Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 10:23 AM BST

PDB ID	:	3WIE
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)

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.33 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		6.8%
RSRZ outliers		12.5%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 on 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 <=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	11% / 81% / 14% · ·
1	B	369	6% / 88% / 8% · ·
1	C	369	12% / 83% / 12% · ·
1	D	369	20% / 74% / 20% · ·

2 Entry composition (i)

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 2827	C 1804	N 473	O 537	S 13	0	0	0
1	B	360	Total 2827	C 1804	N 473	O 537	S 13	0	0	0
1	C	360	Total 2827	C 1804	N 473	O 537	S 13	0	0	0
1	D	360	Total 2827	C 1804	N 473	O 537	S 13	0	0	0

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

Continued on next page...

Continued from previous page...

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 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 (three-letter code: DN4) (formula: $C_{21}H_{27}N_6O_{18}P_3$).
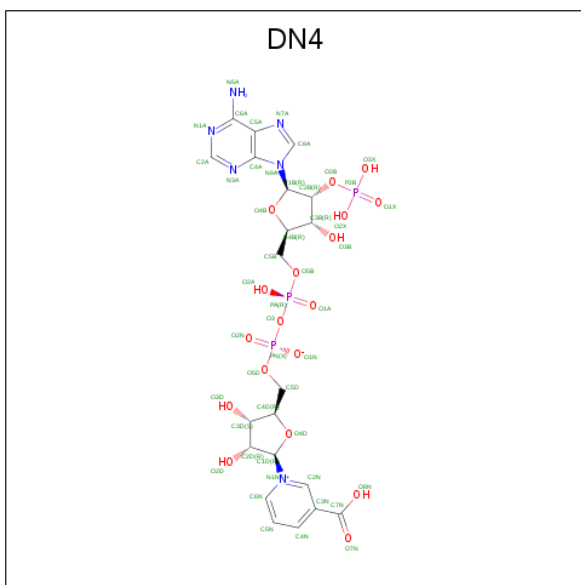
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	6	18	3		

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).
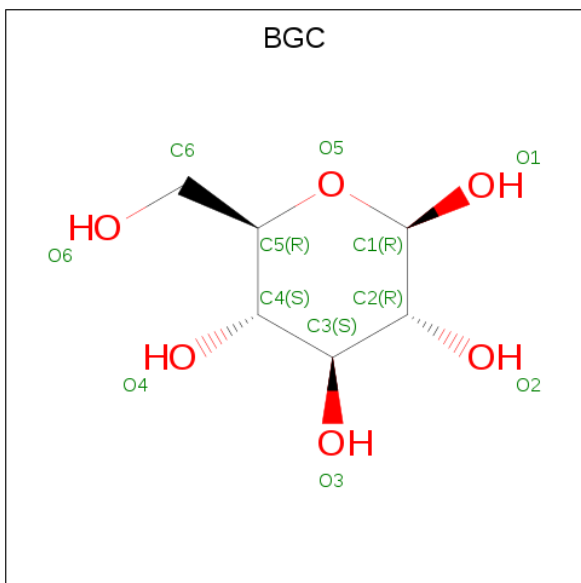
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C O 12 6 6		0	0
4	B	1	Total C O 12 6 6		0	0
4	C	1	Total C O 12 6 6		0	0
4	D	1	Total C O 12 6 6		0	0

- 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.

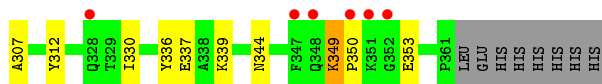- Molecule 1: Glucose 1-dehydrogenase
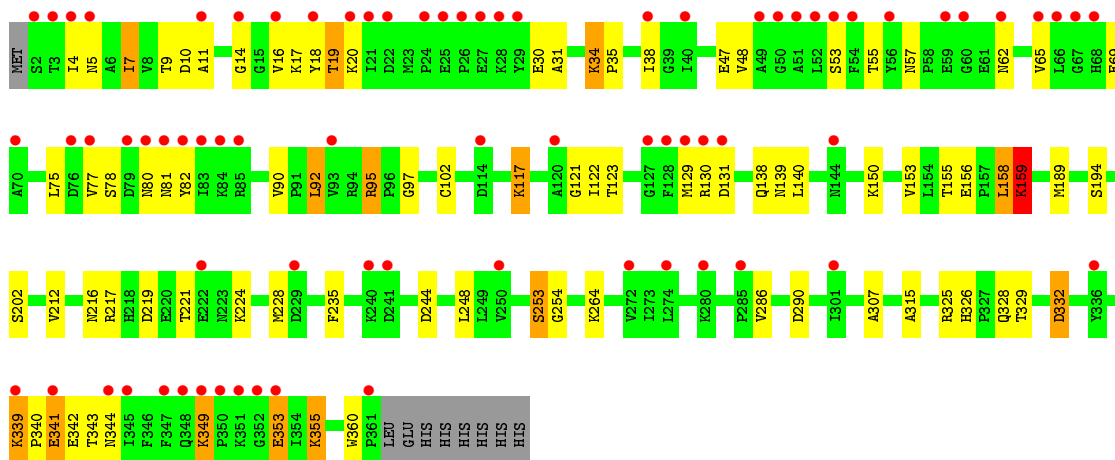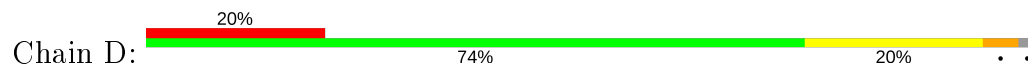

- Molecule 1: Glucose 1-dehydrogenase

- Molecule 1: Glucose 1-dehydrogenase

A307 Y312 Q328 T329 I330 Y336 E337 A338 K339 N344 F347 Q348 K349 P350 K351 G352 E353 P361 LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Glucose 1-dehydrogenase

Chain D:

20%

74% 20%

MET S2 T3 I4 N5 A6 I7 V8 T9 D10 A11 G14 G15 V16 K17 Y18 T19 K20 I21 D22 M23 P24 E25 P26 E27 K28 Y29 E30 A31 K34 P35 I38 G39 I40 E47 V48 A49 G50 A51 L52 S53 F54 T55 Y56 N57 P58 E59 G60 E61 N62 V65 L66 G67 H68 E69

A70 L75 D76 V77 S78 D79 N80 N81 Y82 I83 K84 R85 V90 P91 L92 V93 R94 R95 P96 G97 C102 D114 K117 A120 G121 I122 T123 G127 F128 M129 R130 D131 Q138 N139 L140 N144 K150 V153 L154 T155 E156 P157 L158 K159 M189 S194

S202 V212 N216 R217 H218 D219 E220 T221 E222 N223 K224 M228 D229 F235 K240 D241 D244 L248 L249 V250 S253 G254 K264 V272 I273 L274 K280 P285 V286 D290 I301 A307 A315 R325 H326 P327 Q328 T329 D332 Y336

