



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:56 AM GMT

PDB ID : 3GIJ  
Title : Dpo4 extension ternary complex with oxoG(syn)-A(anti) and oxoG(anti)-A(syn) pairs  
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Deposited on : 2009-03-05  
Resolution : 2.40 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

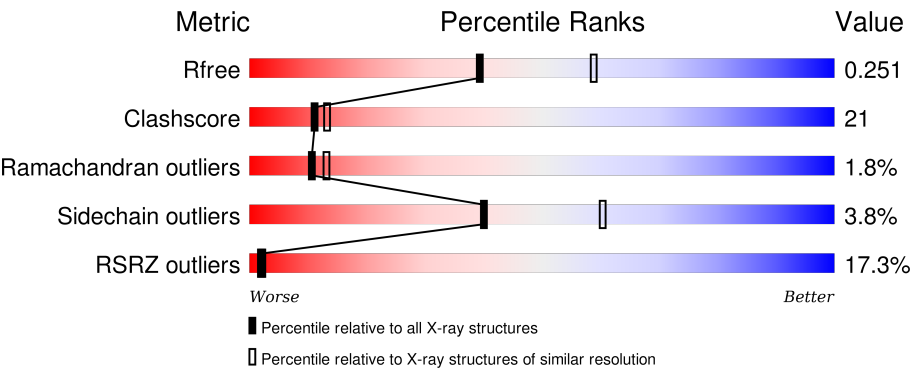
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	341	
1	B	341	
2	D	13	
2	H	13	
3	E	18	

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Mol	Chain	Length	Quality of chain
3	J	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2DA	D	814[B]	-	-	X	-
3	8OG	E	906[A]	X	-	-	-
3	8OG	E	906[B]	X	-	-	-
3	8OG	J	1906	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7025 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	1	0
			2750	1763	475	506	6			
1	B	341	Total	C	N	O	S	0	0	0
			2740	1757	472	505	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q97W02
B	1001	GLY	-	EXPRESSION TAG	UNP Q97W02

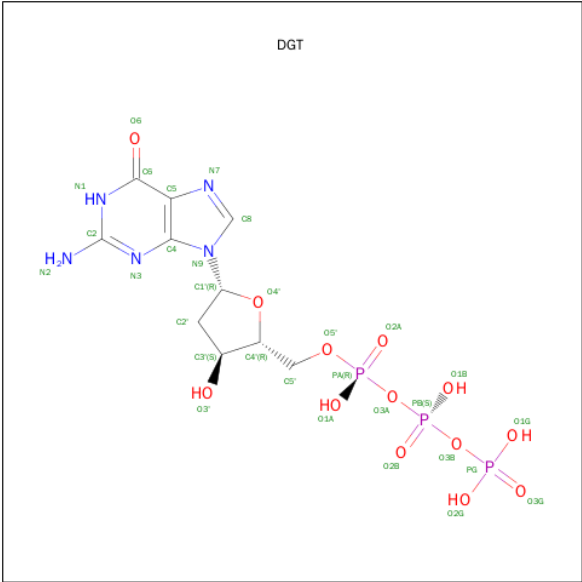
- Molecule 2 is a DNA chain called 5'-D(\*GP\*TP\*TP\*GP\*GP\*AP\*TP\*GP\*GP\*TP\*AP\*GP\*(2DA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	1	0
			291	140	58	80	13			
2	H	13	Total	C	N	O	P	0	0	0
			271	130	53	76	12			

- Molecule 3 is a DNA chain called 5'-D(\*CP\*TP\*AP\*AP\*CP\*(8OG)P\*CP\*TP\*AP\*CP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	18	Total	C	N	O	P	0	1	0
			381	182	70	111	18			
3	J	14	Total	C	N	O	P	0	0	0
			280	133	50	83	14			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		
5	A	3	Total	Ca	0	0
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	D	20	Total	O	0	0
			20	20		
6	E	20	Total	O	0	0
			20	20		
6	B	61	Total	O	0	0
			61	61		
6	H	8	Total	O	0	0
			8	8		

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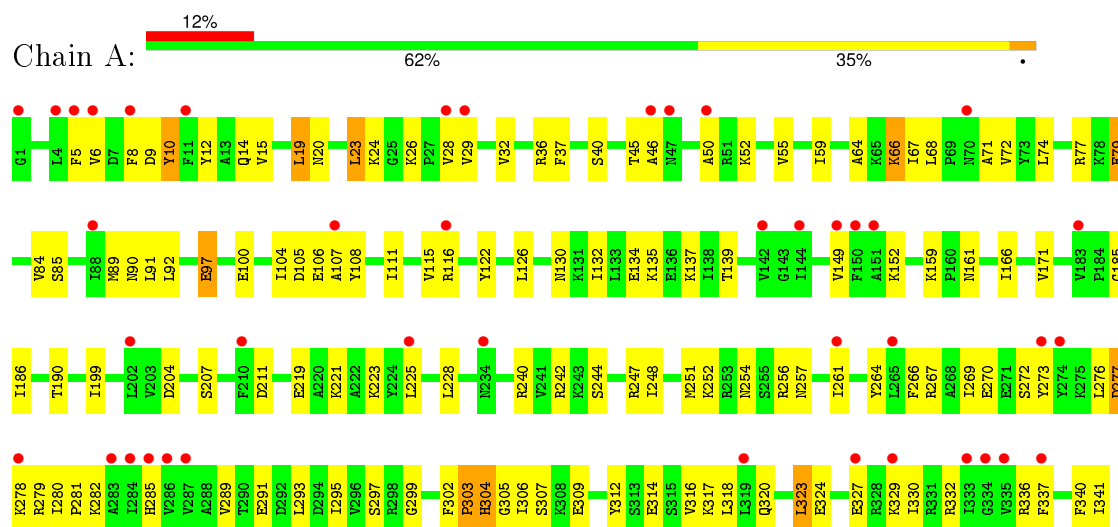
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	6	Total	O	0	0
			6	6		

