



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

PDB ID : 3EPG  
Title : Structure of Human DNA Polymerase Iota complexed with N2-ethylguanine  
Authors : Pence, M.G.  
Deposited on : 2008-09-29  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

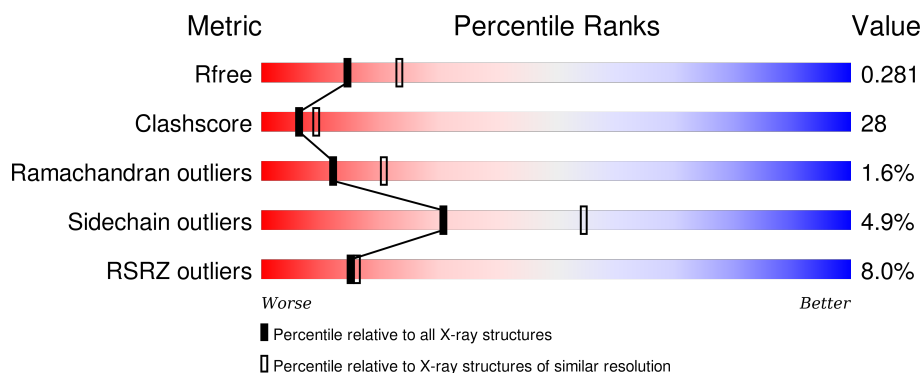
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

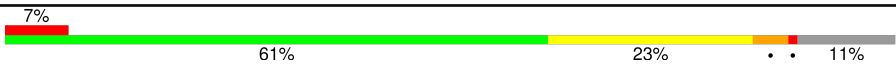


The reported resolution of this entry is 2.50 Å.

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	420	
2	B	18	
2	C	18	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3307 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.

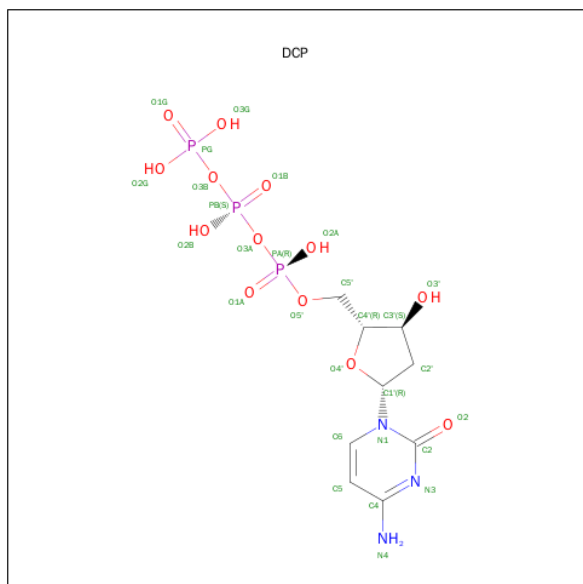
- Molecule 1 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2896	1825	504	546	21			

- Molecule 2 is a DNA chain called 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			142	67	29	39	7			
2	C	8	Total	C	N	O	P	0	0	0
			168	80	30	50	8			

- Molecule 3 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		
4	C	1	Total	Na	0	0
			1	1		

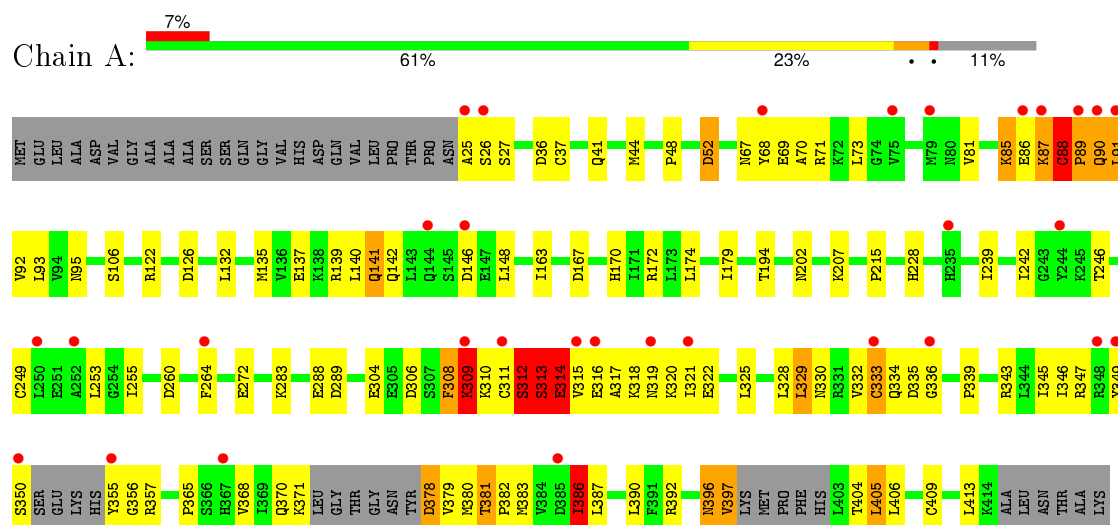
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	C	2	Total	O	0	0
			2	2		