K339 P340 E341 E342 T343 N344 I345 F346 F347 Q348 K349 P350 K351 G352 E353 I354 K355 W360 P361 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 28.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.01-2.33) 98.6 (28.00-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [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 (5.01%)	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)	0.42 , 59.5	EDS
L-test for twinning [2]	$<|L|> = 0.51, <L^2> = 0.35$	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.88	0/2887	0.88	1/3904 (0.0%)
1	B	0.92	1/2887 (0.0%)	0.93	3/3904 (0.1%)
1	C	0.83	2/2887 (0.1%)	0.87	5/3904 (0.1%)
1	D	0.79	0/2887	0.86	1/3904 (0.0%)
All	All	0.85	3/11548 (0.0%)	0.88	10/15616 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CD-OE2	-5.44	1.19	1.25
1	C	350	PRO	N-CD	5.36	1.55	1.47
1	C	96	PRO	N-CD	5.11	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	306	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C	95	ARG	C-N-CD	5.35	139.63	128.40
1	C	349	LYS	C-N-CD	5.18	139.28	128.40
1	C	148	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	208	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	87	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	D	159	LYS	CA-CB-CG	5.02	124.44	113.40
1	B	217	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2827	0	2808	33	0
1	B	2827	0	2807	15	0
1	C	2827	0	2807	27	0
1	D	2827	0	2807	54	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
3	A	48	0	24	1	0
3	B	48	0	24	1	0
3	C	48	0	24	1	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	0	0
All	All	11772	0	11371	130	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 (130) 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:D:329:THR:HA	1:D:332:ASP:OD2	1.75	0.87
1:D:19:THR:OG1	1:D:20:LYS:N	2.15	0.80
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:A:99:CYS:SG	1:A:102:CYS:HB2	2.27	0.73
1:D:353:GLU:HG3	1:D:353:GLU:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:CYS:HB3	1:A:69:GLU:OE2	1.90	0.71
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:D:7:ILE:HG23	1:D:129:MET:HB3	1.84	0.60
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: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:156:GLU:C	1:A:156:GLU:OE2	2.44	0.56
1:A:3:THR:HG23	1:A:22:ASP:OD1	2.05	0.56
1:A:224:LYS:HA	1:A:227:MET:HE3	1.89	0.54
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: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: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:5:ASN:N	1:D:131:ASP:OD2	2.36	0.51
1:A:227:MET:CE	1:A:354:ILE:HD11	2.40	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: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

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:THR:HG22	1:D:122:ILE:CG2	2.39	0.49
1:A:224:LYS:HA	1:A:227:MET:CE	2.42	0.49
1:A:227:MET:HE1	1:A:354:ILE:HD11	1.94	0.49
1:C:159:LYS:HD3	1:C:307:ALA:HB3	1.94	0.49
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
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: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:HD2	1:D:117:LYS:O	2.16	0.46
1:D:202:SER:HA	1:D:212:VAL:HG11	1.96	0.46
1:D:18:TYR:HE2	1:D:341:GLU:HG3	1.79	0.46
1:A:223:ASN:C	1:A:227:MET:HE2	2.36	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:D:18:TYR:CE2	1:D:340:PRO:HB2	2.51	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:D:253:SER:OG	1:D:254:GLY:N	2.50	0.45
1:A:29:TYR:OH	1:A:76:ASP:OD2	2.24	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:339:LYS:HD3	1:A:341:GLU:OE2	2.17	0.44
1:A:58:PRO:HG2	1:A:126:HIS:CE1	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HE	1:C:85:ARG:HB2	1.63	0.43
1:D:95:ARG:HH11	1:D:95:ARG:HG2	1.82	0.43
1:A:223:ASN:O	1:A:227:MET:HE2	2.18	0.43
1:D:34:LYS:HG2	1:D:75:LEU:HD11	2.01	0.43
1:C:228:MET:SD	1:C:235:PHE:HB2	2.58	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:326:HIS:HB3	1:A:329:THR:CG2	2.49	0.43
1:A:35:PRO:HB2	1:A:38:ILE:HD11	2.00	0.43
1:C:197:GLU:OE1	1:C:197:GLU:HA	2.18	0.43
1:A:189:MET:HA	1:A:248:LEU:O	2.19	0.42
1:A:326:HIS:HB3	1:A:329:THR:HG22	2.01	0.42
1:A:77:VAL:O	1:A:77:VAL:HG13	2.18	0.42
1:A:240:LYS:C	1:A:241:ASP:OD1	2.58	0.42
1:C:92:LEU:O	1:C:95:ARG:NH2	2.33	0.42
1:C:25:GLU:HG2	1:C:26:PRO:O	2.19	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: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:HA	1:B:75:LEU:HD23	1.87	0.42
1:B:23:MET:CE	1:B:23:MET:HA	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: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:132:VAL:C	1:A:133:ILE:HG13	2.40	0.41
1:A:156:GLU:O	1:A:159:LYS:HE3	2.21	0.40
1:B:77:VAL:HG13	1:B:77:VAL:O	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
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%)	291 (93%)	22 (7%)	15	16
1	B	313/322 (97%)	297 (95%)	16 (5%)	24	29
1	C	313/322 (97%)	290 (93%)	23 (7%)	14	14
1	D	313/322 (97%)	289 (92%)	24 (8%)	13	13
All	All	1252/1288 (97%)	1167 (93%)	85 (7%)	16	17

