



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:07 PM UTC

PDB ID : 3WIE / pdb_00003wie
Title : Structure of a glucose dehydrogenase T277F mutant in complex with D-glucose and NAADP
Authors : Sakuraba, H.; Kanoh, Y.; Yoneda, K.; Ohshima, T.
Deposited on : 2013-09-10
Resolution : 2.33 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

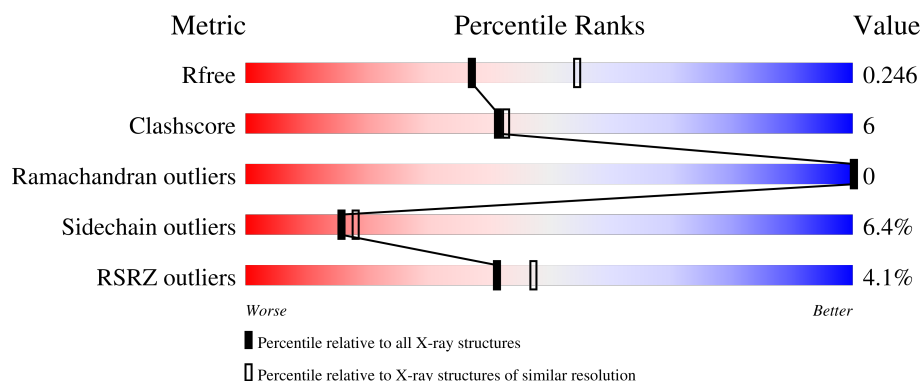
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

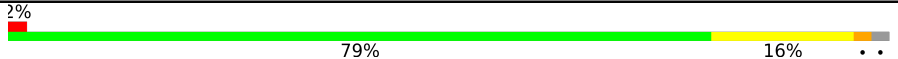
The reported resolution of this entry is 2.33 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	369	
1	B	369	
1	C	369	
1	D	369	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11772 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 Glucose 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	B	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	C	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	D	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	PHE	THR	engineered mutation	UNP Q979W2
A	362	LEU	-	expression tag	UNP Q979W2
A	363	GLU	-	expression tag	UNP Q979W2
A	364	HIS	-	expression tag	UNP Q979W2
A	365	HIS	-	expression tag	UNP Q979W2
A	366	HIS	-	expression tag	UNP Q979W2
A	367	HIS	-	expression tag	UNP Q979W2
A	368	HIS	-	expression tag	UNP Q979W2
A	369	HIS	-	expression tag	UNP Q979W2
B	277	PHE	THR	engineered mutation	UNP Q979W2
B	362	LEU	-	expression tag	UNP Q979W2
B	363	GLU	-	expression tag	UNP Q979W2
B	364	HIS	-	expression tag	UNP Q979W2
B	365	HIS	-	expression tag	UNP Q979W2
B	366	HIS	-	expression tag	UNP Q979W2
B	367	HIS	-	expression tag	UNP Q979W2
B	368	HIS	-	expression tag	UNP Q979W2
B	369	HIS	-	expression tag	UNP Q979W2
C	277	PHE	THR	engineered mutation	UNP Q979W2
C	362	LEU	-	expression tag	UNP Q979W2
C	363	GLU	-	expression tag	UNP Q979W2

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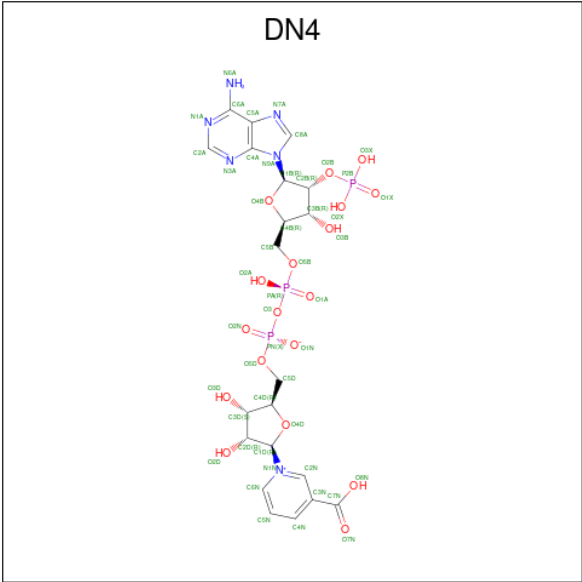
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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	HIS	-	expression tag	UNP Q979W2
C	365	HIS	-	expression tag	UNP Q979W2
C	366	HIS	-	expression tag	UNP Q979W2
C	367	HIS	-	expression tag	UNP Q979W2
C	368	HIS	-	expression tag	UNP Q979W2
C	369	HIS	-	expression tag	UNP Q979W2
D	277	PHE	THR	engineered mutation	UNP Q979W2
D	362	LEU	-	expression tag	UNP Q979W2
D	363	GLU	-	expression tag	UNP Q979W2
D	364	HIS	-	expression tag	UNP Q979W2
D	365	HIS	-	expression tag	UNP Q979W2
D	366	HIS	-	expression tag	UNP Q979W2
D	367	HIS	-	expression tag	UNP Q979W2
D	368	HIS	-	expression tag	UNP Q979W2
D	369	HIS	-	expression tag	UNP Q979W2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

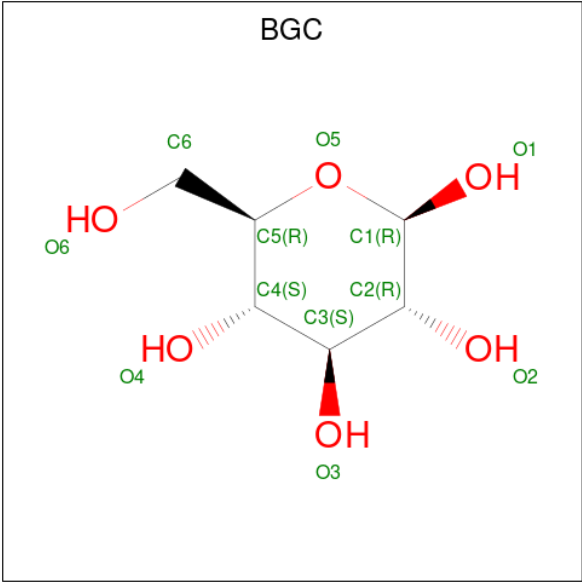
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is [[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-3-oxidanyl-4-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3S,4R,5R)-5-(3-carboxypyridin-1-ium-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphate (CCD ID: DN4) (formula: C₂₁H₂₇N₆O₁₈P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	6	18	3		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0
4	B	1	Total C O 12 6 6	0	0
4	C	1	Total C O 12 6 6	0	0
4	D	1	Total C O 12 6 6	0	0

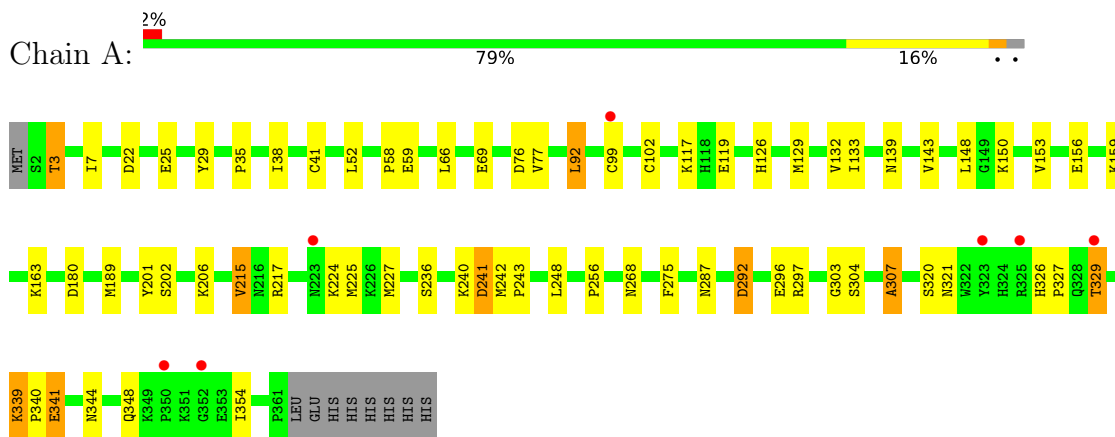
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	60	Total O 60 60	0	0
5	B	61	Total O 61 61	0	0
5	C	51	Total O 51 51	0	0
5	D	44	Total O 44 44	0	0

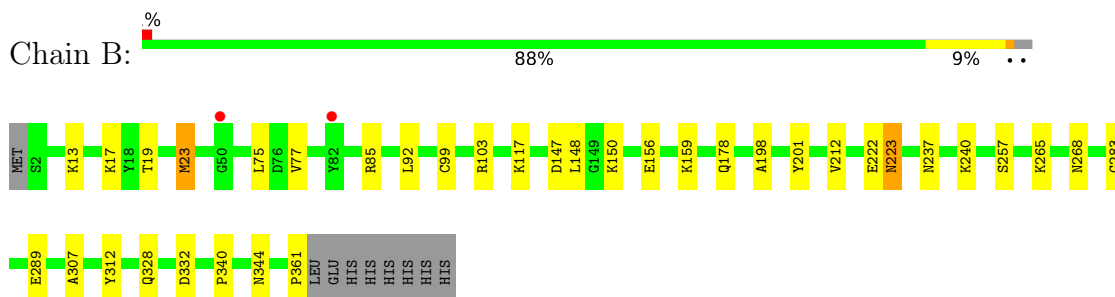
3 Residue-property plots [i](#)

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.