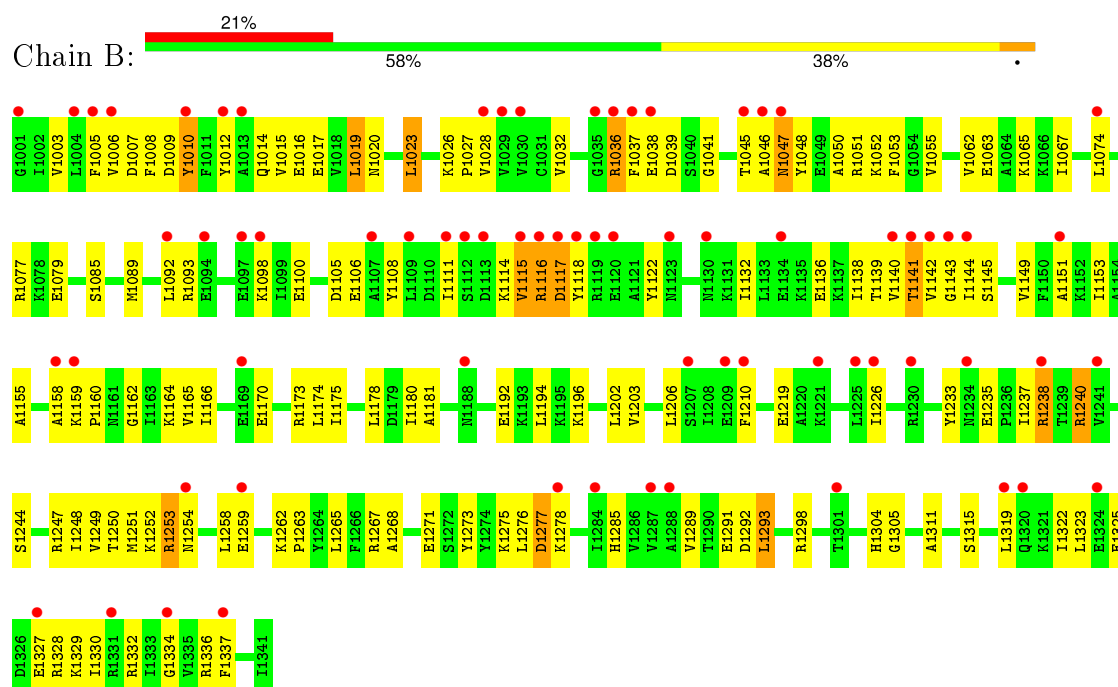
### 3 Residue-property plots

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

#### • Molecule 1: DNA polymerase IV



#### • Molecule 1: DNA polymerase IV



- |       |
|-------|
| DC    |
| DT    |
| DA    |
| DA    |
| C1905 |
| G1906 |
| C1907 |
| T1908 |
| A1909 |
| C1910 |
| C1911 |
| A1912 |
| T1913 |
| C1914 |
| C1915 |
| A1916 |
| A1917 |
| C1918 |



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.26 Å 107.41 Å 97.87 Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.40) 92.6 (19.97-2.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.35 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.209 , 0.253 0.205 , 0.251	Depositor DCC
$R_{free}$ test set	1950 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 40096 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: 8OG, CA, 2DA, DGT

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	0.52	0/2790	0.60	0/3746
1	B	0.38	0/2779	0.49	0/3731
2	D	0.72	0/282	1.48	5/436 (1.1%)
2	H	0.54	0/282	1.15	1/436 (0.2%)
3	E	0.86	0/373	1.53	10/568 (1.8%)
3	J	0.60	0/285	1.21	1/432 (0.2%)
All	All	0.51	0/6791	0.79	17/9349 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	2	0
3	J	2	0
All	All	4	0

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	907	DC	C1'-O4'-C4'	-7.77	102.33	110.10
2	D	805	DG	O4'-C1'-N9	7.60	113.32	108.00
2	H	1813	DG	O4'-C1'-N9	7.03	112.92	108.00
2	D	813	DG	O4'-C1'-N9	6.74	112.72	108.00
3	E	913	DT	P-O3'-C3'	6.54	127.55	119.70
3	E	913	DT	O4'-C1'-N1	6.24	112.36	108.00
2	D	808	DT	C1'-O4'-C4'	-6.12	103.98	110.10
3	E	907	DC	O4'-C4'-C3'	-6.07	102.07	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	907	DC	O4'-C1'-N1	5.98	112.19	108.00
3	E	908	DT	O4'-C1'-N1	-5.94	103.84	108.00
3	E	915	DC	O4'-C1'-N1	5.85	112.09	108.00
3	J	1914	DC	O4'-C1'-N1	5.58	111.91	108.00
3	E	913	DT	C1'-O4'-C4'	-5.40	104.70	110.10
2	D	811	DT	O4'-C1'-N1	-5.19	104.36	108.00
3	E	904	DA	O4'-C4'-C3'	-5.18	102.43	104.50
3	E	901	DC	C1'-O4'-C4'	-5.17	104.93	110.10
2	D	807	DA	O4'-C1'-N9	-5.17	104.38	108.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	906[A]	8OG	C1'
3	E	906[B]	8OG	C1'
3	J	1906	8OG	C4',C1'