All (85) 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	143	VAL
1	A	148	LEU
1	A	159	LYS
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	306	ASP
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	148	LEU
1	B	150	LYS
1	B	159	LYS
1	B	163	LYS
1	B	178	GLN
1	B	222	GLU
1	B	223	ASN
1	B	229	ASP
1	B	257	SER
1	B	289	GLU
1	B	344	ASN
1	B	361	PRO
1	C	29	TYR
1	C	32	LYS
1	C	34	LYS
1	C	79	ASP
1	C	81	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	85	ARG
1	C	92	LEU
1	C	95	ARG
1	C	117	LYS
1	C	140	LEU
1	C	148	LEU
1	C	150	LYS
1	C	159	LYS
1	C	163	LYS
1	C	194	SER
1	C	225	MET
1	C	229	ASP
1	C	248	LEU
1	C	249	LEU
1	C	257	SER
1	C	264	LYS
1	C	339	LYS
1	C	344	ASN
1	D	7	ILE
1	D	19	THR
1	D	34	LYS
1	D	53	SER
1	D	78	SER
1	D	92	LEU
1	D	95	ARG
1	D	117	LYS
1	D	138	GLN
1	D	140	LEU
1	D	158	LEU
1	D	159	LYS
1	D	194	SER
1	D	219	ASP
1	D	244	ASP
1	D	253	SER
1	D	332	ASP
1	D	339	LYS
1	D	341	GLU
1	D	343	THR
1	D	344	ASN
1	D	349	LYS
1	D	353	GLU
1	D	355	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	118	HIS
1	A	268	ASN
1	A	269	ASN
1	A	324	HIS
1	A	344	ASN
1	A	348	GLN
1	B	118	HIS
1	B	144	ASN
1	B	223	ASN
1	B	269	ASN
1	C	68	HIS
1	C	118	HIS
1	C	138	GLN
1	C	267	ASN
1	C	268	ASN
1	C	269	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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	#$|Z| > 2$
3	DN4	A	1003	-	43,52,52	2.13	12 (27%)	53,80,80	1.40	5 (9%)
4	BGC	A	1004	-	12,12,12	1.89	4 (33%)	17,17,17	1.50	3 (17%)
4	BGC	B	1004	-	12,12,12	1.57	3 (25%)	17,17,17	1.37	2 (11%)
4	BGC	C	1004	-	12,12,12	0.86	1 (8%)	17,17,17	0.61	0
3	DN4	C	1003	-	43,52,52	1.84	11 (25%)	53,80,80	1.87	7 (13%)
3	DN4	D	1003	-	43,52,52	2.08	10 (23%)	53,80,80	1.63	10 (18%)
4	BGC	D	1004	-	12,12,12	1.20	1 (8%)	17,17,17	1.67	5 (29%)
3	DN4	B	1003	-	43,52,52	1.88	8 (18%)	53,80,80	2.15	9 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DN4	A	1003	-	-	16/27/67/67	0/5/5/5
4	BGC	A	1004	-	-	2/2/22/22	0/1/1/1
4	BGC	B	1004	-	-	2/2/22/22	0/1/1/1
4	BGC	C	1004	-	-	2/2/22/22	0/1/1/1
3	DN4	C	1003	-	-	12/27/67/67	0/5/5/5
3	DN4	D	1003	-	-	14/27/67/67	0/5/5/5
4	BGC	D	1004	-	-	2/2/22/22	0/1/1/1
3	DN4	B	1003	-	-	5/27/67/67	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	DN4	C3N-C7N	-6.82	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	DN4	C2A-N3A	6.64	1.42	1.32
3	D	1003	DN4	C2N-N1N	5.74	1.42	1.35
3	D	1003	DN4	P2B-O2B	5.61	1.69	1.59
3	B	1003	DN4	P2B-O2B	4.81	1.68	1.59
3	A	1003	DN4	C2N-N1N	4.75	1.40	1.35
3	C	1003	DN4	P2B-O2B	4.75	1.68	1.59
3	B	1003	DN4	O4B-C1B	4.71	1.47	1.41
3	B	1003	DN4	C2A-N3A	4.40	1.39	1.32
3	B	1003	DN4	O4D-C1D	4.38	1.47	1.41
3	A	1003	DN4	P2B-O2B	4.36	1.67	1.59
3	A	1003	DN4	C2A-N3A	4.24	1.38	1.32
3	C	1003	DN4	C2N-N1N	4.05	1.39	1.35
3	B	1003	DN4	C2N-N1N	3.94	1.39	1.35
4	A	1004	BGC	O2-C2	-3.94	1.33	1.43
3	A	1003	DN4	C2D-C1D	-3.84	1.47	1.53
3	C	1003	DN4	C3N-C7N	-3.73	1.43	1.47
3	A	1003	DN4	C2A-N1A	3.43	1.40	1.33
3	C	1003	DN4	C2A-N3A	3.40	1.37	1.32
3	C	1003	DN4	C2D-C1D	-3.34	1.48	1.53
3	C	1003	DN4	C6A-C5A	-3.18	1.31	1.43
3	C	1003	DN4	C5A-C4A	-3.17	1.32	1.40
3	A	1003	DN4	O4D-C1D	3.16	1.45	1.41
3	D	1003	DN4	C3N-C7N	-3.07	1.44	1.47
3	D	1003	DN4	C2A-N1A	3.06	1.39	1.33
3	A	1003	DN4	C6A-C5A	-2.89	1.32	1.43
3	B	1003	DN4	C3N-C7N	-2.84	1.44	1.47
4	A	1004	BGC	C1-C2	-2.82	1.45	1.52
3	D	1003	DN4	O4D-C1D	2.79	1.45	1.41
3	A	1003	DN4	P2B-O3X	2.77	1.65	1.54
3	B	1003	DN4	C5A-C4A	-2.63	1.34	1.40
3	C	1003	DN4	C6N-N1N	2.58	1.41	1.35
4	B	1004	BGC	C1-C2	-2.51	1.46	1.52
3	C	1003	DN4	C2A-N1A	2.48	1.38	1.33
4	D	1004	BGC	O5-C1	2.40	1.48	1.42
3	D	1003	DN4	C2D-C1D	-2.40	1.50	1.53
4	B	1004	BGC	O5-C5	-2.37	1.38	1.44
3	B	1003	DN4	C6A-C5A	-2.37	1.34	1.43
3	C	1003	DN4	P2B-O2X	2.36	1.63	1.54
3	C	1003	DN4	O4B-C1B	2.32	1.44	1.41
4	A	1004	BGC	C4-C5	-2.29	1.48	1.53
3	A	1003	DN4	C5A-C4A	-2.29	1.34	1.40
3	D	1003	DN4	C5A-C4A	-2.21	1.35	1.40