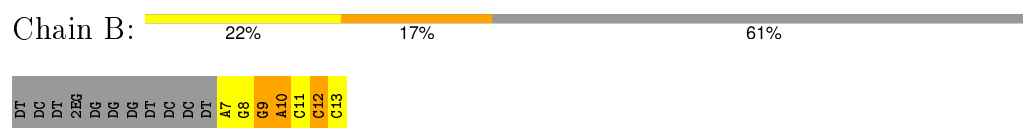
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

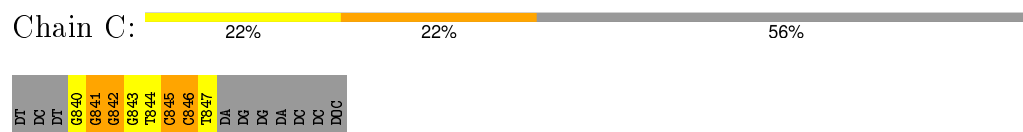
- Molecule 1: DNA polymerase iota



- Molecule 2: 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'



- Molecule 2: 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.53Å 98.53Å 202.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.50) 99.7 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.18 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.283 0.240 , 0.281	Depositor DCC
$R_{free}$ test set	942 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 18423 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 2EG, DCP, DOC

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	0.72	0/2934	0.77	2/3964 (0.1%)
2	B	3.17	21/139 (15.1%)	3.35	22/212 (10.4%)
2	C	4.69	44/160 (27.5%)	4.57	42/245 (17.1%)
All	All	1.41	65/3233 (2.0%)	1.49	66/4421 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	842	DG	P-O5'	-17.45	1.42	1.59
2	C	842	DG	N7-C5	-16.99	1.29	1.39
2	C	845	DC	C4'-O4'	-13.33	1.31	1.45
2	C	842	DG	N9-C8	-12.87	1.28	1.37
2	B	12	DC	N3-C4	12.57	1.42	1.33
2	C	846	DC	N3-C4	9.59	1.40	1.33
2	C	845	DC	O4'-C1'	-9.51	1.30	1.42
2	C	845	DC	C4-C5	-9.43	1.35	1.43
2	C	842	DG	N9-C4	-8.98	1.30	1.38
2	B	12	DC	N1-C6	8.76	1.42	1.37
2	B	11	DC	N3-C4	8.62	1.40	1.33
2	C	844	DT	N3-C4	-8.28	1.32	1.38
2	C	844	DT	P-O5'	-7.97	1.51	1.59
2	C	842	DG	C6-N1	-7.88	1.34	1.39
2	B	11	DC	C5-C6	7.82	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	844	DT	C4-O4	-7.81	1.16	1.23
2	B	9	DG	N7-C5	-7.68	1.34	1.39
2	C	843	DG	N7-C5	-7.55	1.34	1.39
2	C	846	DC	C2-N3	7.44	1.41	1.35
2	B	8	DG	C6-N1	-7.33	1.34	1.39
2	B	11	DC	N1-C6	7.26	1.41	1.37
2	C	842	DG	O3'-P	-7.18	1.52	1.61
2	C	841	DG	C8-N7	-7.17	1.26	1.30
2	C	844	DT	C2-N3	-7.13	1.32	1.37
2	C	844	DT	C4-C5	-6.89	1.38	1.45
2	B	11	DC	C2-N3	6.80	1.41	1.35
2	C	843	DG	C8-N7	6.78	1.35	1.30
2	C	842	DG	P-OP2	-6.77	1.37	1.49
2	B	8	DG	N7-C5	-6.74	1.35	1.39
2	C	841	DG	C6-N1	-6.60	1.34	1.39
2	C	841	DG	N9-C8	-6.60	1.33	1.37
2	B	9	DG	N9-C8	-6.59	1.33	1.37
2	B	9	DG	N9-C4	-6.59	1.32	1.38
2	C	846	DC	C5-C6	6.41	1.39	1.34
2	C	844	DT	P-OP1	-6.35	1.38	1.49
2	C	845	DC	C4-N4	-6.34	1.28	1.33
2	C	841	DG	N7-C5	-6.31	1.35	1.39
2	C	841	DG	N1-C2	-6.29	1.32	1.37
2	C	843	DG	O3'-P	-6.21	1.53	1.61
2	B	12	DC	C5-C6	6.20	1.39	1.34
2	C	846	DC	N1-C6	6.10	1.40	1.37
2	C	842	DG	P-OP1	-6.02	1.38	1.49
2	C	844	DT	C2-O2	-6.02	1.17	1.22
2	C	845	DC	N1-C2	-6.00	1.34	1.40
2	C	844	DT	P-OP2	-5.85	1.39	1.49
2	B	12	DC	C4-C5	-5.82	1.38	1.43
2	B	8	DG	N9-C8	-5.82	1.33	1.37
2	C	845	DC	C2'-C1'	-5.75	1.46	1.52
2	C	843	DG	N9-C4	-5.72	1.33	1.38
2	C	841	DG	C5-C4	-5.72	1.34	1.38
2	C	842	DG	O4'-C1'	-5.71	1.35	1.42
2	B	9	DG	C8-N7	5.66	1.34	1.30
2	C	841	DG	P-O5'	-5.64	1.54	1.59
2	B	8	DG	N3-C4	-5.49	1.31	1.35
2	B	8	DG	C5-C4	-5.48	1.34	1.38
2	C	845	DC	C2-O2	-5.47	1.19	1.24
2	B	12	DC	C2-N3	5.36	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	DG	N1-C2	5.36	1.42	1.37
2	B	8	DG	C2-N3	-5.33	1.28	1.32
2	B	11	DC	C4-C5	-5.32	1.38	1.43
2	C	841	DG	O3'-P	-5.29	1.54	1.61
2	C	842	DG	C2-N2	-5.17	1.29	1.34
2	C	842	DG	N3-C4	-5.16	1.31	1.35