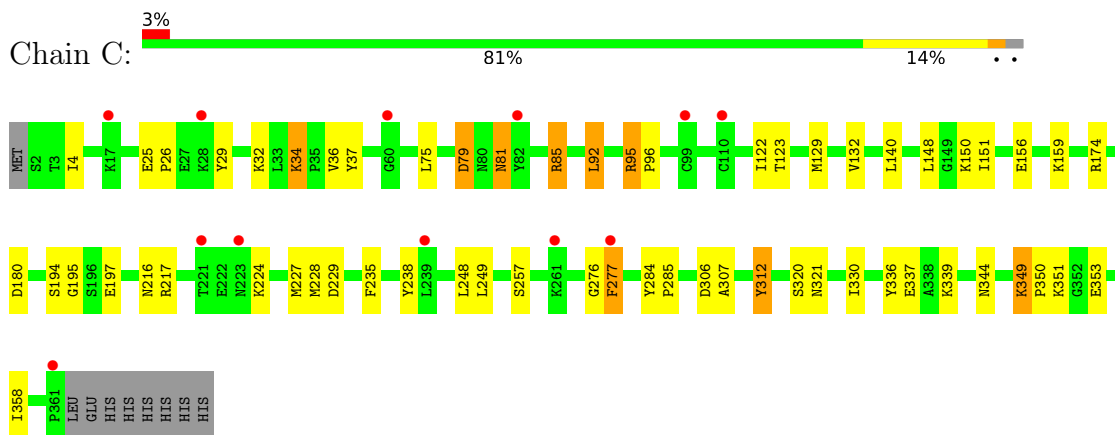
- Molecule 1: Glucose 1-dehydrogenase



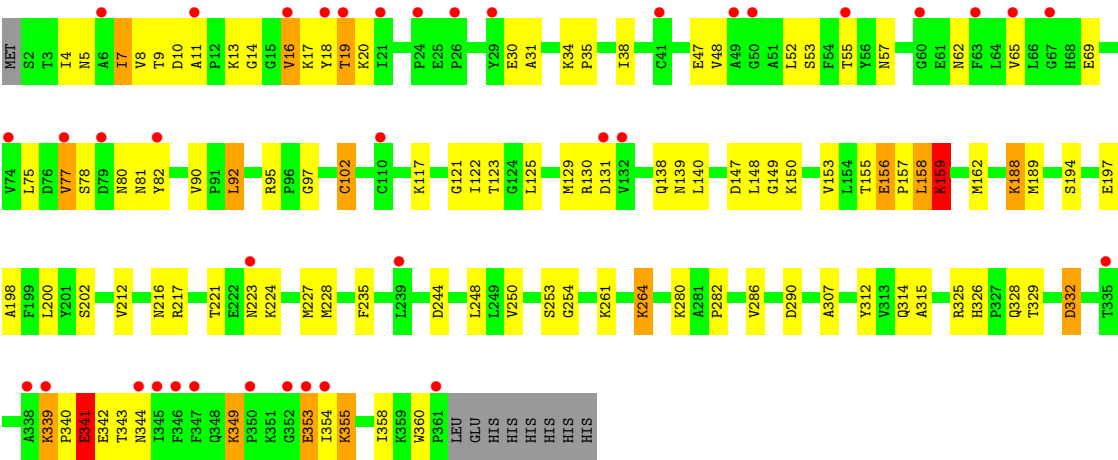
- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase



● Molecule 1: Glucose 1-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.91Å 92.33Å 120.47Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	28.01 – 2.33 28.01 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.01-2.33) 98.8 (28.01-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.244 0.200 , 0.246	Depositor DCC
R_{free} test set	3752 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DN4, ZN, BGC

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	1.20	4/2887 (0.1%)	1.10	4/3904 (0.1%)
1	B	1.25	4/2887 (0.1%)	1.14	0/3904
1	C	1.13	4/2887 (0.1%)	1.12	9/3904 (0.2%)
1	D	1.11	4/2887 (0.1%)	1.16	9/3904 (0.2%)
All	All	1.18	16/11548 (0.1%)	1.13	22/15616 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	200	LEU	CA-C	6.54	1.61	1.52
1	B	212	VAL	C-O	-6.04	1.18	1.24
1	B	198	ALA	CA-C	-5.63	1.45	1.52
1	C	195	GLY	C-O	-5.49	1.18	1.23
1	C	95	ARG	C-N	5.45	1.40	1.33
1	A	206	LYS	CA-C	-5.43	1.45	1.52
1	C	350	PRO	N-CD	5.43	1.55	1.47
1	B	201	TYR	C-O	5.38	1.30	1.24
1	D	157	PRO	C-O	-5.27	1.18	1.24
1	D	147	ASP	CA-C	-5.23	1.45	1.52
1	A	215	VAL	N-CA	-5.19	1.40	1.46
1	C	96	PRO	N-CD	5.18	1.55	1.47
1	A	307	ALA	C-O	-5.17	1.17	1.23
1	D	250	VAL	CA-CB	-5.12	1.47	1.54
1	A	202	SER	CA-C	-5.08	1.46	1.52
1	B	268	ASN	C-O	5.06	1.29	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	GLU	CA-C-N	-7.61	111.12	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	GLU	C-N-CA	-7.61	111.12	119.19
1	A	242	MET	CA-C-N	-7.05	113.05	120.03
1	A	242	MET	C-N-CA	-7.05	113.05	120.03
1	C	349	LYS	CA-C-N	-6.19	113.40	119.78
1	C	349	LYS	C-N-CA	-6.19	113.40	119.78
1	C	95	ARG	CA-C-N	-5.89	113.90	120.14
1	C	95	ARG	C-N-CA	-5.89	113.90	120.14
1	D	341	GLU	N-CA-C	-5.77	104.99	111.28
1	C	276	GLY	N-CA-C	5.71	119.30	111.54
1	C	79	ASP	N-CA-C	5.43	118.05	109.96
1	A	321	ASN	N-CA-C	-5.34	105.35	111.07
1	C	277	PHE	CB-CA-C	-5.29	101.01	109.75
1	D	282	PRO	CA-C-N	5.22	125.30	120.34
1	D	282	PRO	C-N-CA	5.22	125.30	120.34
1	D	159	LYS	CA-CB-CG	5.17	124.44	114.10
1	C	96	PRO	N-CA-C	5.16	120.30	111.68
1	D	312	TYR	N-CA-C	-5.16	105.73	111.36
1	A	296	GLU	CA-CB-CG	5.13	124.37	114.10
1	C	312	TYR	N-CA-C	-5.08	105.65	111.14
1	D	102	CYS	CB-CA-C	-5.07	102.92	110.88
1	D	77	VAL	N-CA-C	5.01	114.87	107.75