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1004	BGC	O5-C5	-2.20	1.39	1.44
4	B	1004	BGC	O2-C2	-2.19	1.37	1.43
3	A	1003	DN4	C6N-N1N	2.19	1.40	1.35
3	D	1003	DN4	C6N-N1N	2.19	1.40	1.35
3	D	1003	DN4	C6A-C5A	-2.16	1.35	1.43
4	C	1004	BGC	O1-C1	2.08	1.46	1.39
3	A	1003	DN4	C4A-N3A	-2.01	1.32	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	DN4	C1B-N9A-C4A	-8.57	111.58	126.64
3	B	1003	DN4	N3A-C2A-N1A	-8.28	115.74	128.68
3	C	1003	DN4	N3A-C2A-N1A	-7.40	117.11	128.68
3	C	1003	DN4	C1B-N9A-C4A	-6.89	114.54	126.64
3	D	1003	DN4	N3A-C2A-N1A	-5.48	120.12	128.68
3	A	1003	DN4	N3A-C2A-N1A	-4.86	121.08	128.68
3	D	1003	DN4	C1B-N9A-C4A	-4.63	118.51	126.64
3	C	1003	DN4	O4D-C1D-C2D	-4.38	100.52	106.93
3	A	1003	DN4	C1B-N9A-C4A	-4.37	118.97	126.64
3	D	1003	DN4	C4A-C5A-N7A	-3.99	105.24	109.40
4	D	1004	BGC	O5-C5-C6	3.81	115.90	106.44
4	B	1004	BGC	O5-C5-C6	-3.53	97.67	106.44
4	A	1004	BGC	O5-C5-C6	-3.51	97.71	106.44
3	B	1003	DN4	PN-O3-PA	-3.42	121.08	132.83
4	A	1004	BGC	O1-C1-O5	-2.89	101.71	110.38
4	B	1004	BGC	C1-O5-C5	2.71	118.77	113.66
3	B	1003	DN4	C3D-C2D-C1D	-2.68	96.94	100.98
3	B	1003	DN4	C2N-C3N-C7N	2.58	124.81	119.84
4	D	1004	BGC	C4-C3-C2	-2.58	106.33	110.82
3	B	1003	DN4	C5N-C6N-N1N	-2.57	116.71	120.40
3	A	1003	DN4	C3B-C2B-C1B	-2.51	98.18	102.89
3	C	1003	DN4	C3D-C2D-C1D	-2.43	97.32	100.98
3	C	1003	DN4	C2N-N1N-C1D	-2.37	113.85	119.14
4	D	1004	BGC	C3-C4-C5	-2.37	106.01	110.24
4	D	1004	BGC	O5-C5-C4	-2.30	105.52	109.69
3	D	1003	DN4	O4D-C4D-C5D	2.29	116.92	109.37
3	C	1003	DN4	O4B-C1B-C2B	-2.28	102.63	106.59
3	D	1003	DN4	C3B-C2B-C1B	-2.27	98.62	102.89
3	A	1003	DN4	O2A-PA-O1A	2.26	123.41	112.24
3	B	1003	DN4	O3X-P2B-O2X	-2.20	99.22	107.64
3	D	1003	DN4	O3X-P2B-O1X	2.19	119.27	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1004	BGC	O5-C1-C2	2.15	114.13	110.28
3	B	1003	DN4	C5N-C4N-C3N	2.15	123.26	120.56
3	D	1003	DN4	O4B-C1B-C2B	-2.13	102.90	106.59
4	A	1004	BGC	C3-C4-C5	-2.08	106.52	110.24
3	C	1003	DN4	C3B-C2B-C1B	-2.07	99.00	102.89
3	D	1003	DN4	O3D-C3D-C4D	-2.04	105.16	111.05
3	D	1003	DN4	O2A-PA-O1A	2.04	122.30	112.24
3	B	1003	DN4	C2N-N1N-C1D	-2.03	114.62	119.14
3	A	1003	DN4	O4B-C1B-C2B	-2.02	103.08	106.59
3	D	1003	DN4	C5N-C6N-N1N	-2.01	117.53	120.40

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1003	DN4	C5B-O5B-PA-O1A
3	C	1003	DN4	C5B-O5B-PA-O2A
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	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	D	1003	DN4	C5B-O5B-PA-O1A
3	D	1003	DN4	C5B-O5B-PA-O2A
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
3	A	1003	DN4	C5B-O5B-PA-O2A
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
4	D	1004	BGC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1003	DN4	C3D-C4D-C5D-O5D
4	A	1004	BGC	C4-C5-C6-O6
4	D	1004	BGC	C4-C5-C6-O6
4	C	1004	BGC	O5-C5-C6-O6
4	A	1004	BGC	O5-C5-C6-O6
4	C	1004	BGC	C4-C5-C6-O6
4	B	1004	BGC	O5-C5-C6-O6
3	D	1003	DN4	O4D-C4D-C5D-O5D
3	D	1003	DN4	C3D-C4D-C5D-O5D
4	B	1004	BGC	C4-C5-C6-O6
3	D	1003	DN4	C3B-C4B-C5B-O5B
3	C	1003	DN4	PN-O3-PA-O5B
3	C	1003	DN4	C2B-O2B-P2B-O1X
3	C	1003	DN4	C2B-O2B-P2B-O3X
3	A	1003	DN4	C5B-O5B-PA-O3
3	D	1003	DN4	O4B-C4B-C5B-O5B
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	C	1003	DN4	C5B-O5B-PA-O3
3	D	1003	DN4	C5B-O5B-PA-O3
3	C	1003	DN4	PN-O3-PA-O1A
3	D	1003	DN4	PA-O3-PN-O1N
3	D	1003	DN4	PA-O3-PN-O2N
3	A	1003	DN4	PA-O3-PN-O1N
3	C	1003	DN4	O4B-C4B-C5B-O5B
3	B	1003	DN4	O4B-C4B-C5B-O5B
3	A	1003	DN4	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 5 short contacts:

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

Ligand DN4 A 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand DN4 C 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand DN4 D 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand DN4 B 1003