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	2750	0	2889	124	0
1	B	2740	0	2880	123	0
2	D	291	0	160	14	0
2	H	271	0	149	0	0
3	E	381	0	207	19	0
3	J	280	0	155	4	0
4	A	31	0	12	4	0
4	B	31	0	12	5	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	129	0	0	16	0
6	B	61	0	0	10	0
6	D	20	0	0	2	0
6	E	20	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	8	0	0	0	0
6	J	6	0	0	0	0
All	All	7025	0	6464	269	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 21.

All (269) 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:B:1116:ARG:HE	1:B:1116:ARG:H	1.04	1.00
1:A:14:GLN:HE22	1:A:139:THR:H	1.02	0.94
1:B:1014:GLN:HE22	1:B:1139:THR:H	1.16	0.93
1:A:130:ASN:O	1:A:134:GLU:HG3	1.71	0.90
1:B:1115:VAL:HG13	1:B:1116:ARG:HH21	1.36	0.89
1:A:270:GLU:HG2	1:A:312:TYR:OH	1.73	0.86
1:A:293:LEU:HD11	3:E:904:DA:C8	2.11	0.86
1:B:1289:VAL:HB	1:B:1332:ARG:HB2	1.56	0.85
1:B:1116:ARG:O	1:B:1117:ASP:HB2	1.78	0.84
1:B:1267:ARG:O	1:B:1271:GLU:HG3	1.78	0.83
1:A:316:VAL:O	1:A:320:GLN:HG3	1.82	0.80
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.62	0.80
1:A:66:LYS:HB3	1:A:66:LYS:HZ2	1.47	0.78
1:A:267:ARG:HD2	6:A:709:HOH:O	1.82	0.78
1:A:97:GLU:CD	1:A:97:GLU:H	1.85	0.77
1:A:26:LYS:CG	6:A:729:HOH:O	2.33	0.76
1:B:1180:ILE:HG12	1:B:1194:LEU:HD13	1.67	0.76
1:A:277:ASP:O	1:A:278:LYS:HB2	1.85	0.76
1:A:79:GLU:H	1:A:79:GLU:CD	1.85	0.76
2:D:813:DG:H2''	2:D:814[B]:2DA:C5'	2.16	0.75
1:B:1285:HIS:HD2	6:B:713:HOH:O	1.69	0.75
1:B:1116:ARG:NE	1:B:1116:ARG:H	1.81	0.75
1:B:1116:ARG:HE	1:B:1116:ARG:N	1.84	0.75
1:A:285:HIS:HD2	6:A:507:HOH:O	1.70	0.74
2:D:813:DG:H2''	2:D:814[B]:2DA:O5'	1.87	0.74
1:A:291:GLU:HG3	1:A:329:LYS:HB2	1.69	0.74
1:A:111:ILE:O	1:A:115:VAL:HG22	1.87	0.73
1:B:1115:VAL:HG13	1:B:1116:ARG:NH2	2.05	0.71
1:B:1111:ILE:HG23	1:B:1114:LYS:HB2	1.71	0.70
2:D:813:DG:H2''	2:D:814[B]:2DA:H5'	1.72	0.69
2:D:814[A]:2DA:N7	3:E:906[A]:8OG:N2	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:HG12	1:A:320:GLN:HE21	1.57	0.68
1:A:14:GLN:NE2	1:A:139:THR:H	1.85	0.68
1:A:37:PHE:CE2	3:E:902:DT:H5'	2.28	0.68
1:A:256:ARG:HG3	1:A:329:LYS:HG2	1.75	0.68
1:A:266:PHE:HB3	1:A:312:TYR:HE1	1.59	0.67
1:B:1046:ALA:HB1	1:B:1050:ALA:HB3	1.76	0.67
1:B:1026:LYS:O	1:B:1047:ASN:ND2	2.27	0.67
1:A:324:GLU:HB3	6:A:606:HOH:O	1.95	0.66
1:B:1192:GLU:O	1:B:1196:LYS:HG2	1.94	0.66
2:D:813:DG:H2'	2:D:814[A]:2DA:H2	1.78	0.66
1:B:1304:HIS:HD2	1:B:1305:GLY:O	1.79	0.66
1:A:46:ALA:HB1	1:A:50:ALA:CB	2.26	0.65
1:A:19:LEU:HD23	1:A:77:ARG:NH2	2.12	0.65
1:A:26:LYS:HG2	6:A:729:HOH:O	1.94	0.65
1:A:336:ARG:NH2	3:E:908:DT:OP2	2.30	0.65
1:A:273:TYR:HA	1:A:276:LEU:HD12	1.77	0.65
1:A:186:ILE:HD11	1:A:225:LEU:HD21	1.78	0.64
1:B:1273:TYR:HE1	6:B:724:HOH:O	1.79	0.64
1:B:1012:TYR:HB2	1:B:1045:THR:CG2	2.26	0.64
1:B:1149:VAL:O	1:B:1153:ILE:HG13	1.98	0.64
3:E:916:DA:H1'	3:E:917:DA:H5'	1.80	0.64
1:A:20:ASN:HB3	1:A:23:LEU:HD22	1.79	0.64
1:A:242:ARG:HH11	3:E:908:DT:H5''	1.63	0.63
1:B:1028:VAL:H	1:B:1047:ASN:HD22	1.46	0.63
1:B:1311:ALA:O	1:B:1315:SER:HB3	1.99	0.62
2:D:813:DG:H2'	2:D:814[A]:2DA:C2	2.29	0.62
1:A:26:LYS:HG3	6:A:729:HOH:O	1.95	0.62
1:B:1052:LYS:HD3	6:B:712:HOH:O	1.99	0.62
1:A:12:TYR:HB2	1:A:45:THR:CG2	2.30	0.62