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	2827	0	2808	35	0
1	B	2827	0	2807	16	0
1	C	2827	0	2807	32	0
1	D	2827	0	2807	63	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	24	1	0
3	B	48	0	24	1	0
3	C	48	0	24	2	0
3	D	48	0	24	1	0
4	A	12	0	10	1	0
4	B	12	0	12	1	0
4	C	12	0	12	2	0
4	D	12	0	12	1	0
5	A	60	0	0	0	0
5	B	61	0	0	0	0
5	C	51	0	0	0	0
5	D	44	0	0	1	0
All	All	11772	0	11371	147	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 (147) 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:D:264:LYS:HE3	1:D:290:ASP:OD1	1.68	0.92
1:A:227:MET:HE1	1:A:354:ILE:HD11	1.54	0.89
1:D:329:THR:HA	1:D:332:ASP:OD2	1.75	0.87
1:A:224:LYS:HA	1:A:227:MET:HE3	1.57	0.87
1:D:55:THR:HG22	1:D:122:ILE:HG23	1.65	0.78
1:A:150:LYS:O	1:A:153:VAL:HG12	1.85	0.76
1:D:19:THR:OG1	1:D:20:LYS:N	2.15	0.75
1:C:224:LYS:HA	1:C:227:MET:HE3	1.68	0.74
1:A:99:CYS:SG	1:A:102:CYS:HB2	2.27	0.73
1:D:353:GLU:O	1:D:353:GLU:HG3	1.89	0.71
1:A:41:CYS:HB3	1:A:69:GLU:OE2	1.90	0.71
1:D:227:MET:HE1	1:D:354:ILE:HD12	1.75	0.68
1:D:264:LYS:CE	1:D:290:ASP:OD1	2.40	0.68
1:B:75:LEU:O	1:B:85:ARG:HG3	1.94	0.67
3:A:1003:DN4:C4N	4:A:1004:BGC:H1	2.26	0.65
1:D:69:GLU:OE1	1:D:355:LYS:NZ	2.30	0.65
1:D:156:GLU:O	1:D:159:LYS:HD2	1.97	0.64
1:D:17:LYS:HG3	1:D:19:THR:HG22	1.79	0.63
1:D:92:LEU:HD22	1:D:139:ASN:HA	1.80	0.62
1:A:156:GLU:OE2	1:A:156:GLU:C	2.44	0.61
1:D:7:ILE:HG23	1:D:129:MET:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ALA:O	1:D:57:ASN:ND2	2.33	0.60
1:A:268:ASN:ND2	1:A:297:ARG:HG2	2.16	0.60
1:D:227:MET:HE1	1:D:354:ILE:CD1	2.32	0.59
1:D:19:THR:OG1	1:D:20:LYS:O	2.21	0.58
1:C:34:LYS:HE3	1:C:75:LEU:HD21	1.85	0.58
1:D:349:LYS:HB2	1:D:353:GLU:HG2	1.87	0.57
1:D:221:THR:O	1:D:224:LYS:N	2.38	0.57
1:A:303:GLY:O	1:C:174:ARG:NH2	2.23	0.57
1:D:35:PRO:HB2	1:D:38:ILE:HD11	1.87	0.56
1:A:3:THR:HG23	1:A:22:ASP:OD1	2.05	0.56
1:A:227:MET:HE1	1:A:354:ILE:CD1	2.33	0.55
1:C:36:VAL:HG12	1:C:37:TYR:CD2	2.43	0.54
1:D:47:GLU:OE1	1:D:121:GLY:O	2.26	0.54
1:D:162:MET:HE2	1:D:314:GLN:HB3	1.90	0.54
1:A:159:LYS:HD3	1:A:307:ALA:HB3	1.88	0.54
3:D:1003:DN4:C4N	4:D:1004:BGC:H1	2.38	0.53
1:A:29:TYR:OH	1:A:76:ASP:OD2	2.24	0.53
1:C:34:LYS:CE	1:C:75:LEU:HD21	2.39	0.53
1:D:4:ILE:O	1:D:20:LYS:HA	2.09	0.52
1:D:16:VAL:HG22	1:D:48:VAL:HG22	1.92	0.52
1:C:81:ASN:N	1:C:81:ASN:OD1	2.43	0.52
1:B:159:LYS:HD2	1:B:307:ALA:HB3	1.91	0.52
1:D:188:LYS:NZ	1:D:244:ASP:O	2.22	0.52
1:D:5:ASN:N	1:D:131:ASP:OD2	2.36	0.51
1:B:159:LYS:CD	1:B:307:ALA:HB3	2.40	0.51
1:D:65:VAL:HG21	1:D:130:ARG:HD3	1.93	0.51
1:D:325:ARG:HG2	1:D:326:HIS:CD2	2.45	0.50
3:B:1003:DN4:C4N	4:B:1004:BGC:H1	2.41	0.50
1:D:129:MET:HE2	1:D:358:ILE:HD12	1.94	0.50
1:D:339:LYS:O	1:D:342:GLU:N	2.43	0.50
1:B:99:CYS:O	1:B:103:ARG:HD3	2.12	0.50
1:D:30:GLU:O	1:D:77:VAL:HG23	2.12	0.50
1:D:122:ILE:HG22	1:D:123:THR:HG23	1.94	0.49
1:D:18:TYR:CE2	1:D:341:GLU:HG3	2.47	0.49
1:C:284:TYR:CD1	1:C:285:PRO:HD2	2.48	0.49
1:D:55:THR:HG22	1:D:122:ILE:CG2	2.39	0.49
1:C:159:LYS:HD3	1:C:307:ALA:HB3	1.94	0.49
1:C:129:MET:HE2	1:C:358:ILE:HD12	1.95	0.48
1:D:31:ALA:HB2	1:D:77:VAL:HG23	1.95	0.48
1:D:328:GLN:O	1:D:332:ASP:OD2	2.32	0.48
1:D:18:TYR:CZ	1:D:340:PRO:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:O	1:C:85:ARG:HG2	2.14	0.48
1:D:90:VAL:HG21	1:D:155:THR:HB	1.96	0.48
1:D:158:LEU:HB3	1:D:315:ALA:HB1	1.96	0.47
3:C:1003:DN4:C4N	4:C:1004:BGC:H1	2.44	0.47
1:C:156:GLU:O	1:C:159:LYS:HG3	2.14	0.47
1:C:349:LYS:HE2	1:C:353:GLU:OE1	2.15	0.47
1:D:150:LYS:O	1:D:153:VAL:HG12	2.14	0.47
1:A:7:ILE:HG22	1:A:66:LEU:HD12	1.95	0.47
1:A:240:LYS:C	1:A:241:ASP:OD1	2.58	0.47
1:C:306:ASP:OD2	4:C:1004:BGC:O4	2.22	0.47
1:D:228:MET:SD	1:D:235:PHE:HB2	2.54	0.47
1:C:4:ILE:HG21	1:C:132:VAL:HG12	1.96	0.46
1:D:117:LYS:O	1:D:117:LYS:HD2	2.16	0.46
1:D:18:TYR:HE2	1:D:341:GLU:HG3	1.79	0.46
1:D:202:SER:HA	1:D:212:VAL:HG11	1.96	0.46
1:C:216:ASN:OD1	1:C:217:ARG:NH2	2.48	0.46
1:C:34:LYS:HD2	1:C:75:LEU:HD21	1.98	0.46
1:C:238:TYR:OH	3:C:1003:DN4:N1A	2.46	0.46
1:B:23:MET:HE3	1:B:23:MET:HA	1.98	0.46
1:D:18:TYR:CE2	1:D:340:PRO:HB2	2.51	0.46
1:D:261:LYS:NZ	5:D:1110:HOH:O	2.48	0.46
1:B:223:ASN:H	1:B:223:ASN:HD22	1.62	0.46
1:B:328:GLN:O	1:B:332:ASP:OD2	2.33	0.46
1:C:159:LYS:HE2	1:C:312:TYR:CZ	2.51	0.45
1:D:159:LYS:HG2	1:D:307:ALA:HB3	1.98	0.45
1:A:132:VAL:C	1:A:133:ILE:HG13	2.40	0.45
1:D:253:SER:OG	1:D:254:GLY:N	2.50	0.45
1:C:336:TYR:CE1	1:C:337:GLU:O	2.70	0.45
1:A:25:GLU:O	1:A:25:GLU:HG3	2.17	0.44
1:A:292:ASP:OD1	1:C:277:PHE:CD1	2.69	0.44
1:A:58:PRO:HG2	1:A:126:HIS:CE1	2.53	0.44
1:A:339:LYS:HD3	1:A:341:GLU:OE2	2.17	0.44
1:D:9:THR:OG1	1:D:14:GLY:HA2	2.18	0.44
1:D:325:ARG:CG	1:D:326:HIS:CD2	3.01	0.44
1:B:283:GLY:HA2	1:D:286:VAL:O	2.18	0.44
1:D:329:THR:CA	1:D:332:ASP:OD2	2.57	0.44
1:C:159:LYS:HE2	1:C:312:TYR:OH	2.18	0.44
1:C:85:ARG:HE	1:C:85:ARG:HB2	1.63	0.43
1:C:180:ASP:OD1	1:C:180:ASP:C	2.60	0.43
1:D:95:ARG:HH11	1:D:95:ARG:HG2	1.82	0.43
1:D:34:LYS:HG2	1:D:75:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:MET:SD	1:C:235:PHE:HB2	2.58	0.43
1:A:339:LYS:O	1:A:340:PRO:C	2.60	0.43
1:C:4:ILE:HD13	1:C:132:VAL:CG1	2.48	0.43
1:C:75:LEU:O	1:C:85:ARG:CG	2.66	0.43
1:D:97:GLY:N	1:D:102:CYS:SG	2.89	0.43
1:A:92:LEU:HD22	1:A:139:ASN:HA	2.01	0.43
1:D:10:ASP:OD1	1:D:62:ASN:O	2.36	0.43
1:A:35:PRO:HB2	1:A:38:ILE:HD11	2.00	0.43
1:A:326:HIS:HB3	1:A:329:THR:CG2	2.49	0.43
1:C:197:GLU:HA	1:C:197:GLU:OE1	2.18	0.43
1:A:189:MET:HA	1:A:248:LEU:O	2.19	0.42
1:A:77:VAL:O	1:A:77:VAL:HG13	2.18	0.42
1:A:326:HIS:HB3	1:A:329:THR:HG22	2.01	0.42
1:D:197:GLU:O	1:D:198:ALA:C	2.62	0.42
1:C:92:LEU:O	1:C:95:ARG:NH2	2.33	0.42
1:A:326:HIS:O	1:A:327:PRO:C	2.63	0.42
1:C:25:GLU:HG2	1:C:26:PRO:O	2.19	0.42
1:D:156:GLU:OE2	1:D:156:GLU:C	2.63	0.42
1:A:215:VAL:HA	1:A:236:SER:O	2.19	0.42
1:B:17:LYS:HG2	1:B:19:THR:HB	2.01	0.42
1:C:320:SER:O	1:C:321:ASN:C	2.61	0.42
1:A:201:TYR:OH	1:A:275:PHE:CD1	2.66	0.42
1:B:159:LYS:HD3	1:B:312:TYR:CE1	2.54	0.42
1:C:122:ILE:HG22	1:C:123:THR:HG23	2.02	0.42
1:D:81:ASN:HD22	1:D:81:ASN:N	2.17	0.42
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.87	0.42
1:A:38:ILE:HG21	1:A:129:MET:HE3	2.01	0.41
1:B:23:MET:HA	1:B:23:MET:CE	2.50	0.41
1:D:216:ASN:OD1	1:D:217:ARG:NH1	2.52	0.41
1:A:153:VAL:HG22	1:A:153:VAL:O	2.21	0.41
1:D:80:ASN:OD1	1:D:82:TYR:N	2.37	0.41
1:D:148:LEU:O	1:D:149:GLY:C	2.62	0.41
1:D:35:PRO:HG2	1:D:360:TRP:CG	2.56	0.41
1:D:189:MET:HA	1:D:248:LEU:O	2.21	0.41
1:A:287:ASN:OD1	1:A:287:ASN:C	2.63	0.41
1:A:156:GLU:O	1:A:159:LYS:HE3	2.21	0.40
1:A:180:ASP:OD1	1:A:180:ASP:C	2.64	0.40
1:B:77:VAL:O	1:B:77:VAL:HG13	2.22	0.40
1:B:156:GLU:O	1:B:159:LYS:HE3	2.21	0.40
1:B:340:PRO:CG	1:B:361:PRO:HD3	2.51	0.40
1:A:215:VAL:HG11	1:A:243:PRO:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASN:ND2	1:B:240:LYS:HE3	2.37	0.40
1:D:9:THR:OG1	1:D:10:ASP:N	2.54	0.40
1:C:151:ILE:HD12	1:C:330:ILE:HG22	2.04	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	358/369 (97%)	344 (96%)	14 (4%)	0	100	100
1	B	358/369 (97%)	348 (97%)	10 (3%)	0	100	100
1	C	358/369 (97%)	338 (94%)	20 (6%)	0	100	100
1	D	358/369 (97%)	342 (96%)	16 (4%)	0	100	100
All	All	1432/1476 (97%)	1372 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	313/322 (97%)	292 (93%)	21 (7%)	15	16
1	B	313/322 (97%)	299 (96%)	14 (4%)	24	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	313/322 (97%)	295 (94%)	18 (6%)	18	22
1	D	313/322 (97%)	286 (91%)	27 (9%)	10	10
All	All	1252/1288 (97%)	1172 (94%)	80 (6%)	16	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	52	LEU
1	A	59	GLU
1	A	92	LEU
1	A	117	LYS
1	A	119	GLU
1	A	143	VAL
1	A	148	LEU
1	A	163	LYS
1	A	217	ARG
1	A	225	MET
1	A	241	ASP
1	A	256	PRO
1	A	292	ASP
1	A	304	SER
1	A	320	SER
1	A	329	THR
1	A	339	LYS
1	A	341	GLU
1	A	344	ASN
1	A	348	GLN
1	B	13	LYS
1	B	23	MET
1	B	92	LEU
1	B	117	LYS
1	B	147	ASP
1	B	148	LEU
1	B	150	LYS
1	B	178	GLN
1	B	222	GLU
1	B	223	ASN
1	B	257	SER
1	B	265	LYS
1	B	289	GLU