Bond lengths

Bond angles

Torsions

Rings
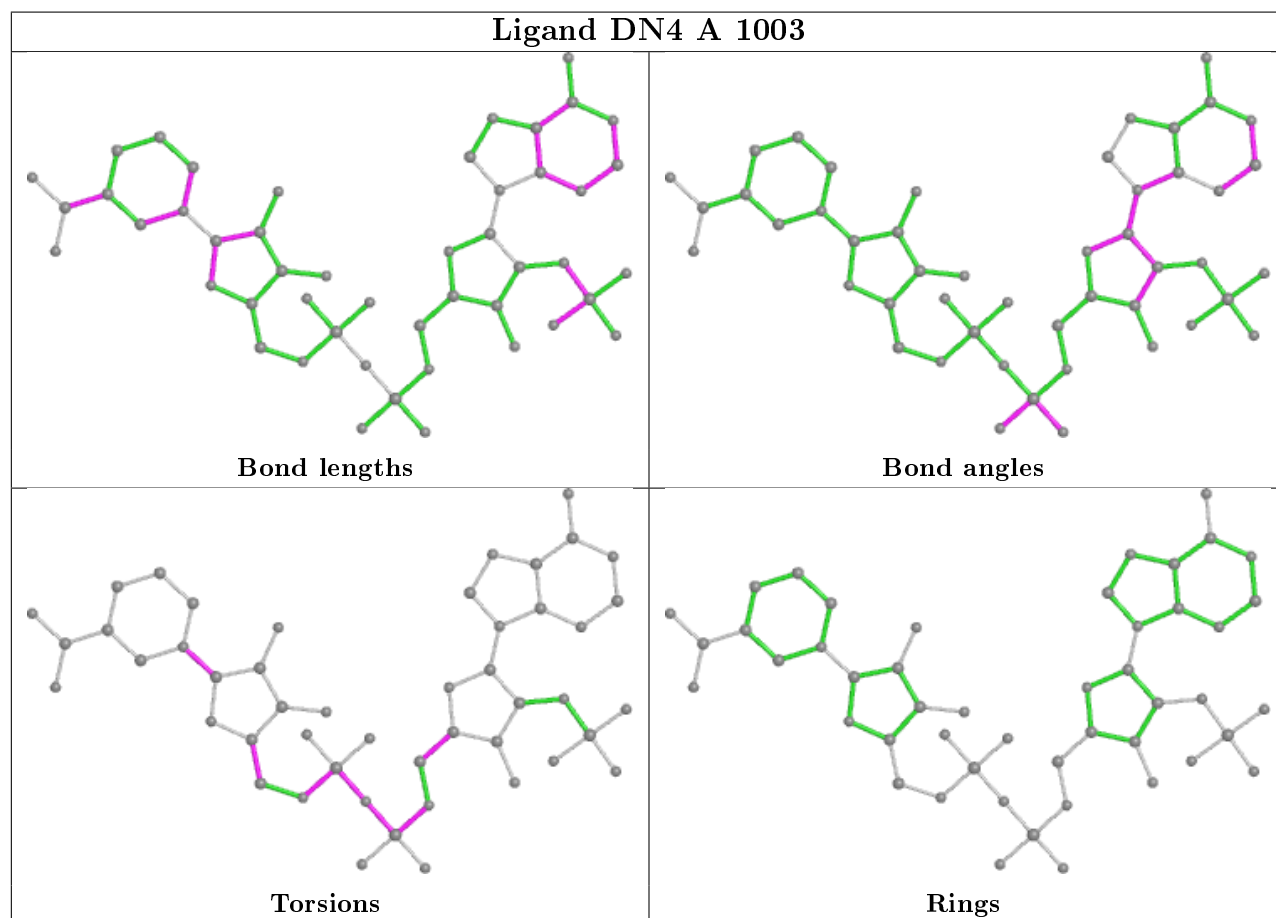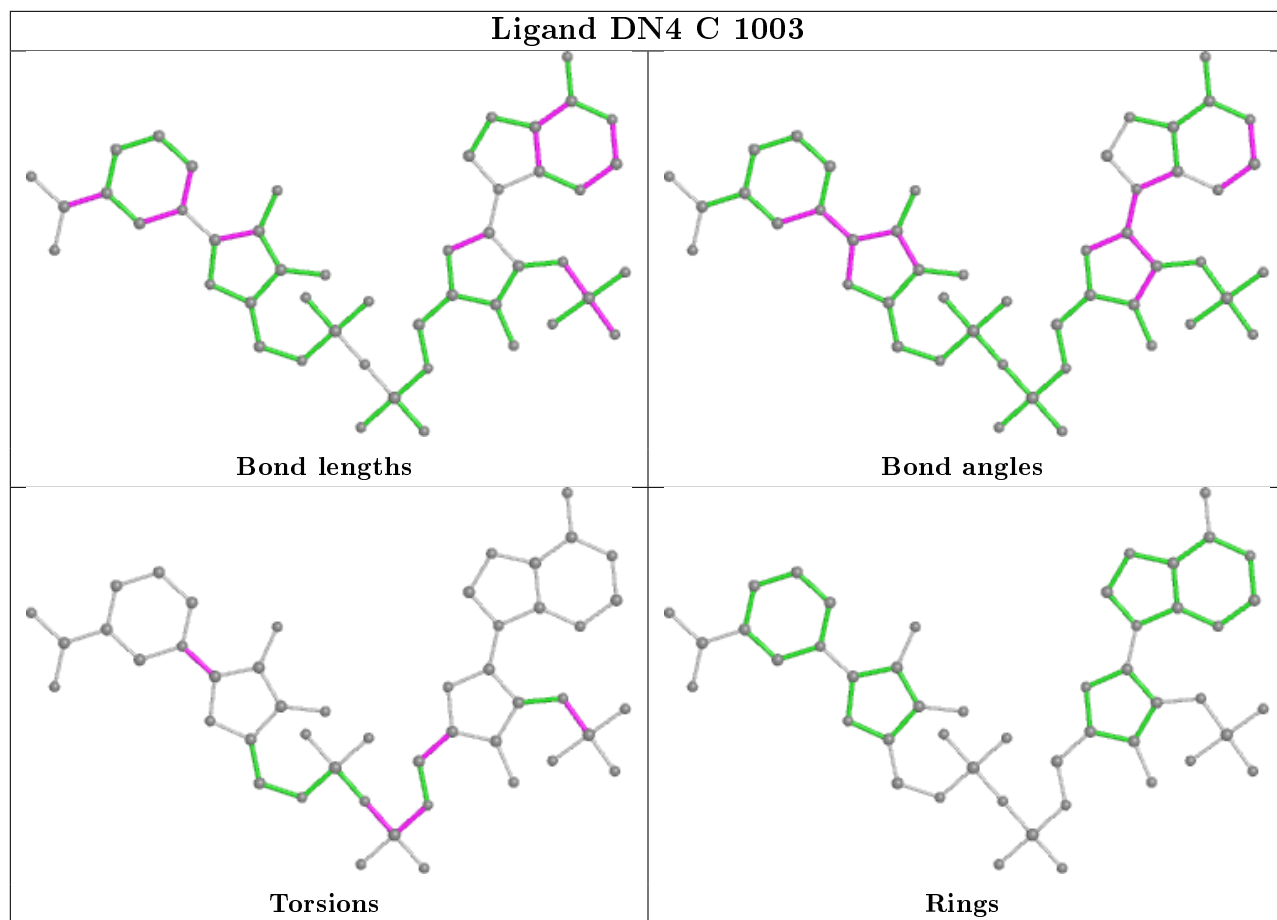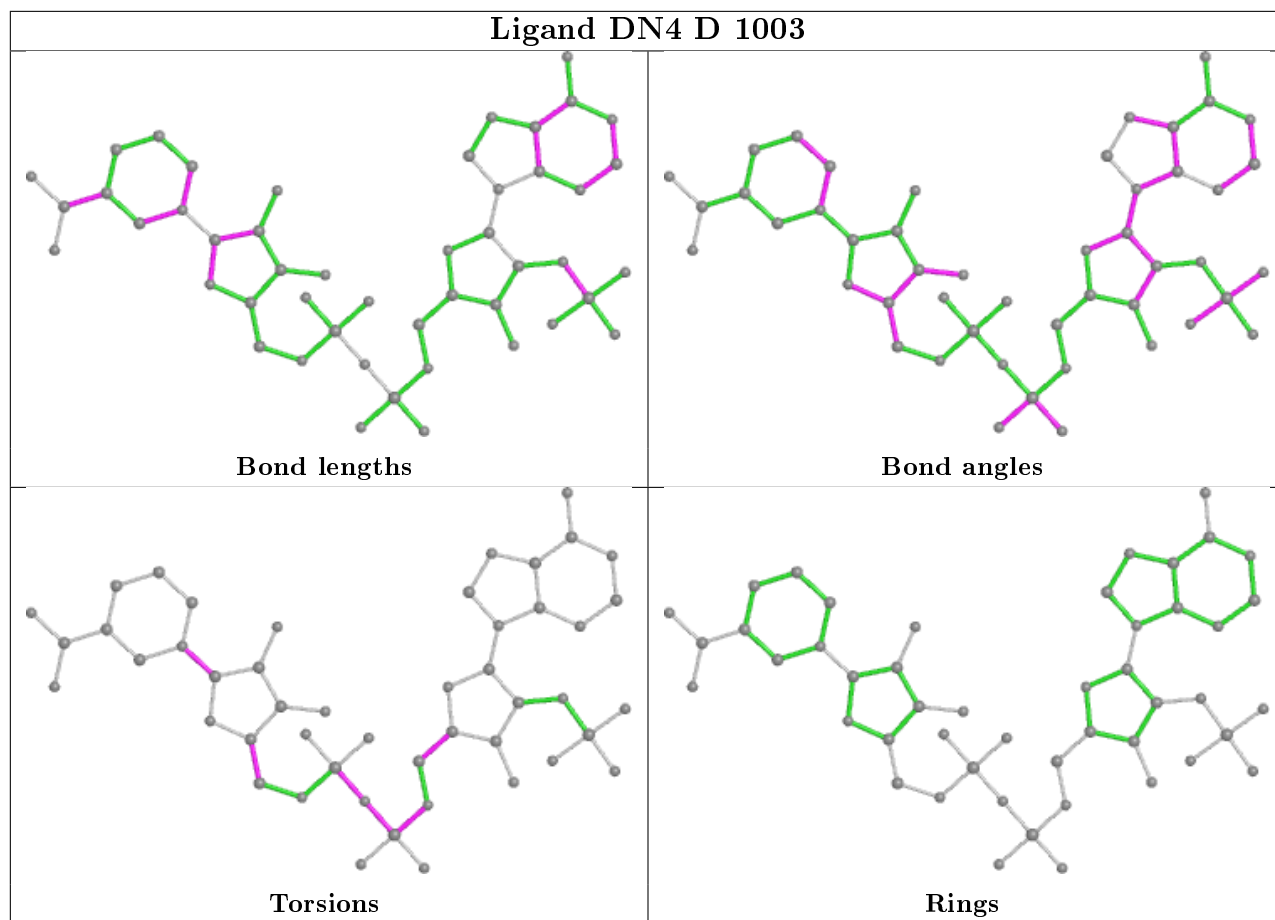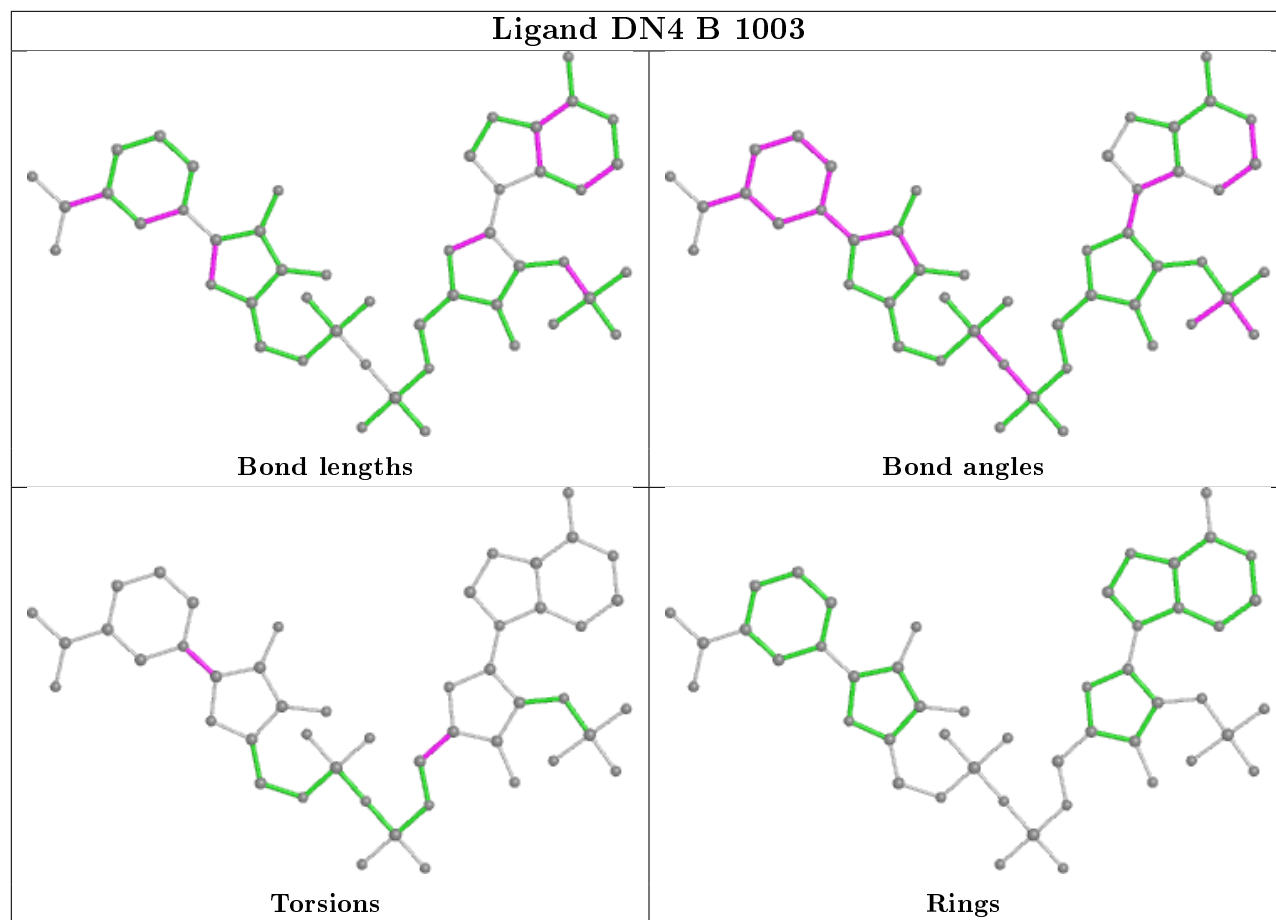
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.52	41 (11%)	5	8	24, 45, 74, 95	0
1	B	360/369 (97%)	0.21	21 (5%)	23	32	23, 38, 68, 96	0
1	C	360/369 (97%)	0.52	43 (11%)	4	7	25, 47, 77, 114	0
1	D	360/369 (97%)	0.93	75 (20%)	1	1	25, 55, 95, 126	0
All	All	1440/1476 (97%)	0.55	180 (12%)	3	6	23, 46, 82, 126	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	351	LYS	7.8
1	D	26	PRO	7.3
1	D	352	GLY	7.3
1	D	60	GLY	7.2
1	D	79	ASP	7.0
1	D	28	LYS	6.1
1	B	28	LYS	5.2
1	C	240	LYS	4.8
1	D	29	TYR	4.7
1	C	27	GLU	4.7
1	A	60	GLY	4.6
1	D	128	PHE	4.5
1	D	27	GLU	4.5
1	D	50	GLY	4.5
1	D	85	ARG	4.4
