79	114.10	106.98
4	A	262	NAG	O3-C3-C2	-6.59	95.24	109.09
4	A	262	NAG	O7-C7-C8	6.19	134.13	122.04
4	A	262	NAG	O3-C3-C4	6.06	123.93	110.35
4	A	262	NAG	C8-C7-N2	-5.91	104.55	116.11
4	A	262	NAG	O5-C5-C4	-3.98	105.61	110.65
4	A	261	NAG	O3-C3-C4	-3.86	101.71	110.35
4	A	262	NAG	O4-C4-C3	3.70	118.66	110.35
4	A	261	NAG	C8-C7-N2	3.08	122.13	116.11
4	A	262	NAG	C3-C4-C5	2.96	115.49	110.20
4	A	261	NAG	C3-C4-C5	2.84	115.28	110.20
4	A	261	NAG	O5-C5-C4	-2.37	107.64	110.65
4	A	261	NAG	O3-C3-C2	2.31	113.95	109.09
4	A	261	NAG	C4-C3-C2	2.13	116.54	111.32
4	A	262	NAG	C6-C5-C4	-2.13	107.86	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	261	NAG	C2

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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.