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Mol	Chain	Res	Type
1	B	344	ASN
1	C	29	TYR
1	C	32	LYS
1	C	34	LYS
1	C	79	ASP
1	C	81	ASN
1	C	85	ARG
1	C	92	LEU
1	C	140	LEU
1	C	148	LEU
1	C	150	LYS
1	C	194	SER
1	C	229	ASP
1	C	248	LEU
1	C	249	LEU
1	C	257	SER
1	C	339	LYS
1	C	344	ASN
1	C	351	LYS
1	D	7	ILE
1	D	8	VAL
1	D	13	LYS
1	D	16	VAL
1	D	19	THR
1	D	52	LEU
1	D	53	SER
1	D	78	SER
1	D	92	LEU
1	D	125	LEU
1	D	138	GLN
1	D	140	LEU
1	D	158	LEU
1	D	159	LYS
1	D	188	LYS
1	D	194	SER
1	D	223	ASN
1	D	264	LYS
1	D	280	LYS
1	D	332	ASP
1	D	339	LYS
1	D	341	GLU
1	D	343	THR

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Mol	Chain	Res	Type
1	D	344	ASN
1	D	349	LYS
1	D	353	GLU
1	D	355	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	81	ASN
1	A	118	HIS
1	A	178	GLN
1	A	268	ASN
1	A	314	GLN
1	A	324	HIS
1	A	328	GLN
1	A	344	ASN
1	A	348	GLN
1	B	118	HIS
1	B	144	ASN
1	B	223	ASN
1	B	268	ASN
1	C	68	HIS
1	C	118	HIS
1	C	138	GLN
1	C	267	ASN
1	C	268	ASN
1	C	321	ASN
1	C	324	HIS
1	D	5	ASN
1	D	81	ASN
1	D	268	ASN
1	D	321	ASN
1	D	324	HIS
1	D	326	HIS
1	D	348	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
4	BGC	C	1004	-	12,12,12	0.87	1 (8%)	17,17,17	0.61	0
4	BGC	A	1004	-	12,12,12	1.85	4 (33%)	17,17,17	1.51	3 (17%)
4	BGC	B	1004	-	12,12,12	1.55	3 (25%)	17,17,17	1.36	2 (11%)
3	DN4	C	1003	-	50,52,52	2.63	14 (28%)	71,80,80	2.07	18 (25%)
4	BGC	D	1004	-	12,12,12	1.21	1 (8%)	17,17,17	1.67	5 (29%)
3	DN4	A	1003	-	50,52,52	2.61	15 (30%)	71,80,80	1.71	17 (23%)
3	DN4	D	1003	-	50,52,52	2.42	15 (30%)	71,80,80	1.97	23 (32%)
3	DN4	B	1003	-	50,52,52	2.17	13 (26%)	71,80,80	2.25	20 (28%)