1	D	62	ASN	4.3
1	A	352	GLY	4.3
1	C	82	TYR	4.3
1	D	76	ASP	4.3
1	D	25	GLU	4.2
1	D	350	PRO	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	13	LYS	4.1
1	D	38	ILE	4.1
1	D	129	MET	4.1
1	D	66	LEU	4.0
1	D	16	VAL	3.9
1	A	274	LEU	3.9
1	D	82	TYR	3.9
1	D	2	SER	3.9
1	D	84	LYS	3.8
1	D	240	LYS	3.8
1	A	351	LYS	3.8
1	D	5	ASN	3.8
1	C	280	LYS	3.8
1	A	53	SER	3.8
1	C	60	GLY	3.7
1	B	50	GLY	3.7
1	D	51	ALA	3.7
1	D	18	TYR	3.7
1	D	336	TYR	3.7
1	C	348	GLN	3.7
1	D	24	PRO	3.6
1	D	344	ASN	3.6
1	A	49	ALA	3.6
1	D	22	ASP	3.6
1	A	59	GLU	3.5
1	C	79	ASP	3.5
1	D	127	GLY	3.5
1	D	222	GLU	3.5
1	B	280	LYS	3.5
1	A	79	ASP	3.5
1	D	20	LYS	3.4
1	A	222	GLU	3.4
1	A	280	LYS	3.4
1	D	280	LYS	3.4
1	C	272	VAL	3.4
1	A	81	ASN	3.3
1	C	351	LYS	3.3
1	D	347	PHE	3.3
1	D	68	HIS	3.2
1	C	28	LYS	3.2
1	D	250	VAL	3.2
1	C	84	LYS	3.2