2	C	844	DT	C5-C6	-5.07	1.30	1.34
2	C	846	DC	C4-C5	-5.06	1.39	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	842	DG	N3-C4-C5	-20.42	118.39	128.60
2	C	842	DG	C2-N3-C4	18.99	121.39	111.90
2	C	843	DG	C2-N3-C4	18.14	120.97	111.90
2	B	9	DG	C2-N3-C4	17.12	120.46	111.90
2	C	842	DG	C5-C6-N1	15.02	119.01	111.50
2	C	843	DG	C5-C6-N1	14.96	118.98	111.50
2	C	843	DG	N3-C4-C5	-14.87	121.17	128.60
2	B	9	DG	N3-C4-C5	-14.53	121.34	128.60
2	C	845	DC	O4'-C4'-C3'	-13.48	97.91	106.00
2	B	9	DG	C5-C6-N1	13.24	118.12	111.50
2	C	842	DG	N3-C4-N9	12.71	133.63	126.00
2	C	845	DC	C5'-C4'-C3'	-12.48	91.64	114.10
2	C	844	DT	O4'-C4'-C3'	-12.27	98.64	106.00
2	C	842	DG	C4-C5-N7	-12.02	105.99	110.80
2	B	9	DG	C4-C5-N7	-11.83	106.07	110.80
2	C	842	DG	C6-N1-C2	-10.98	118.51	125.10
2	C	843	DG	C5-C6-O6	-10.89	122.07	128.60
2	C	845	DC	O4'-C1'-N1	-10.53	100.63	108.00
2	C	845	DC	O4'-C1'-C2'	-10.35	97.62	105.90
2	B	9	DG	C5-C6-O6	-10.18	122.49	128.60
2	B	9	DG	O4'-C4'-C3'	-9.61	100.23	106.00
2	C	842	DG	C5-N7-C8	9.38	108.99	104.30
2	C	843	DG	C6-N1-C2	-9.15	119.61	125.10
2	C	842	DG	O5'-P-OP1	8.97	121.46	110.70
2	C	843	DG	N3-C4-N9	8.97	131.38	126.00
2	B	9	DG	C6-N1-C2	-8.87	119.78	125.10
2	C	843	DG	C4-C5-N7	-8.67	107.33	110.80
2	B	9	DG	C5-N7-C8	8.54	108.57	104.30
2	B	9	DG	N7-C8-N9	-8.54	108.83	113.10
2	B	9	DG	O4'-C1'-N9	8.40	113.88	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	DG	N3-C4-N9	8.38	131.03	126.00
2	B	8	DG	O4'-C1'-C2'	-8.29	99.27	105.90
2	C	846	DC	O4'-C1'-N1	-8.26	102.22	108.00
2	B	12	DC	O4'-C4'-C3'	-7.81	101.31	106.00
2	C	842	DG	C5-C6-O6	-7.54	124.08	128.60
2	C	845	DC	C6-N1-C2	-7.48	117.31	120.30
2	C	843	DG	N7-C8-N9	-7.28	109.46	113.10
2	C	846	DC	N1-C2-O2	7.01	123.11	118.90
2	C	842	DG	C5'-C4'-C3'	6.85	126.44	114.10
2	B	11	DC	N3-C4-C5	-6.83	119.17	121.90
2	C	843	DG	C5-N7-C8	6.57	107.58	104.30
2	C	842	DG	N7-C8-N9	-6.47	109.87	113.10
2	B	9	DG	C6-C5-N7	6.42	134.25	130.40
2	C	842	DG	N9-C4-C5	6.39	107.96	105.40
2	C	844	DT	C4'-C3'-C2'	-6.26	97.46	103.10
2	C	845	DC	N3-C4-C5	-6.26	119.39	121.90
2	B	9	DG	C8-N9-C4	6.24	108.90	106.40
2	B	9	DG	C1'-O4'-C4'	-6.24	103.86	110.10
2	C	845	DC	N3-C2-O2	-6.18	117.57	121.90
2	C	841	DG	O3'-P-O5'	-6.13	92.36	104.00
2	C	843	DG	O4'-C1'-N9	-6.08	103.74	108.00
2	C	843	DG	C6-C5-N7	6.01	134.00	130.40
2	C	842	DG	P-O5'-C5'	5.98	130.47	120.90
1	A	313	SER	CB-CA-C	-5.83	99.02	110.10
2	B	9	DG	N9-C4-C5	5.58	107.63	105.40
2	C	845	DC	C1'-O4'-C4'	-5.53	104.57	110.10
2	C	843	DG	N1-C2-N3	-5.50	120.60	123.90
2	B	9	DG	N1-C2-N3	-5.46	120.62	123.90
2	B	10	DA	O4'-C4'-C3'	-5.44	102.32	104.50
2	C	842	DG	C6-C5-N7	5.36	133.62	130.40
1	A	392	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	C	841	DG	P-O3'-C3'	5.24	125.98	119.70
2	B	9	DG	P-O3'-C3'	5.23	125.98	119.70
2	C	843	DG	N9-C4-C5	5.12	107.45	105.40
2	C	847	DT	C6-C5-C7	-5.11	119.84	122.90
2	B	7	DA	P-O3'-C3'	5.10	125.83	119.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	309	LYS	Peptide
1	A	312	SER	Peptide
1	A	313	SER	Peptide
1	A	314	GLU	Peptide
1	A	378	ASP	Peptide
1	A	396	ASN	Peptide
1	A	52	ASP	Peptide
1	A	87	LYS	Peptide
1	A	88	CYS	Peptide
1	A	89	PRO	Peptide
1	A	90	GLN	Peptide