1:A:323:LEU:CD1	1:A:330:ILE:HD12	2.30	0.61
3:J:1910:DC:H2''	3:J:1911:DC:C6	2.35	0.61
1:B:1039:ASP:OD1	1:B:1065:LYS:HE3	1.99	0.61
1:A:36:ARG:NH2	1:A:254:ASN:OD1	2.34	0.61
1:B:1012:TYR:HB2	1:B:1045:THR:HG21	1.83	0.60
1:B:1336:ARG:HG2	6:B:636:HOH:O	2.01	0.60
1:B:1028:VAL:N	1:B:1047:ASN:HD22	1.99	0.60
1:B:1100:GLU:HB2	1:B:1237:ILE:HG23	1.85	0.59
2:D:813:DG:H2''	2:D:814[A]:2DA:O5'	2.03	0.59
1:B:1136:GLU:O	1:B:1138:ILE:HG12	2.03	0.59
1:A:85:SER:O	1:A:89:MET:HG2	2.03	0.59
1:A:285:HIS:ND1	1:A:299:GLY:HA3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:916:DA:H2''	3:E:917:DA:OP2	2.02	0.59
1:A:20:ASN:O	1:A:23:LEU:HB2	2.02	0.59
1:B:1038:GLU:HB2	6:B:668:HOH:O	2.01	0.58
1:A:304[B]:HIS:HD2	1:A:305:GLY:O	1.85	0.58
1:B:1048:TYR:CE2	1:B:1160:PRO:HG3	2.39	0.58
3:E:913:DT:H2''	3:E:914:DC:C6	2.38	0.58
1:A:336:ARG:HD2	6:A:516:HOH:O	2.03	0.58
1:B:1206:LEU:HD23	1:B:1226:ILE:HG13	1.86	0.58
1:B:1336:ARG:NH2	3:J:1908:DT:OP2	2.32	0.58
1:B:1020:ASN:O	1:B:1023:LEU:HB2	2.05	0.57
3:J:1910:DC:H2''	3:J:1911:DC:H6	1.70	0.57
1:B:1100:GLU:HB3	1:B:1108:TYR:HB2	1.86	0.57
1:A:277:ASP:O	1:A:278:LYS:CB	2.52	0.57
1:B:1010:TYR:HA	4:B:1414:DGT:O2B	2.04	0.56
1:A:91:LEU:HD11	1:A:135:LYS:HB2	1.86	0.56
1:A:12:TYR:HB2	1:A:45:THR:HG22	1.87	0.56
1:B:1015:VAL:HG12	1:B:1019:LEU:HD22	1.86	0.56
1:A:66:LYS:HB3	1:A:66:LYS:NZ	2.10	0.56
1:A:256:ARG:NH2	1:A:323:LEU:O	2.25	0.56
1:B:1118:TYR:HB3	1:B:1165:VAL:HG11	1.86	0.55
1:A:291:GLU:CG	1:A:329:LYS:HB2	2.35	0.55
4:B:1414:DGT:O1B	4:B:1414:DGT:H5'A	2.05	0.55
1:B:1298:ARG:HG2	1:B:1322:ILE:HG12	1.90	0.54
2:D:803:DT:H3	3:E:917:DA:H61	1.54	0.54
1:B:1008:PHE:HB2	1:B:1105:ASP:HB2	1.90	0.54
1:B:1079:GLU:H	1:B:1079:GLU:CD	2.11	0.54
1:B:1248:ILE:HA	1:B:1334:GLY:HA3	1.90	0.53
1:A:186:ILE:HD12	1:A:190:THR:HG21	1.90	0.53
1:B:1028:VAL:H	1:B:1047:ASN:ND2	2.07	0.53
1:A:244:SER:OG	1:A:336:ARG:NH1	2.42	0.53
1:A:52:LYS:HE3	6:A:646:HOH:O	2.08	0.53
2:D:813:DG:H2''	2:D:814[B]:2DA:H8	1.91	0.53
1:B:1009:ASP:O	1:B:1010:TYR:C	2.46	0.52
1:A:293:LEU:CD1	3:E:904:DA:C8	2.91	0.52
1:B:1012:TYR:CD2	4:B:1414:DGT:H2'	2.44	0.52
1:A:19:LEU:HD23	1:A:77:ARG:HH22	1.74	0.52
1:A:10:TYR:HA	4:A:414:DGT:O2B	2.10	0.52
1:A:314:GLU:O	1:A:318:LEU:HG	2.09	0.52
1:A:270:GLU:CG	1:A:312:TYR:OH	2.53	0.51
1:B:1014:GLN:NE2	1:B:1139:THR:H	1.95	0.51
1:A:242:ARG:HA	3:E:909:DA:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1275:LYS:HG2	6:B:538:HOH:O	2.09	0.51
1:B:1003:VAL:HG13	1:B:1237:ILE:HD11	1.93	0.51
1:B:1122:TYR:HD1	1:B:1165:VAL:HG23	1.76	0.50
1:A:85:SER:OG	1:A:104:ILE:O	2.21	0.50
1:B:1238:ARG:HD2	1:B:1240:ARG:HE	1.77	0.50
1:B:1233:TYR:CE2	1:B:1235:GLU:HB2	2.46	0.50
1:A:6:VAL:O	1:A:106:GLU:HA	2.12	0.50
1:B:1051:ARG:HH22	4:B:1414:DGT:PB	2.35	0.50
1:A:152:LYS:HE3	2:D:814[B]:2DA:OP1	2.11	0.50
1:A:92:LEU:HD21	1:A:132:ILE:HD11	1.94	0.50
1:B:1291:GLU:N	1:B:1329:LYS:O	2.39	0.50
3:E:915:DC:H2''	3:E:916:DA:C8	2.46	0.49
1:B:1158:ALA:HB2	1:B:1164:LYS:HB2	1.94	0.49
1:B:1141:THR:OG1	1:B:1159:LYS:O	2.21	0.49
1:A:12:TYR:HB2	1:A:45:THR:HG21	1.94	0.49
1:B:1289:VAL:CB	1:B:1332:ARG:HB2	2.35	0.49
1:B:1252:LYS:O	1:B:1253:ARG:HB3	2.12	0.49
1:A:32:VAL:HG21	3:E:905:DC:O2	2.13	0.49
1:A:219:GLU:HG2	1:A:223:LYS:HE2	1.93	0.49
1:A:282:LYS:HG2	1:A:303:PRO:O	2.12	0.49