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	3	THR	3.1
1	C	281	ALA	3.1
1	C	2	SER	3.1
1	C	22	ASP	3.1
1	A	40	ILE	3.1
1	B	82	TYR	3.1
1	C	85	ARG	3.0
1	D	54	PHE	3.0
1	A	348	GLN	3.0
1	D	120	ALA	3.0
1	D	53	SER	3.0
1	A	20	LYS	3.0
1	B	13	LYS	3.0
1	A	223	ASN	2.9
1	C	223	ASN	2.9
1	C	249	LEU	2.9
1	D	348	GLN	2.9
1	A	85	ARG	2.9
1	B	351	LYS	2.8
1	A	240	LYS	2.8
1	B	81	ASN	2.8
1	D	67	GLY	2.8
1	D	241	ASP	2.8
1	D	49	ALA	2.8
1	B	79	ASP	2.8
1	D	70	ALA	2.8
1	D	81	ASN	2.8
1	C	301	ILE	2.8
1	C	26	PRO	2.7
1	D	341	GLU	2.8
1	A	347	PHE	2.7
1	A	62	ASN	2.7
1	A	250	VAL	2.7
1	C	93	VAL	2.7
1	A	68	HIS	2.7
1	C	350	PRO	2.7
1	B	53	SER	2.6
1	A	241	ASP	2.6
1	C	81	ASN	2.6
1	D	77	VAL	2.6
1	D	301	ILE	2.6
1	D	59	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	2.6
1	B	272	VAL	2.5
1	C	77	VAL	2.5
1	A	38	ILE	2.5
1	B	59	GLU	2.5
1	A	127	GLY	2.5
1	D	11	ALA	2.5
1	B	348	GLN	2.5
1	C	68	HIS	2.5
1	A	273	ILE	2.5
1	B	249	LEU	2.5
1	B	274	LEU	2.5
1	A	128	PHE	2.5
1	B	93	VAL	2.5
1	C	347	PHE	2.4
1	C	24	PRO	2.4
1	D	229	ASP	2.4
1	C	29	TYR	2.4
1	C	40	ILE	2.4
1	C	157	PRO	2.4
1	C	283	GLY	2.4
1	C	80	ASN	2.4
1	A	272	VAL	2.4
1	A	67	GLY	2.4
1	D	14	GLY	2.3
1	D	361	PRO	2.3
1	A	70	ALA	2.3
1	D	40	ILE	2.3
1	D	345	ILE	2.3
1	C	154	LEU	2.3
1	A	219	ASP	2.3
1	D	130	ARG	2.3
1	B	128	PHE	2.3
1	D	21	ILE	2.3
1	A	239	LEU	2.3
1	C	352	GLY	2.3
1	C	229	ASP	2.3
1	B	273	ILE	2.3
1	A	323	TYR	2.2
1	D	131	ASP	2.2
1	C	328	GLN	2.2
1	A	325	ARG	2.2