## 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	2896	0	2929	168	0
2	B	142	0	78	4	0
2	C	168	0	90	4	0
3	A	28	0	12	8	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
5	A	67	0	0	5	0
5	C	2	0	0	0	0
All	All	3307	0	3109	176	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 28.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD22	1:A:406:LEU:N	1.04	1.37
1:A:44:MET:CE	1:A:67:ASN:HD22	1.37	1.35
1:A:405:LEU:CD2	1:A:406:LEU:N	1.94	1.29
1:A:316:GLU:HA	1:A:319:ASN:OD1	1.37	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD22	1:A:405:LEU:C	1.58	1.16
1:A:386:ILE:CD1	1:A:386:ILE:H	1.56	1.14
1:A:44:MET:HE1	1:A:67:ASN:HD22	1.13	1.12
1:A:306:ASP:O	1:A:405:LEU:HD23	1.49	1.09
1:A:316:GLU:O	1:A:319:ASN:HB2	1.53	1.09
1:A:91:LEU:HD23	1:A:91:LEU:O	1.51	1.09
1:A:167:ASP:CB	1:A:170:HIS:HD2	1.66	1.07
1:A:167:ASP:HB3	1:A:170:HIS:HD2	1.17	1.06
1:A:44:MET:CE	1:A:67:ASN:ND2	2.20	1.05
1:A:386:ILE:N	1:A:386:ILE:HD13	1.62	1.04
1:A:311:CYS:O	1:A:312:SER:HB2	1.24	1.04
1:A:44:MET:HE2	1:A:67:ASN:HD22	1.23	1.04
1:A:349:TYR:HA	1:A:350:SER:HB3	1.36	1.03
1:A:167:ASP:HB3	1:A:170:HIS:CD2	1.94	1.01
1:A:396:ASN:O	1:A:397:VAL:O	1.81	0.99
1:A:311:CYS:O	1:A:312:SER:CB	2.11	0.97
1:A:386:ILE:HD13	1:A:386:ILE:H	0.82	0.96
1:A:405:LEU:HD22	1:A:406:LEU:H	1.27	0.96
1:A:44:MET:HE1	1:A:67:ASN:ND2	1.80	0.95
1:A:386:ILE:CD1	1:A:386:ILE:N	2.14	0.95
1:A:405:LEU:HD22	1:A:406:LEU:CA	1.99	0.91
1:A:91:LEU:C	1:A:91:LEU:HD23	1.91	0.91
1:A:167:ASP:CB	1:A:170:HIS:CD2	2.51	0.90
1:A:318:LYS:O	1:A:322:GLU:CG	2.20	0.89
1:A:396:ASN:HB3	1:A:397:VAL:HA	1.55	0.88
1:A:41:GLN:HE22	1:A:194:THR:H	1.22	0.85
1:A:318:LYS:O	1:A:322:GLU:HG2	1.80	0.82
1:A:371:LYS:CB	1:A:379:VAL:CG2	2.59	0.81
1:A:316:GLU:O	1:A:319:ASN:CB	2.28	0.80
1:A:318:LYS:O	1:A:322:GLU:HG3	1.80	0.80
1:A:405:LEU:CD2	1:A:406:LEU:H	1.81	0.77
1:A:371:LYS:CB	1:A:379:VAL:HG21	2.14	0.77
1:A:44:MET:HE3	1:A:67:ASN:HB3	1.67	0.76
1:A:316:GLU:O	1:A:319:ASN:N	2.21	0.74
1:A:85:LYS:O	1:A:89:PRO:HG3	1.89	0.72
1:A:378:ASP:O	1:A:382:PRO:HD2	1.91	0.70
1:A:25:ALA:O	1:A:26:SER:HB2	1.89	0.70
3:A:875:DCP:O1B	3:A:875:DCP:H3'	1.92	0.70
1:A:255:ILE:HD11	1:A:264:PHE:CE2	2.27	0.69
1:A:365:PRO:HB2	1:A:368:VAL:HG23	1.74	0.68
1:A:325:LEU:HD21	1:A:383:MET:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:O	1:A:335:ASP:C	2.31	0.67
2:C:845:DC:H2''	2:C:846:DC:O5'	1.95	0.66
2:C:841:DG:H2''	2:C:842:DG:O5'	1.96	0.66
1:A:319:ASN:O	1:A:322:GLU:N	2.28	0.66
1:A:71:ARG:NH2	3:A:875:DCP:O3G	2.29	0.66
1:A:309:LYS:HE3	1:A:309:LYS:H	1.60	0.65
1:A:386:ILE:N	1:A:386:ILE:HD12	2.11	0.63
1:A:88:CYS:O	1:A:90:GLN:C	2.38	0.62
1:A:67:ASN:HB2	1:A:69:GLU:OE1	2.00	0.62