1:A:185:GLY:O	1:A:221:LYS:HE3	2.13	0.49
1:B:1143:GLY:HA3	1:B:1151:ALA:O	2.12	0.49
1:A:304[A]:HIS:HE1	6:A:685:HOH:O	1.95	0.49
1:A:256:ARG:HD2	1:A:327:GLU:O	2.13	0.48
1:B:1012:TYR:CE2	4:B:1414:DGT:H2'	2.48	0.48
1:B:1038:GLU:O	1:B:1039:ASP:HB2	2.12	0.48
1:B:1098:LYS:HD2	6:B:543:HOH:O	2.13	0.48
1:B:1085:SER:O	1:B:1089:MET:HG2	2.14	0.48
1:A:332:ARG:NH1	3:E:906[A]:8OG:O8	2.46	0.48
1:A:126:LEU:O	1:A:130:ASN:ND2	2.47	0.48
1:A:159:LYS:NZ	6:D:502:HOH:O	2.47	0.47
1:B:1244:SER:HA	1:B:1337:PHE:O	2.14	0.47
1:A:281:PRO:O	1:A:306:ILE:N	2.43	0.47
1:B:1012:TYR:HB2	1:B:1045:THR:HG22	1.97	0.47
1:B:1298:ARG:NE	1:B:1325:GLU:OE1	2.44	0.47
1:B:1159:LYS:HE2	6:B:1503:HOH:O	2.15	0.47
1:A:37:PHE:HB3	3:E:901:DC:H1'	1.97	0.47
1:A:105:ASP:CG	4:A:414:DGT:H5'	2.35	0.46
1:B:1141:THR:HA	1:B:1162:GLY:O	2.15	0.46
1:B:1005:PHE:CE2	1:B:1007:ASP:HB2	2.50	0.46
1:B:1005:PHE:HE1	1:B:1106:GLU:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CD1	1:A:8:PHE:N	2.83	0.46
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.97	0.46
1:A:248:ILE:HG22	6:E:582:HOH:O	2.15	0.46
1:A:320:GLN:O	1:A:324:GLU:HG3	2.15	0.46
1:B:1008:PHE:CD2	1:B:1105:ASP:HA	2.50	0.46
1:B:1251:MET:C	1:B:1253:ARG:H	2.19	0.46
2:D:814[B]:2DA:N1	3:E:906[B]:8OG:N7	2.52	0.46
1:B:1141:THR:CG2	1:B:1155:ALA:HA	2.45	0.46
1:A:90:ASN:ND2	6:A:691:HOH:O	2.21	0.46
1:B:1249:VAL:HG23	1:B:1268:ALA:HB2	1.97	0.46
2:D:813:DG:C2'	2:D:814[B]:2DA:H8	2.45	0.46
1:B:1153:ILE:HD13	1:B:1178:LEU:CD2	2.46	0.46
1:B:1262:LYS:N	1:B:1263:PRO:HD2	2.31	0.46
1:A:122:TYR:CE2	1:A:126:LEU:HD11	2.51	0.46
1:A:280:ILE:O	1:A:340:PHE:HA	2.16	0.46
1:A:251:MET:HG2	1:A:264:TYR:CG	2.51	0.46
1:A:100:GLU:HG3	1:A:240:ARG:HG3	1.96	0.46
1:B:1026:LYS:HB2	1:B:1027:PRO:HD2	1.98	0.45
1:B:1265:LEU:HD22	1:B:1319:LEU:HD22	1.97	0.45
1:B:1026:LYS:HB2	1:B:1027:PRO:CD	2.46	0.45
1:B:1005:PHE:CD1	1:B:1108:TYR:CE1	3.04	0.45
1:A:323:LEU:CD1	1:A:330:ILE:CD1	2.94	0.45
1:B:1166:ILE:HD13	1:B:1174:LEU:CD1	2.46	0.45
1:A:285:HIS:CE1	1:A:299:GLY:HA3	2.52	0.45
1:A:336:ARG:HD2	6:A:693:HOH:O	2.17	0.45
1:B:1175:ILE:HG22	1:B:1203:VAL:HB	1.97	0.45
1:A:59:ILE:HD11	1:A:64:ALA:HB2	1.98	0.45
1:A:317:LYS:O	1:A:320:GLN:HB2	2.17	0.45
1:B:1170:GLU:HA	1:B:1173:ARG:HB3	1.99	0.45
1:B:1235:GLU:HA	1:B:1235:GLU:OE1	2.17	0.45
1:A:282:LYS:HE3	1:A:341:ILE:HG12	1.99	0.44
1:B:1053:PHE:O	1:B:1067:ILE:HG21	2.17	0.44
1:B:1028:VAL:N	1:B:1047:ASN:ND2	2.65	0.44
1:B:1174:LEU:O	1:B:1178:LEU:N	2.44	0.44
1:A:9:ASP:O	1:A:10:TYR:C	2.55	0.44
1:B:1233:TYR:CZ	1:B:1235:GLU:HG3	2.52	0.44
1:B:1210:PHE:HZ	1:B:1219:GLU:HG3	1.83	0.44
1:B:1032:VAL:O	1:B:1041:GLY:HA3	2.18	0.44
1:B:1116:ARG:O	1:B:1117:ASP:CB	2.55	0.44
1:B:1005:PHE:CE1	1:B:1106:GLU:HB3	2.52	0.44
1:A:166:ILE:HG22	1:A:171:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1238:ARG:HB2	1:B:1238:ARG:HH21	1.83	0.44
1:B:1051:ARG:HA	1:B:1055:VAL:O	2.17	0.44
1:B:1250:THR:HA	1:B:1332:ARG:HG2	2.00	0.44
1:B:1036:ARG:HB3	1:B:1037:PHE:H	1.63	0.44
1:B:1247:ARG:NE	1:B:1271:GLU:OE1	2.42	0.43
1:B:1016:GLU:OE1	1:B:1077:ARG:NH2	2.47	0.43
1:A:289:VAL:HG22	1:A:295:ILE:HG12	2.00	0.43
1:B:1008:PHE:N	1:B:1008:PHE:CD1	2.83	0.43
1:A:29:VAL:HG22	1:A:55:VAL:HG11	1.99	0.43