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	BGC	C	1004	-	-	2/2/22/22	0/1/1/1
4	BGC	A	1004	-	-	2/2/22/22	0/1/1/1
4	BGC	B	1004	-	-	2/2/22/22	0/1/1/1
3	DN4	C	1003	-	-	9/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	D	1004	-	-	2/2/22/22	0/1/1/1
3	DN4	A	1003	-	-	15/35/67/67	0/5/5/5
3	DN4	D	1003	-	-	14/35/67/67	0/5/5/5
3	DN4	B	1003	-	-	4/35/67/67	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	DN4	PN-O3	12.10	1.72	1.59
3	A	1003	DN4	PN-O3	11.52	1.71	1.59
3	B	1003	DN4	PN-O3	7.88	1.68	1.59
3	D	1003	DN4	PN-O3	7.27	1.67	1.59
3	D	1003	DN4	C2N-N1N	6.35	1.42	1.35
3	C	1003	DN4	PA-O3	6.33	1.66	1.59
3	A	1003	DN4	PA-O3	6.21	1.66	1.59
3	D	1003	DN4	P2B-O2B	5.92	1.69	1.59
3	D	1003	DN4	PA-O3	5.52	1.65	1.59
3	A	1003	DN4	C2N-N1N	5.25	1.40	1.35
3	B	1003	DN4	P2B-O2B	5.06	1.68	1.59
3	D	1003	DN4	C2A-N3A	4.99	1.42	1.33
3	C	1003	DN4	P2B-O2B	4.99	1.68	1.59
3	B	1003	DN4	O4D-C1D	4.80	1.47	1.40
3	A	1003	DN4	P2B-O2B	4.57	1.67	1.59
3	C	1003	DN4	C2N-N1N	4.47	1.39	1.35
3	B	1003	DN4	C2N-N1N	4.34	1.39	1.35
3	B	1003	DN4	O7N-C7N	4.04	1.34	1.22
3	A	1003	DN4	C3N-C7N	-4.04	1.40	1.49
4	A	1004	BGC	O2-C2	-3.74	1.33	1.43
3	C	1003	DN4	C5A-C4A	-3.67	1.32	1.39
3	A	1003	DN4	C2A-N1A	3.58	1.40	1.33
3	D	1003	DN4	C8A-N9A	-3.58	1.31	1.37
3	A	1003	DN4	O4D-C1D	3.50	1.45	1.40
3	C	1003	DN4	C5A-C6A	-3.41	1.31	1.41
3	C	1003	DN4	O7N-C7N	3.30	1.32	1.22
3	D	1003	DN4	C2A-N1A	3.19	1.39	1.33
3	D	1003	DN4	O4D-C1D	3.11	1.45	1.40
3	A	1003	DN4	C5A-C6A	-3.03	1.32	1.41
3	B	1003	DN4	C2A-N3A	2.96	1.39	1.33
4	A	1004	BGC	C1-C2	-2.94	1.45	1.52
3	A	1003	DN4	P2B-O3X	2.89	1.65	1.54
3	B	1003	DN4	C5A-C4A	-2.87	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	DN4	C2A-N3A	2.81	1.38	1.33
3	C	1003	DN4	C6N-N1N	2.80	1.41	1.35
3	D	1003	DN4	O7N-C7N	2.80	1.30	1.22
3	B	1003	DN4	C2B-C1B	-2.80	1.46	1.53
3	C	1003	DN4	C3N-C7N	-2.64	1.43	1.49
4	B	1004	BGC	C1-C2	-2.62	1.46	1.52
3	C	1003	DN4	C5A-N7A	-2.60	1.34	1.39
3	D	1003	DN4	C8A-N7A	2.59	1.36	1.31
3	C	1003	DN4	C2A-N1A	2.59	1.38	1.33
3	D	1003	DN4	C5A-N7A	-2.55	1.34	1.39
3	B	1003	DN4	C4A-N9A	-2.49	1.32	1.37
3	A	1003	DN4	O7N-C7N	2.49	1.30	1.22
4	D	1004	BGC	O5-C1	2.46	1.48	1.42
3	C	1003	DN4	P2B-O2X	2.46	1.63	1.54
3	B	1003	DN4	O4B-C1B	2.45	1.47	1.42
3	A	1003	DN4	C4A-N9A	-2.40	1.32	1.37
3	C	1003	DN4	C4A-N9A	-2.40	1.32	1.37
3	A	1003	DN4	C6N-N1N	2.39	1.40	1.35
3	D	1003	DN4	C6N-N1N	2.38	1.40	1.35
3	A	1003	DN4	C5A-C4A	-2.37	1.34	1.39
4	B	1004	BGC	O5-C5	-2.36	1.38	1.44
3	D	1003	DN4	C3N-C7N	-2.34	1.44	1.49
3	B	1003	DN4	C5A-C6A	-2.33	1.34	1.41
3	B	1003	DN4	C8A-N9A	-2.33	1.33	1.37
4	A	1004	BGC	C4-C5	-2.26	1.48	1.53
3	D	1003	DN4	C5A-C4A	-2.24	1.35	1.39
3	B	1003	DN4	C3N-C7N	-2.24	1.44	1.49
4	A	1004	BGC	O5-C5	-2.20	1.39	1.44
4	C	1004	BGC	O1-C1	2.12	1.46	1.39
3	A	1003	DN4	C5A-N7A	-2.09	1.35	1.39
4	B	1004	BGC	O2-C2	-2.08	1.37	1.43
3	D	1003	DN4	C5A-C6A	-2.05	1.35	1.41
3	C	1003	DN4	C2A-N3A	2.05	1.37	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	DN4	N3A-C2A-N1A	-8.48	115.74	128.58
3	C	1003	DN4	N3A-C2A-N1A	-7.58	117.11	128.58
3	B	1003	DN4	C4A-N9A-C1B	-6.43	111.58	126.63
3	C	1003	DN4	C4D-O4D-C1D	-5.78	104.63	109.92
3	D	1003	DN4	N3A-C2A-N1A	-5.59	120.12	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	DN4	C1B-N9A-C8A	5.49	139.27	127.09
3	B	1003	DN4	C4D-O4D-C1D	-5.46	104.92	109.92
3	A	1003	DN4	C4D-O4D-C1D	-5.36	105.02	109.92
3	C	1003	DN4	N9A-C8A-N7A	-5.31	106.40	113.94
3	C	1003	DN4	C4A-N9A-C1B	-5.17	114.54	126.63
3	D	1003	DN4	N9A-C8A-N7A	-5.04	106.78	113.94
3	A	1003	DN4	N3A-C2A-N1A	-4.96	121.08	128.58
3	D	1003	DN4	C4A-C5A-N7A	-4.67	105.24	110.58
3	D	1003	DN4	C5A-C4A-N3A	-4.46	120.58	126.72
3	A	1003	DN4	N9A-C8A-N7A	-4.39	107.71	113.94
3	C	1003	DN4	C1B-N9A-C8A	4.25	136.53	127.09
3	B	1003	DN4	N9A-C8A-N7A	-4.17	108.02	113.94
3	D	1003	DN4	C5A-N7A-C8A	4.06	109.83	103.45
4	D	1004	BGC	O5-C5-C6	3.82	115.90	106.44
3	B	1003	DN4	C2A-N3A-C4A	3.69	120.85	111.83
3	C	1003	DN4	C5A-C4A-N3A	-3.64	121.70	126.72
4	B	1004	BGC	O5-C5-C6	-3.54	97.67	106.44
4	A	1004	BGC	O5-C5-C6	-3.52	97.71	106.44
3	C	1003	DN4	C2A-N3A-C4A	3.52	120.43	111.83
3	D	1003	DN4	C4A-N9A-C1B	-3.47	118.51	126.63
3	D	1003	DN4	C5A-C4A-N9A	3.32	109.43	105.81
3	A	1003	DN4	C5A-C4A-N3A	-3.32	122.15	126.72
3	A	1003	DN4	C4A-N9A-C1B	-3.28	118.97	126.63
3	B	1003	DN4	C4A-N9A-C8A	3.20	109.10	105.74
3	B	1003	DN4	C5A-C4A-N3A	-3.16	122.36	126.72
3	C	1003	DN4	C5A-N7A-C8A	3.11	108.33	103.45
3	C	1003	DN4	C4A-N9A-C8A	3.00	108.89	105.74
3	B	1003	DN4	C5N-C4N-C3N	2.95	123.26	120.36
3	B	1003	DN4	C2N-C3N-C7N	2.93	124.81	119.78
4	A	1004	BGC	O1-C1-O5	-2.93	101.71	110.41
3	A	1003	DN4	C4A-N9A-C8A	2.89	108.77	105.74
3	D	1003	DN4	C6A-C5A-C4A	2.87	121.10	117.18
3	D	1003	DN4	C4A-N9A-C8A	2.84	108.72	105.74
3	D	1003	DN4	C2A-N3A-C4A	2.72	118.47	111.83
3	D	1003	DN4	C4D-O4D-C1D	-2.71	107.44	109.92
3	B	1003	DN4	C5N-C6N-N1N	-2.69	116.71	120.38
3	A	1003	DN4	C5A-N7A-C8A	2.69	107.67	103.45
3	B	1003	DN4	C4A-C5A-N7A	-2.66	107.54	110.58
4	B	1004	BGC	C1-O5-C5	2.65	118.77	113.65
3	D	1003	DN4	C5N-C4N-C3N	2.61	122.93	120.36
3	A	1003	DN4	C6A-C5A-C4A	2.60	120.73	117.18
4	D	1004	BGC	C4-C3-C2	-2.57	106.33	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1003	DN4	C1B-N9A-C8A	2.56	132.77	127.09
3	B	1003	DN4	C2N-C3N-C4N	-2.55	115.29	118.26
3	C	1003	DN4	C5A-C4A-N9A	2.55	108.59	105.81
3	A	1003	DN4	C4A-C5A-N7A	-2.52	107.70	110.58
3	C	1003	DN4	C4A-C5A-N7A	-2.45	107.78	110.58
3	C	1003	DN4	C5A-C6A-N1A	2.44	123.70	117.51
3	A	1003	DN4	C3B-C2B-C1B	-2.42	98.18	102.81
3	D	1003	DN4	C2N-C3N-C4N	-2.41	115.45	118.26
3	C	1003	DN4	C6N-N1N-C1D	2.40	124.43	119.73
3	C	1003	DN4	C2N-N1N-C1D	-2.39	113.85	119.13
3	D	1003	DN4	O4D-C4D-C5D	2.37	116.92	109.33
3	A	1003	DN4	O2A-PA-O1A	2.36	123.41	112.44
3	B	1003	DN4	C5A-N7A-C8A	2.36	107.15	103.45
4	D	1004	BGC	C3-C4-C5	-2.33	106.01	110.23
3	A	1003	DN4	C1B-N9A-C8A	2.32	132.25	127.09
4	D	1004	BGC	O5-C5-C4	-2.32	105.52	109.70
3	A	1003	DN4	C5A-C6A-N6A	-2.32	117.55	123.29
3	C	1003	DN4	C5A-C6A-N6A	-2.31	117.58	123.29
3	C	1003	DN4	O4B-C1B-C2B	-2.30	102.63	106.59
3	B	1003	DN4	O3X-P2B-O2X	-2.29	99.22	107.80
3	D	1003	DN4	O4B-C1B-N9A	-2.26	103.74	108.09
3	C	1003	DN4	O2X-P2B-O2B	-2.24	97.10	105.85
3	B	1003	DN4	O4B-C1B-N9A	2.22	112.35	108.09
3	D	1003	DN4	C3B-C2B-C1B	-2.19	98.62	102.81
3	A	1003	DN4	C4B-O4B-C1B	-2.19	104.64	109.47
4	D	1004	BGC	O5-C1-C2	2.18	114.13	110.30
3	B	1003	DN4	C5A-C4A-N9A	2.17	108.17	105.81
3	D	1003	DN4	O3X-P2B-O1X	2.17	119.27	110.83
3	D	1003	DN4	O4B-C1B-C2B	-2.14	102.90	106.59
3	A	1003	DN4	C5A-C4A-N9A	2.14	108.14	105.81
3	D	1003	DN4	O2A-PA-O1A	2.12	122.30	112.44
3	D	1003	DN4	C5N-C6N-N1N	-2.09	117.53	120.38
3	B	1003	DN4	C5A-C6A-N6A	-2.09	118.12	123.29
3	D	1003	DN4	O3D-C3D-C4D	-2.06	105.16	111.08
3	B	1003	DN4	O1N-PN-O2N	2.06	122.01	112.44
4	A	1004	BGC	C3-C4-C5	-2.05	106.52	110.23
3	B	1003	DN4	C2N-N1N-C1D	-2.04	114.62	119.13
3	A	1003	DN4	O4B-C1B-C2B	-2.04	103.08	106.59
3	A	1003	DN4	C2A-N3A-C4A	2.04	116.80	111.83
3	D	1003	DN4	C4B-O4B-C1B	-2.02	105.00	109.47
3	C	1003	DN4	O4D-C4D-C5D	2.01	115.78	109.33