1:A:325:LEU:HD23	1:A:380:MET:HG2	1.82	0.61
1:A:349:TYR:HA	1:A:350:SER:CB	2.17	0.61
1:A:81:VAL:O	1:A:85:LYS:HB2	2.00	0.61
1:A:316:GLU:CA	1:A:319:ASN:OD1	2.30	0.61
2:B:9:DG:H2'	2:B:10:DA:C8	2.36	0.61
1:A:315:VAL:O	1:A:318:LYS:HB3	2.01	0.61
1:A:167:ASP:HB2	1:A:170:HIS:HD2	1.63	0.61
1:A:325:LEU:HG	1:A:329:LEU:CD1	2.31	0.60
1:A:396:ASN:HB3	1:A:397:VAL:CA	2.20	0.60
1:A:346:ILE:HG22	1:A:406:LEU:HD23	1.84	0.60
1:A:85:LYS:O	1:A:89:PRO:HA	2.01	0.60
1:A:71:ARG:NH1	3:A:875:DCP:O3G	2.35	0.60
1:A:44:MET:HE2	1:A:67:ASN:ND2	2.00	0.60
1:A:383:MET:O	1:A:386:ILE:HB	2.02	0.60
1:A:308:PHE:CB	1:A:309:LYS:HE3	2.32	0.59
1:A:207:LYS:NZ	2:B:13:DOC:OP1	2.27	0.59
1:A:86:GLU:CD	1:A:86:GLU:C	2.60	0.59
3:A:875:DCP:N4	2:C:840:2EG:O6	2.33	0.59
1:A:313:SER:O	1:A:315:VAL:N	2.35	0.59
1:A:355:TYR:CE2	1:A:357:ARG:HD2	2.36	0.59
1:A:381:THR:HB	1:A:382:PRO:CD	2.32	0.59
1:A:316:GLU:C	1:A:319:ASN:H	2.06	0.59
1:A:349:TYR:CA	1:A:350:SER:HB3	2.24	0.59
1:A:319:ASN:HA	1:A:322:GLU:HG3	1.84	0.58
1:A:325:LEU:O	1:A:329:LEU:HD12	2.03	0.58
1:A:81:VAL:O	1:A:85:LYS:CB	2.51	0.58
1:A:88:CYS:HB3	1:A:91:LEU:HB3	1.85	0.58
1:A:334:GLN:O	1:A:336:GLY:N	2.37	0.58
1:A:106:SER:OG	1:A:122:ARG:NH2	2.37	0.58
1:A:396:ASN:C	1:A:397:VAL:O	2.41	0.58
1:A:44:MET:CE	1:A:67:ASN:CB	2.82	0.57
1:A:260:ASP:O	1:A:264:PHE:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:382:PRO:CD	2.53	0.57
1:A:91:LEU:C	1:A:91:LEU:CD2	2.63	0.57
1:A:249:CYS:O	1:A:253:LEU:HD12	2.04	0.56
1:A:311:CYS:SG	1:A:312:SER:N	2.77	0.56
1:A:308:PHE:HB2	1:A:309:LYS:HE3	1.89	0.55
2:B:9:DG:H4'	2:B:10:DA:OP1	2.06	0.55
1:A:95:ASN:ND2	5:A:480:HOH:O	2.37	0.55
1:A:85:LYS:O	1:A:89:PRO:CA	2.55	0.55
1:A:405:LEU:HD21	1:A:406:LEU:O	2.08	0.54
1:A:41:GLN:NE2	5:A:458:HOH:O	2.26	0.54
1:A:381:THR:HB	1:A:382:PRO:HD3	1.89	0.54
1:A:44:MET:CE	1:A:67:ASN:HB3	2.38	0.53
1:A:355:TYR:HE2	1:A:357:ARG:HD2	1.72	0.53
1:A:137:GLU:CD	1:A:172:ARG:HH12	2.11	0.53
1:A:370:GLN:O	1:A:371:LYS:CB	2.55	0.53
1:A:146:ASP:C	1:A:148:LEU:H	2.11	0.53
1:A:41:GLN:NE2	1:A:194:THR:H	2.02	0.52
1:A:85:LYS:O	1:A:89:PRO:CG	2.56	0.52
1:A:318:LYS:HG2	1:A:322:GLU:OE2	2.09	0.52
1:A:239:ILE:HB	1:A:242:ILE:HD12	1.90	0.52
1:A:246:THR:O	1:A:249:CYS:HB2	2.10	0.52
1:A:88:CYS:SG	1:A:91:LEU:HB3	2.51	0.51
1:A:313:SER:O	1:A:314:GLU:C	2.48	0.51
1:A:316:GLU:O	1:A:319:ASN:CA	2.59	0.50
1:A:85:LYS:O	1:A:89:PRO:CB	2.60	0.50
1:A:172:ARG:HD3	5:A:450:HOH:O	2.11	0.50
1:A:68:TYR:C	1:A:70:ALA:H	2.16	0.50
1:A:405:LEU:CD2	1:A:406:LEU:C	2.81	0.49
1:A:242:ILE:HG23	1:A:246:THR:CG2	2.42	0.49
1:A:343:ARG:HB3	1:A:409:CYS:HB3	1.94	0.49
1:A:202:ASN:ND2	1:A:289:ASP:HB3	2.27	0.49
1:A:319:ASN:O	1:A:320:LYS:C	2.50	0.49
1:A:126:ASP:OD1	3:A:875:DCP:O1A	2.31	0.49