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	241	ASP	2.2
1	B	12	PRO	2.2
1	D	274	LEU	2.2
1	C	250	VAL	2.2
1	D	65	VAL	2.2
1	C	248	LEU	2.2
1	A	78	SER	2.2
1	D	114	ASP	2.2
1	A	84	LYS	2.2
1	C	192	ILE	2.2
1	B	26	PRO	2.2
1	B	250	VAL	2.1
1	D	272	VAL	2.1
1	D	83	ILE	2.1
1	D	285	PRO	2.1
1	D	80	ASN	2.1
1	A	39	GLY	2.1
1	D	4	ILE	2.1
1	D	56	TYR	2.1
1	B	344	ASN	2.1
1	D	144	ASN	2.1
1	A	82	TYR	2.1
1	D	339	LYS	2.1
1	D	349	LYS	2.1
1	A	249	LEU	2.1
1	D	353	GLU	2.1
1	C	273	ILE	2.0
1	D	52	LEU	2.0
1	A	301	ILE	2.0
1	A	344	ASN	2.0
1	C	67	GLY	2.0
1	C	120	ALA	2.0
1	C	302	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	1001	1/1	0.76	0.17	89,89,89,89	0
2	ZN	B	1001	1/1	0.88	0.05	65,65,65,65	0
3	DN4	D	1003	48/48	0.88	0.15	44,68,92,101	0
2	ZN	A	1001	1/1	0.89	0.15	71,71,71,71	0
4	BGC	B	1004	12/12	0.90	0.23	51,64,73,73	0
2	ZN	D	1002	1/1	0.91	0.10	34,34,34,34	0
2	ZN	A	1002	1/1	0.91	0.08	34,34,34,34	0
3	DN4	C	1003	48/48	0.91	0.15	43,65,95,109	0
4	BGC	A	1004	12/12	0.91	0.13	48,67,88,93	0
3	DN4	B	1003	48/48	0.92	0.14	40,56,77,80	0
4	BGC	C	1004	12/12	0.92	0.21	61,79,93,93	0
4	BGC	D	1004	12/12	0.92	0.18	66,77,85,91	0
3	DN4	A	1003	48/48	0.92	0.13	38,67,85,95	0
2	ZN	C	1001	1/1	0.94	0.15	71,71,71,71	0
2	ZN	C	1002	1/1	0.95	0.08	35,35,35,35	0
2	ZN	B	1002	1/1	1.00	0.08	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
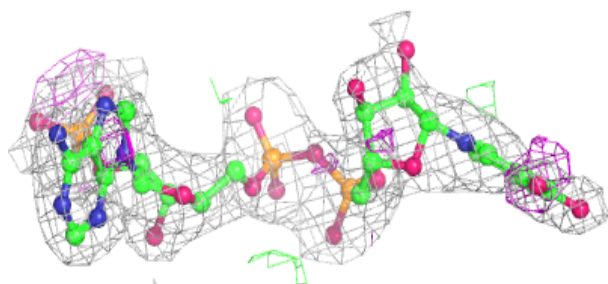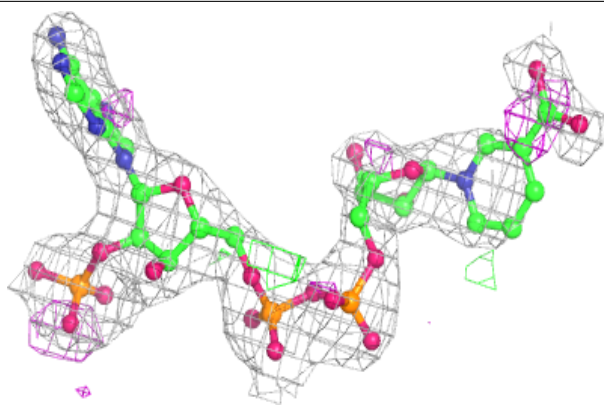mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
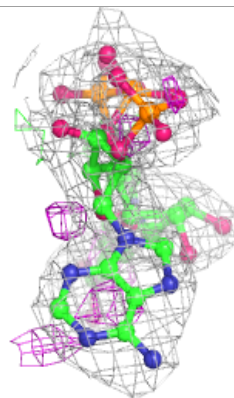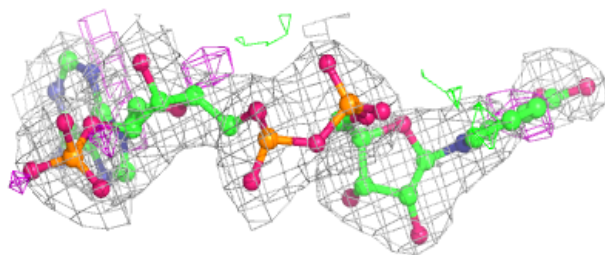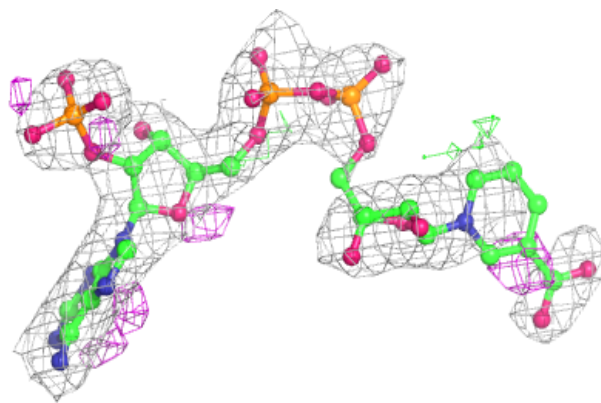
Electron density around DN4 C 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
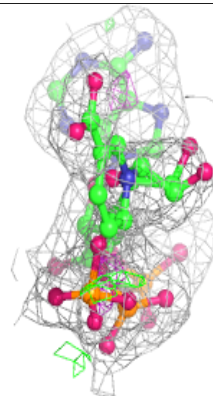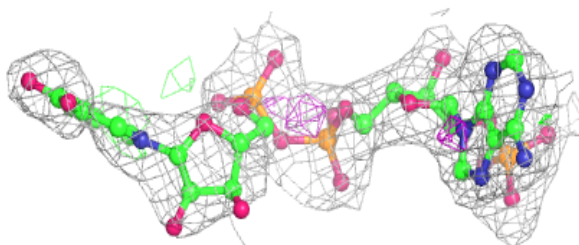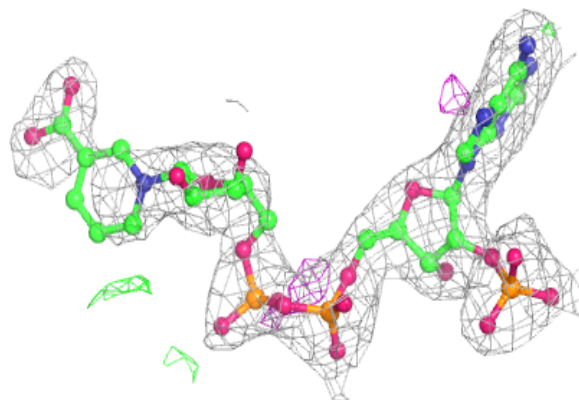mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
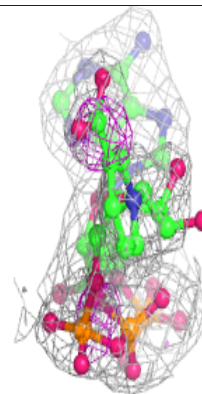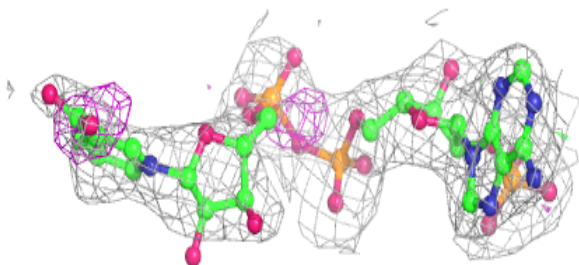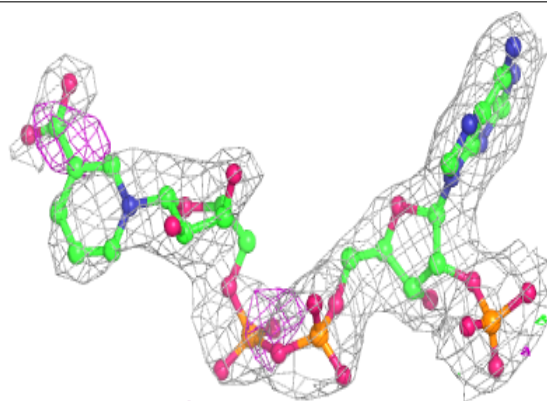
Electron density around DN4 B 1003:

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

Electron density around DN4 A 1003:

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

6.5 Other polymers (i)

There are no such residues in this entry.