1:A:302:PHE:O	1:A:303:PRO:O	2.36	0.43
1:B:1023:LEU:HD21	1:B:1074:LEU:HD11	1.99	0.43
1:B:1020:ASN:HB3	1:B:1023:LEU:HD22	2.00	0.43
1:A:72:VAL:HG12	1:A:74:LEU:HG	2.00	0.43
1:B:1277:ASP:O	1:B:1278:LYS:CB	2.65	0.43
1:A:281:PRO:HB3	1:A:337:PHE:HB3	2.01	0.43
1:A:137:LYS:HD3	1:A:137:LYS:HA	1.90	0.43
1:B:1273:TYR:HA	1:B:1276:LEU:HD12	2.01	0.43
1:A:52:LYS:CE	6:A:646:HOH:O	2.65	0.43
1:A:37:PHE:H	1:A:40:SER:HB3	1.83	0.43
1:A:323:LEU:HD11	1:A:330:ILE:HD12	1.99	0.43
1:B:1111:ILE:HG22	1:B:1111:ILE:O	2.19	0.43
1:A:242:ARG:HG2	6:E:698:HOH:O	2.19	0.43
1:A:36:ARG:HH22	1:A:254:ASN:CG	2.20	0.43
1:B:1181:ALA:O	6:B:1515:HOH:O	2.22	0.43
1:B:1089:MET:O	1:B:1093:ARG:HG3	2.20	0.42
1:A:149:VAL:HG21	1:A:228:LEU:HD21	2.01	0.42
1:B:1142:VAL:HG12	1:B:1144:ILE:CG1	2.49	0.42
1:A:272:SER:HB2	1:A:337:PHE:HE2	1.84	0.42
1:A:29:VAL:CG2	1:A:55:VAL:HG11	2.49	0.42
1:A:116:ARG:HB2	6:A:578:HOH:O	2.18	0.42
1:B:1285:HIS:CD2	6:B:713:HOH:O	2.56	0.42
1:B:1005:PHE:HB2	1:B:1108:TYR:CD1	2.54	0.42
1:B:1017:GLU:OE2	1:B:1047:ASN:OD1	2.38	0.42
1:B:1008:PHE:HA	1:B:1140:VAL:HG12	2.02	0.42
1:B:1292:ASP:OD2	1:B:1328:ARG:HD2	2.20	0.42
1:A:266:PHE:HA	1:A:269:ILE:HD12	2.01	0.42
2:D:802:DG:C2'	2:D:803:DT:H5'	2.49	0.42
1:B:1006:VAL:O	1:B:1106:GLU:HA	2.20	0.42
1:A:5:PHE:CD1	1:A:108:TYR:CE1	3.08	0.42
1:A:251:MET:CE	1:A:330:ILE:HG22	2.49	0.42
1:A:8:PHE:CD2	1:A:105:ASP:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:TYR:CE1	1:B:1014:GLN:HB2	2.55	0.41
1:B:1100:GLU:CB	1:B:1237:ILE:HG23	2.48	0.41
1:B:1202:LEU:HD23	1:B:1202:LEU:HA	1.92	0.41
1:B:1238:ARG:CD	1:B:1240:ARG:HE	2.34	0.41
1:A:137:LYS:HE3	6:A:506:HOH:O	2.20	0.41
1:A:336:ARG:CD	6:A:516:HOH:O	2.66	0.41
1:A:68:LEU:HA	1:A:68:LEU:HD23	1.95	0.41
1:A:28:VAL:O	1:A:46:ALA:HA	2.21	0.41
1:A:15:VAL:HG13	1:A:84:VAL:HG21	2.03	0.41
1:B:1019:LEU:HA	1:B:1019:LEU:HD12	1.91	0.41
1:A:257:ASN:O	1:A:261:ILE:HG13	2.21	0.41
1:A:9:ASP:OD2	1:A:161:ASN:N	2.53	0.41
1:A:66:LYS:HZ3	1:A:67:ILE:HG23	1.85	0.41
1:A:12:TYR:CD2	4:A:414:DGT:H2'	2.56	0.41
1:B:1254:ASN:HA	1:B:1330:ILE:O	2.21	0.41
1:A:279:ARG:HD3	6:A:514:HOH:O	2.20	0.41
1:A:247:ARG:HH11	3:E:907:DC:P	2.44	0.41
1:A:9:ASP:CG	1:A:161:ASN:H	2.24	0.41
3:E:913:DT:C2'	3:E:914:DC:C6	3.03	0.41
1:A:100:GLU:O	1:A:107:ALA:HA	2.21	0.41
1:B:1258:LEU:HD12	1:B:1319:LEU:HG	2.02	0.41
1:A:59:ILE:HD11	1:A:64:ALA:CA	2.50	0.41
1:B:1092:LEU:HD21	1:B:1132:ILE:HD11	2.02	0.41
1:B:1247:ARG:HD2	3:J:1907:DC:OP1	2.20	0.40
1:A:10:TYR:HA	4:A:414:DGT:PB	2.61	0.40
1:B:1277:ASP:O	1:B:1278:LYS:HB2	2.21	0.40
1:A:273:TYR:OH	1:A:307:SER:HA	2.20	0.40
1:B:1293:LEU:HD23	1:B:1293:LEU:HA	1.92	0.40
1:A:66:LYS:NZ	1:A:67:ILE:HG23	2.37	0.40
1:A:242:ARG:CD	6:E:698:HOH:O	2.70	0.40
3:E:915:DC:H2''	3:E:916:DA:OP2	2.21	0.40
1:B:1062:VAL:HG23	1:B:1063:GLU:N	2.36	0.40
2:D:811:DT:H5''	6:D:686:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/341 (100%)	325 (96%)	9 (3%)	6 (2%)	11	13
1	B	339/341 (99%)	312 (92%)	20 (6%)	7 (2%)	9	10
All	All	679/682 (100%)	637 (94%)	29 (4%)	13 (2%)	11	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1036	ARG
1	B	1117	ASP
1	A	303	PRO
1	B	1047	ASN
1	B	1115	VAL
1	B	1277	ASP
1	A	10	TYR
1	A	277	ASP
1	B	1010	TYR
1	B	1253	ARG
1	A	71	ALA
1	A	304[A]	HIS
1	A	304[B]	HIS