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	DN4	C5B-O5B-PA-O2A
3	A	1003	DN4	C5B-O5B-PA-O3
3	A	1003	DN4	PN-O3-PA-O5B
3	A	1003	DN4	C5D-O5D-PN-O3
3	A	1003	DN4	C5D-O5D-PN-O2N
3	A	1003	DN4	O4D-C4D-C5D-O5D
3	A	1003	DN4	O4D-C1D-N1N-C2N
3	A	1003	DN4	O4D-C1D-N1N-C6N
3	A	1003	DN4	C2D-C1D-N1N-C2N
3	A	1003	DN4	C2D-C1D-N1N-C6N
3	B	1003	DN4	O4D-C1D-N1N-C2N
3	B	1003	DN4	O4D-C1D-N1N-C6N
3	B	1003	DN4	C2D-C1D-N1N-C2N
3	B	1003	DN4	C2D-C1D-N1N-C6N
3	C	1003	DN4	C5B-O5B-PA-O1A
3	C	1003	DN4	C5B-O5B-PA-O2A
3	C	1003	DN4	C5B-O5B-PA-O3
3	C	1003	DN4	O4D-C1D-N1N-C2N
3	C	1003	DN4	O4D-C1D-N1N-C6N
3	C	1003	DN4	C2D-C1D-N1N-C2N
3	C	1003	DN4	C2D-C1D-N1N-C6N
3	D	1003	DN4	C5B-O5B-PA-O1A
3	D	1003	DN4	C5B-O5B-PA-O2A
3	D	1003	DN4	C5B-O5B-PA-O3
3	D	1003	DN4	PN-O3-PA-O5B
3	D	1003	DN4	O4D-C1D-N1N-C2N
3	D	1003	DN4	O4D-C1D-N1N-C6N
3	D	1003	DN4	C2D-C1D-N1N-C2N
3	D	1003	DN4	C2D-C1D-N1N-C6N
4	D	1004	BGC	O5-C5-C6-O6
4	D	1004	BGC	C4-C5-C6-O6
4	A	1004	BGC	C4-C5-C6-O6
4	A	1004	BGC	O5-C5-C6-O6
4	C	1004	BGC	O5-C5-C6-O6
4	C	1004	BGC	C4-C5-C6-O6
3	D	1003	DN4	O4D-C4D-C5D-O5D
4	B	1004	BGC	O5-C5-C6-O6
4	B	1004	BGC	C4-C5-C6-O6
3	A	1003	DN4	C3D-C4D-C5D-O5D
3	D	1003	DN4	C3D-C4D-C5D-O5D
3	C	1003	DN4	PN-O3-PA-O5B
3	D	1003	DN4	C3B-C4B-C5B-O5B

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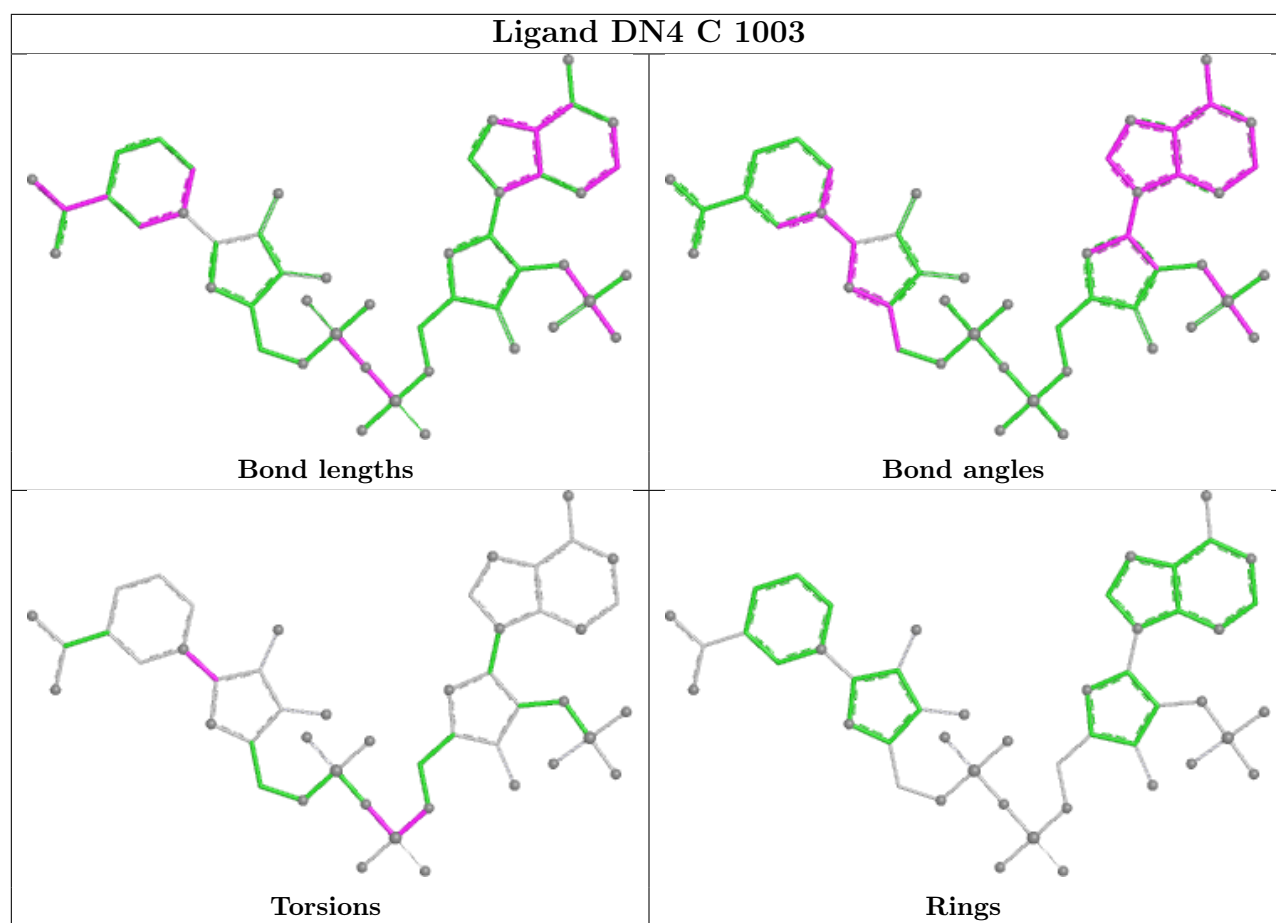
Mol	Chain	Res	Type	Atoms
3	A	1003	DN4	C5B-O5B-PA-O1A
3	A	1003	DN4	C5D-O5D-PN-O1N
3	A	1003	DN4	PA-O3-PN-O2N
3	D	1003	DN4	O4B-C4B-C5B-O5B
3	A	1003	DN4	PA-O3-PN-O1N
3	C	1003	DN4	PN-O3-PA-O1A
3	D	1003	DN4	PA-O3-PN-O1N
3	D	1003	DN4	PA-O3-PN-O2N

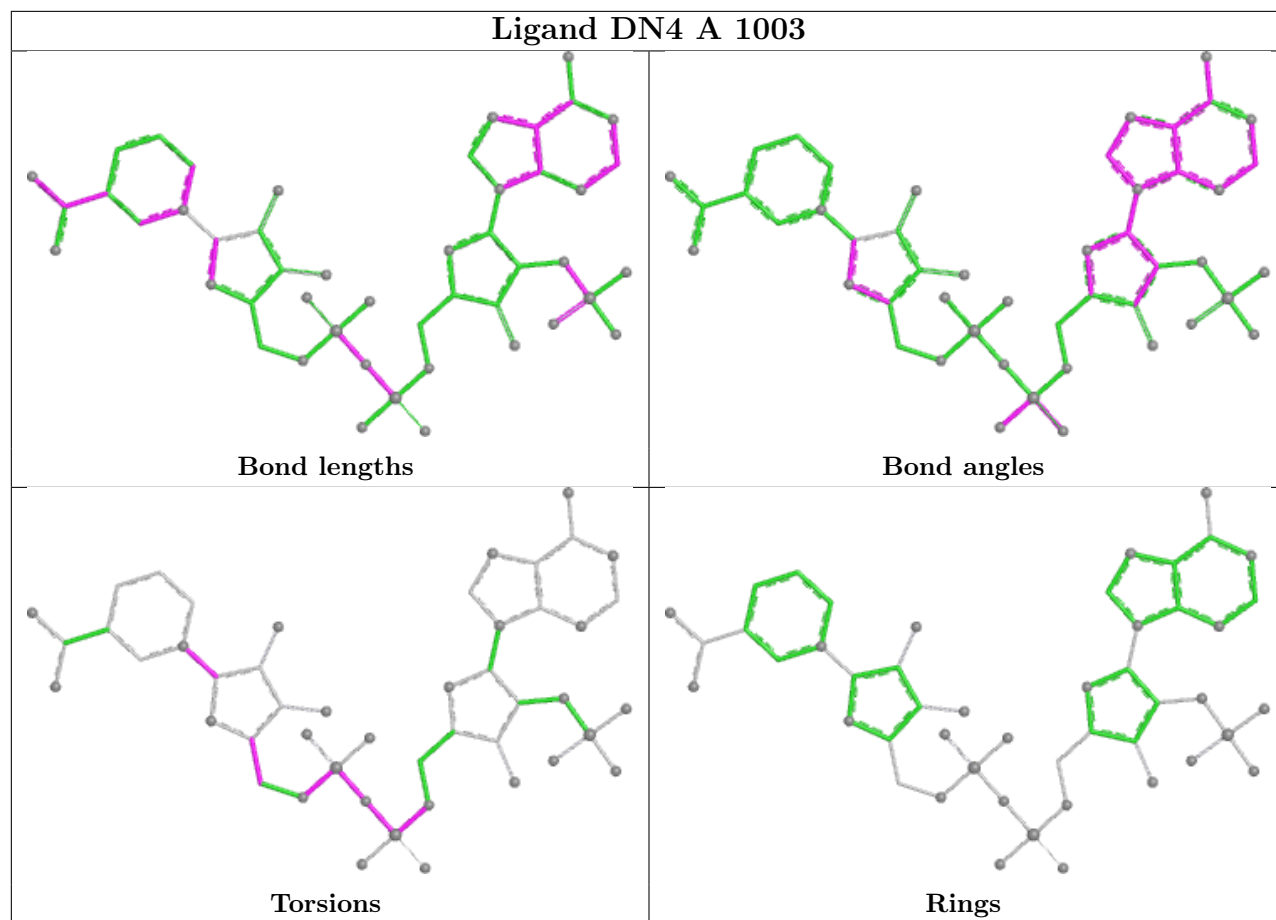
There are no ring outliers.