1:A:52:ASP:O	1:A:52:ASP:OD1	2.30	0.49
1:A:343:ARG:HD2	1:A:345:ILE:HD11	1.93	0.49
1:A:71:ARG:CZ	3:A:875:DCP:O3G	2.61	0.48
1:A:44:MET:HE1	1:A:67:ASN:CB	2.44	0.48
1:A:365:PRO:HB2	1:A:368:VAL:CG2	2.43	0.48
1:A:309:LYS:HE3	1:A:309:LYS:N	2.29	0.48
1:A:332:VAL:HG12	1:A:333:CYS:N	2.20	0.48
1:A:405:LEU:CD2	1:A:406:LEU:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:C	1:A:89:PRO:HG3	2.34	0.48
1:A:370:GLN:OE1	1:A:370:GLN:HA	2.15	0.47
1:A:140:LEU:C	1:A:142:GLN:H	2.18	0.47
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.95	0.47
1:A:339:PRO:HB3	1:A:413:LEU:HD13	1.96	0.47
1:A:86:GLU:O	1:A:89:PRO:HG3	2.15	0.47
1:A:313:SER:C	1:A:315:VAL:N	2.65	0.46
1:A:371:LYS:CB	1:A:379:VAL:HG22	2.42	0.46
1:A:349:TYR:CA	1:A:350:SER:CB	2.91	0.46
1:A:25:ALA:HB1	5:A:448:HOH:O	2.16	0.46
1:A:73:LEU:O	1:A:87:LYS:HG2	2.15	0.46
1:A:405:LEU:HD23	1:A:406:LEU:H	1.72	0.46
1:A:132:LEU:HD22	1:A:179:ILE:HG21	1.97	0.46
1:A:88:CYS:SG	1:A:91:LEU:CB	3.04	0.46
1:A:88:CYS:CB	1:A:91:LEU:HB3	2.44	0.45
1:A:88:CYS:O	1:A:90:GLN:N	2.48	0.45
1:A:355:TYR:HD2	1:A:357:ARG:HG3	1.81	0.45
1:A:347:ARG:HD2	1:A:404:THR:CG2	2.47	0.45
1:A:325:LEU:HG	1:A:329:LEU:HD11	1.99	0.45
1:A:381:THR:CB	1:A:382:PRO:CD	2.95	0.45
1:A:146:ASP:C	1:A:148:LEU:N	2.70	0.45
1:A:228:HIS:HA	5:A:464:HOH:O	2.16	0.44
1:A:405:LEU:HD21	1:A:406:LEU:C	2.37	0.44
1:A:355:TYR:HA	1:A:356:GLY:HA3	1.68	0.44
1:A:272:GLU:O	1:A:272:GLU:HG3	2.17	0.44
1:A:135:MET:O	1:A:139:ARG:HG3	2.17	0.44
1:A:146:ASP:O	1:A:148:LEU:N	2.50	0.44
1:A:140:LEU:C	1:A:142:GLN:N	2.71	0.44
1:A:283:LYS:HE2	1:A:288:GLU:HB3	1.99	0.44
1:A:126:ASP:CG	3:A:875:DCP:C5'	2.86	0.43
1:A:319:ASN:O	1:A:321:ILE:N	2.51	0.43
1:A:313:SER:C	1:A:315:VAL:H	2.22	0.43
1:A:67:ASN:CB	1:A:69:GLU:OE1	2.66	0.43
2:B:12:DC:H2'	2:B:13:DOC:H6	2.00	0.43
1:A:387:LEU:O	1:A:390:LEU:HB2	2.19	0.43
1:A:92:VAL:CG1	1:A:93:LEU:N	2.78	0.43
1:A:163:ILE:HG21	1:A:174:LEU:HD11	2.01	0.42
1:A:36:ASP:C	1:A:37:CYS:SG	2.98	0.42
1:A:309:LYS:CE	1:A:309:LYS:H	2.30	0.42
1:A:317:ALA:O	1:A:321:ILE:HD12	2.19	0.42
1:A:167:ASP:CG	1:A:170:HIS:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:A:215:PRO:O	2.38	0.42
1:A:325:LEU:HD23	1:A:380:MET:CG	2.49	0.42
1:A:304:GLU:HG3	1:A:328:LEU:HG	2.02	0.41
1:A:405:LEU:C	1:A:405:LEU:CD2	2.37	0.41
1:A:382:PRO:O	1:A:386:ILE:CD1	2.68	0.41
1:A:382:PRO:O	1:A:386:ILE:HD13	2.21	0.40
1:A:333:CYS:O	1:A:334:GLN:C	2.60	0.40
3:A:875:DCP:N3	2:C:840:2EG:N7	2.70	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	367/420 (87%)	324 (88%)	37 (10%)	6 (2%)	12 21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	A	313	SER
1	A	386	ILE
1	A	141	GLN
1	A	88	CYS
1	A	48	PRO