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/299 (100%)	288 (96%)	12 (4%)	38	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	299/299 (100%)	288 (96%)	11 (4%)	41	62
All	All	599/598 (100%)	576 (96%)	23 (4%)	40	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	23	LEU
1	A	24	LYS
1	A	66	LYS
1	A	79	GLU
1	A	97	GLU
1	A	207	SER
1	A	211	ASP
1	A	252	LYS
1	A	297	SER
1	A	309	GLU
1	A	323	LEU
1	B	1019	LEU
1	B	1023	LEU
1	B	1116	ARG
1	B	1141	THR
1	B	1145	SER
1	B	1238	ARG
1	B	1240	ARG
1	B	1259	GLU
1	B	1293	LEU
1	B	1323	LEU
1	B	1327	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	130	ASN
1	A	285	HIS
1	A	320	GLN
1	B	1014	GLN
1	B	1047	ASN
1	B	1304	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	2DA	D	814[A]	2,5	14,22,23	0.77	0	13,31,34	1.14	1 (7%)
2	2DA	D	814[B]	2,5	14,22,23	0.63	0	13,31,34	0.82	0
3	8OG	E	906[A]	3	16,25,26	3.35	4 (25%)	21,37,40	4.85	15 (71%)
3	8OG	E	906[B]	3	16,25,26	3.29	4 (25%)	21,37,40	4.74	15 (71%)
2	2DA	H	1814	3,2,5	14,22,23	0.64	0	13,31,34	0.90	0
3	8OG	J	1906	3,2	16,25,26	3.36	4 (25%)	21,37,40	5.16	13 (61%)