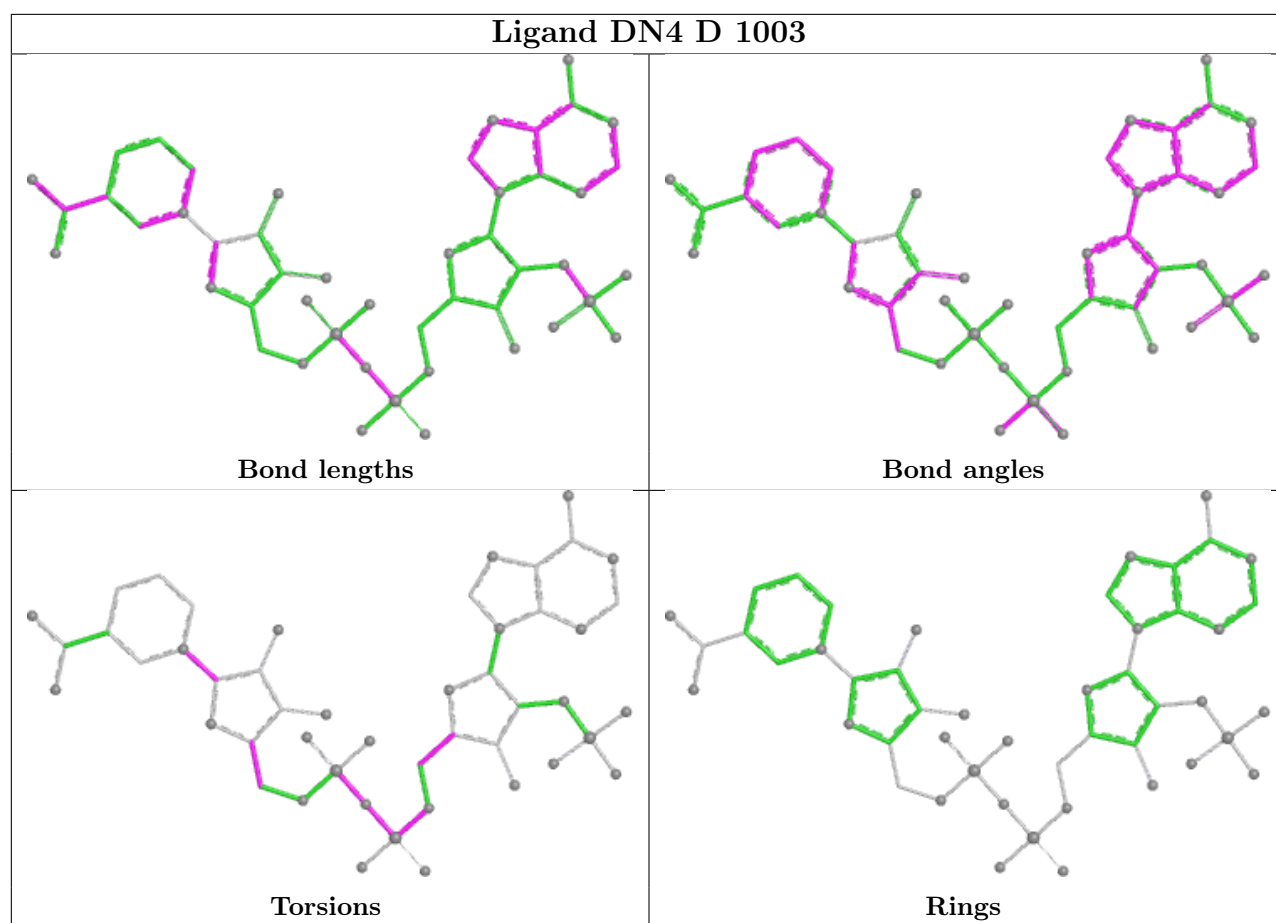
8 monomers are involved in 6 short contacts:

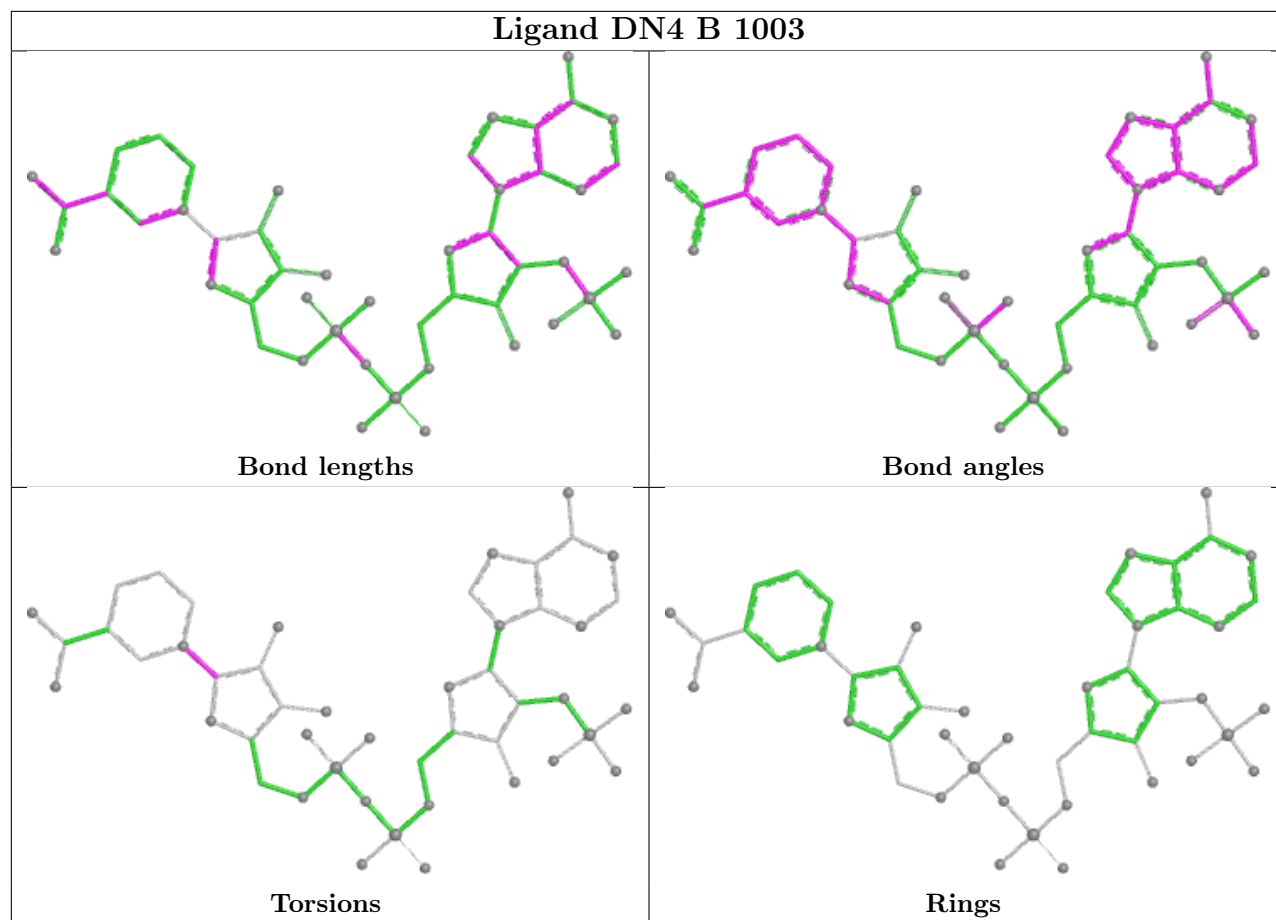
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1004	BGC	2	0
4	A	1004	BGC	1	0
4	B	1004	BGC	1	0
3	C	1003	DN4	2	0
4	D	1004	BGC	1	0
3	A	1003	DN4	1	0
3	D	1003	DN4	1	0
3	B	1003	DN4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	360/369 (97%)	0.13	7 (1%) 66 71	24, 45, 74, 95	0
1	B	360/369 (97%)	-0.16	2 (0%) 85 88	23, 38, 68, 96	0
1	C	360/369 (97%)	0.22	12 (3%) 49 55	25, 47, 77, 114	0
1	D	360/369 (97%)	0.66	38 (10%) 11 13	25, 55, 95, 126	0
All	All	1440/1476 (97%)	0.21	59 (4%) 41 47	23, 46, 82, 126	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	352	GLY	6.0
1	D	26	PRO	4.1
1	D	49	ALA	4.0
1	D	335	THR	3.2
1	D	24	PRO	3.1
1	D	344	ASN	3.1
1	D	82	TYR	3.0
1	D	338	ALA	3.0
1	D	67	GLY	3.0
1	D	19	THR	2.9
1	C	82	TYR	2.9
1	C	60	GLY	2.9
1	A	99	CYS	2.9
1	C	361	PRO	2.8
1	D	29	TYR	2.7
1	D	132	VAL	2.7
1	D	50	GLY	2.6
1	D	16	VAL	2.6
1	C	261	LYS	2.6
1	D	79	ASP	2.6
1	D	361	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	223	ASN	2.6
1	C	17	LYS	2.5
1	D	74	VAL	2.5
1	A	329	THR	2.4
1	C	110	CYS	2.4
1	D	350	PRO	2.4
1	D	63	PHE	2.4
1	D	223	ASN	2.4
1	A	323	TYR	2.3
1	D	131	ASP	2.3
1	D	6	ALA	2.3
1	C	239	LEU	2.3
1	A	350	PRO	2.3
1	D	11	ALA	2.3
1	C	221	THR	2.3
1	D	353	GLU	2.3
1	D	18	TYR	2.3
1	A	325	ARG	2.2
1	B	82	TYR	2.2
1	D	345	ILE	2.2
1	D	354	ILE	2.2
1	D	65	VAL	2.2
1	D	347	PHE	2.2
1	A	352	GLY	2.2
1	D	110	CYS	2.2
1	B	50	GLY	2.2
1	D	60	GLY	2.1
1	D	41	CYS	2.1
1	D	77	VAL	2.1
1	D	55	THR	2.1
1	D	339	LYS	2.1
1	D	239	LEU	2.1
1	A	223	ASN	2.1
1	C	277	PHE	2.1
1	D	346	PHE	2.0
1	C	99	CYS	2.0
1	D	21	ILE	2.0
1	C	28	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