### 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	327/376 (87%)	311 (95%)	16 (5%)	31 55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	85	LYS
1	A	88	CYS
1	A	91	LEU
1	A	308	PHE
1	A	309	LYS
1	A	310	LYS
1	A	312	SER
1	A	314	GLU
1	A	329	LEU
1	A	330	ASN
1	A	333	CYS
1	A	381	THR
1	A	386	ILE
1	A	397	VAL
1	A	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	67	ASN
1	A	189	ASN
1	A	217	GLN
1	A	262	GLN
1	A	279	GLN
1	A	290	ASN
1	A	412	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	DOC	B	13	2	11,19,20	1.35	1 (9%)	14,26,29	3.00	6 (42%)
2	2EG	C	840	2	18,26,27	1.09	1 (5%)	21,37,40	1.98	6 (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
2	DOC	B	13	2	-	0/3/18/19	0/2/2/2
2	2EG	C	840	2	-	0/6/24/25	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	DOC	C5-C4	-2.28	1.35	1.40
2	C	840	2EG	C6-N1	3.76	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DOC	C2'-C1'-N1	-4.62	103.14	112.49
2	B	13	DOC	O4'-C1'-N1	-4.00	100.79	107.72
2	C	840	2EG	N3-C2-N1	-3.74	120.47	126.22
2	C	840	2EG	C5-C6-N1	-3.49	118.81	123.59
2	C	840	2EG	C4-C5-N7	-2.24	107.42	109.48
2	B	13	DOC	C3'-C4'-C5'	-2.14	107.35	116.05
2	C	840	2EG	C4'-O4'-C1'	-2.13	104.07	109.47
2	B	13	DOC	C3'-C2'-C1'	2.31	105.29	102.71
2	C	840	2EG	C6-N1-C2	2.60	119.09	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	DOC	C2-N3-C4	4.14	121.45	115.61
2	C	840	2EG	C2-N3-C4	5.08	121.21	115.09
2	B	13	DOC	O4'-C4'-C5'	7.59	120.74	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	13	DOC	2	0
2	C	840	2EG	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	DCP	A	875	-	21,29,29	1.91	7 (33%)	33,45,45	2.00	7 (21%)

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	DCP	A	875	-	-	0/18/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	875	DCP	PG-O3G	-4.02	1.40	1.54
3	A	875	DCP	PG-O2G	-3.55	1.42	1.54
3	A	875	DCP	PG-O1G	-3.50	1.39	1.51
3	A	875	DCP	PA-O2A	-2.83	1.42	1.54
3	A	875	DCP	PB-O2B	-2.15	1.45	1.54
3	A	875	DCP	PB-O1B	-2.12	1.43	1.51
3	A	875	DCP	C5'-C4'	2.52	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	875	DCP	PB-O3A-PA	-3.31	123.44	132.73
3	A	875	DCP	C6-N1-C2	-2.07	117.93	121.28
3	A	875	DCP	C2-N3-C4	2.12	118.60	115.61
3	A	875	DCP	O5'-C5'-C4'	2.25	117.42	109.12
3	A	875	DCP	C5'-C4'-C3'	2.49	130.42	114.64
3	A	875	DCP	PB-O3B-PG	2.56	141.24	132.67
3	A	875	DCP	O4'-C1'-N1	8.60	122.60	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	875	DCP	8	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/420 (89%)	0.46	31 (8%) 14 15	21, 34, 44, 55	0
2	B	6/18 (33%)	-0.45	0 100 100	30, 32, 39, 40	0
2	C	7/18 (38%)	-0.78	0 100 100	32, 33, 34, 35	0
All	All	388/456 (85%)	0.43	31 (7%) 15 16	21, 34, 44, 55	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	TYR	6.2
1	A	86	GLU	5.6
1	A	25	ALA	5.2
1	A	333	CYS	4.1
1	A	244	TYR	4.1
1	A	336	GLY	3.8
1	A	146	ASP	3.5
1	A	89	PRO	3.4
1	A	90	GLN	3.2
1	A	385	ASP	3.2
1	A	349	TYR	3.0
1	A	26	SER	2.8
1	A	350	SER	2.8
1	A	367	HIS	2.7
1	A	235	HIS	2.7
1	A	348	ARG	2.6
1	A	79	MET	2.6
1	A	316	GLU	2.5
1	A	68	TYR	2.5
1	A	311	CYS	2.5
1	A	315	VAL	2.4
1	A	252	ALA	2.4
1	A	75	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	87	LYS	2.4
1	A	144	GLN	2.4
1	A	319	ASN	2.3
1	A	250	LEU	2.2
1	A	264	PHE	2.2
1	A	321	ILE	2.2
1	A	91	LEU	2.2
1	A	309	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DOC	B	13	18/19	0.97	0.10	-	32,34,36,37	0
2	2EG	C	840	24/25	0.82	0.32	-	20,20,20,20	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DCP	A	875	28/28	0.91	0.27	1.92	43,47,52,54	0
4	NA	A	421	1/1	0.95	0.16	0.64	39,39,39,39	0
4	NA	A	422	1/1	0.85	0.08	-	48,48,48,48	0
4	NA	C	1	1/1	0.96	0.42	-	20,20,20,20	0
4	NA	A	423	1/1	0.93	0.24	-	20,20,20,20	0

## 6.5 Other polymers

There are no such residues in this entry.