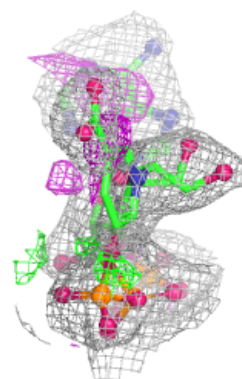
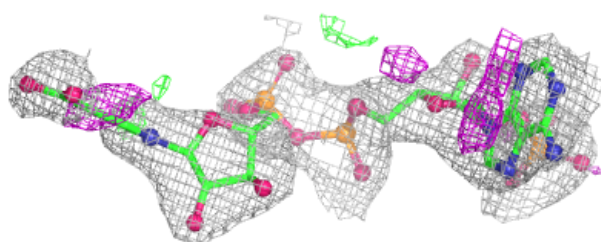
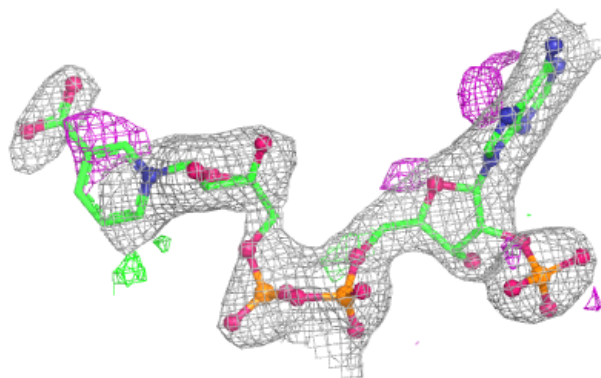
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZN	D	1001	1/1	0.83	0.29	89,89,89,89	0
4	BGC	A	1004	12/12	0.85	0.11	48,67,88,93	0
3	DN4	D	1003	48/48	0.87	0.14	44,68,92,101	0
4	BGC	C	1004	12/12	0.87	0.12	61,79,93,93	0
2	ZN	C	1002	1/1	0.88	0.09	35,35,35,35	0
4	BGC	D	1004	12/12	0.88	0.11	66,77,85,91	0
3	DN4	C	1003	48/48	0.89	0.12	43,65,95,109	0
3	DN4	A	1003	48/48	0.90	0.11	38,67,85,95	0
2	ZN	A	1001	1/1	0.91	0.27	71,71,71,71	0
3	DN4	B	1003	48/48	0.92	0.10	40,56,77,80	0
4	BGC	B	1004	12/12	0.92	0.11	51,64,73,73	0
2	ZN	D	1002	1/1	0.92	0.06	34,34,34,34	0
2	ZN	C	1001	1/1	0.92	0.24	71,71,71,71	0
2	ZN	A	1002	1/1	0.93	0.06	34,34,34,34	0
2	ZN	B	1001	1/1	0.96	0.18	65,65,65,65	0
2	ZN	B	1002	1/1	1.00	0.01	32,32,32,32	0

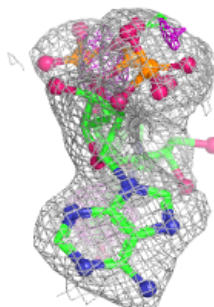
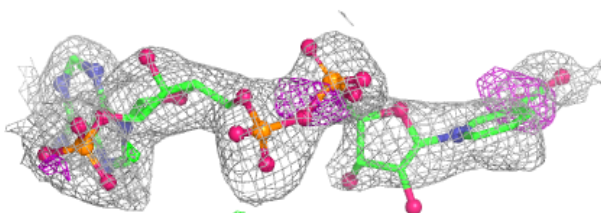
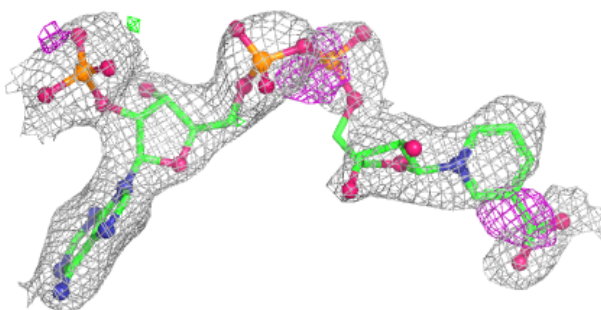
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DN4 D 1003:

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

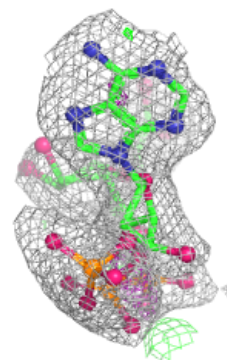
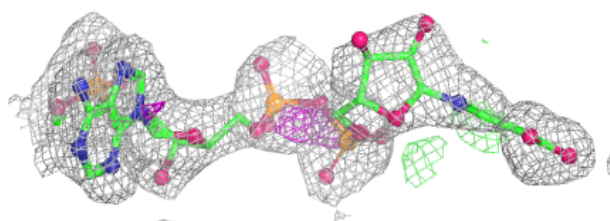
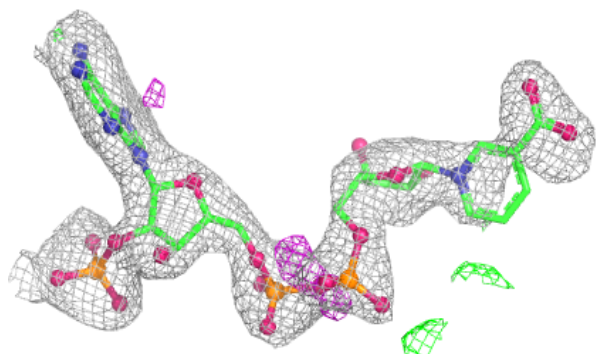
**Electron density around DN4 C 1003:**

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

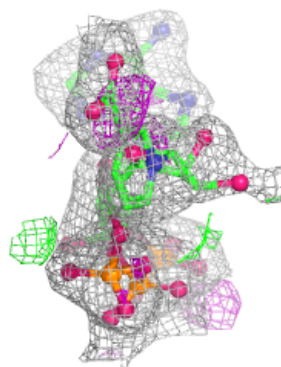
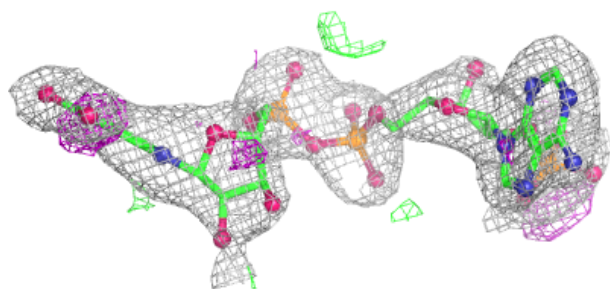
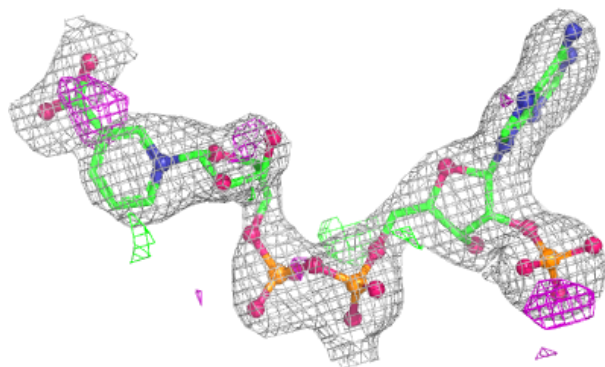


Electron density around DN4 A 1003:

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

**Electron density around DN4 B 1003:**

$2mF_o-DF_c$ (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.