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	2DA	D	814[A]	2,5	-	0/3/18/19	0/3/3/3
2	2DA	D	814[B]	2,5	-	0/3/18/19	0/3/3/3
3	8OG	E	906[A]	3	1/1/4/4	0/3/21/22	0/3/3/3
3	8OG	E	906[B]	3	1/1/4/4	0/3/21/22	0/3/3/3
2	2DA	H	1814	3,2,5	-	0/3/18/19	0/3/3/3
3	8OG	J	1906	3,2	2/2/4/4	0/3/21/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	906[A]	8OG	O3'-C3'	-9.57	1.21	1.43
3	J	1906	8OG	O3'-C3'	-9.28	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	906[B]	8OG	O3'-C3'	-9.16	1.22	1.43
3	J	1906	8OG	C3'-C4'	-7.78	1.31	1.53
3	E	906[A]	8OG	C3'-C4'	-7.63	1.31	1.53
3	E	906[B]	8OG	C3'-C4'	-7.54	1.31	1.53
3	E	906[A]	8OG	C6-C5	2.76	1.46	1.41
3	J	1906	8OG	C6-C5	3.48	1.48	1.41
3	E	906[B]	8OG	C6-C5	3.58	1.48	1.41
3	J	1906	8OG	C5-C4	3.69	1.48	1.40
3	E	906[A]	8OG	C5-C4	3.87	1.49	1.40
3	E	906[B]	8OG	C5-C4	3.87	1.49	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	906[A]	8OG	C6-C5-C4	-4.62	115.38	120.90
3	J	1906	8OG	C5-C6-N1	-4.56	117.35	123.59
3	E	906[A]	8OG	C5-C6-N1	-4.51	117.42	123.59
3	E	906[A]	8OG	C4'-O4'-C1'	-4.19	98.88	109.47
3	J	1906	8OG	C6-C5-C4	-4.06	116.04	120.90
3	E	906[B]	8OG	C4'-O4'-C1'	-4.00	99.35	109.47
3	E	906[B]	8OG	C5-C6-N1	-3.99	118.13	123.59
3	E	906[B]	8OG	C6-C5-C4	-3.93	116.19	120.90
3	E	906[A]	8OG	C1'-N9-C4	-3.84	121.42	127.37
3	J	1906	8OG	C4'-O4'-C1'	-3.67	100.19	109.47
3	J	1906	8OG	N3-C2-N1	-3.06	122.78	127.44
3	J	1906	8OG	C1'-N9-C4	-2.99	122.74	127.37
3	E	906[B]	8OG	N3-C2-N1	-2.97	122.92	127.44
3	E	906[A]	8OG	N3-C2-N1	-2.92	123.00	127.44
3	E	906[B]	8OG	C8-N9-C1'	-2.24	121.92	125.97
3	E	906[A]	8OG	C3'-C2'-C1'	-2.23	97.04	102.40
3	E	906[B]	8OG	C3'-C2'-C1'	-2.10	97.34	102.40
3	E	906[A]	8OG	O3'-C3'-C4'	2.04	118.28	110.05
3	E	906[A]	8OG	O4'-C4'-C3'	2.06	110.84	105.67
3	E	906[B]	8OG	O3'-C3'-C4'	2.11	118.55	110.05
2	D	814[A]	2DA	O4'-C1'-N9	2.18	111.50	107.72
3	E	906[B]	8OG	O4'-C4'-C3'	2.51	111.97	105.67
3	E	906[B]	8OG	C2'-C3'-C4'	2.55	108.07	102.77
3	J	1906	8OG	O4'-C4'-C3'	2.78	112.67	105.67
3	E	906[A]	8OG	C2'-C3'-C4'	2.96	108.91	102.77
3	E	906[A]	8OG	O3'-C3'-C2'	2.97	120.57	110.74
3	J	1906	8OG	O3'-C3'-C2'	3.04	120.80	110.74
3	E	906[B]	8OG	O3'-C3'-C2'	3.10	121.00	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1906	8OG	O4'-C1'-C2'	3.27	112.79	106.27
3	E	906[A]	8OG	O4'-C4'-C5'	3.27	121.03	109.32
3	J	1906	8OG	C2'-C3'-C4'	3.31	109.64	102.77
3	E	906[B]	8OG	O4'-C1'-C2'	3.35	112.96	106.27
3	E	906[B]	8OG	O4'-C4'-C5'	3.37	121.37	109.32
3	E	906[A]	8OG	O4'-C1'-C2'	3.39	113.04	106.27
3	J	1906	8OG	O4'-C4'-C5'	4.02	123.68	109.32
3	E	906[B]	8OG	C6-N1-C2	4.80	122.60	115.94
3	J	1906	8OG	C6-N1-C2	5.00	122.87	115.94
3	E	906[A]	8OG	C6-N1-C2	5.32	123.32	115.94
3	J	1906	8OG	C2'-C1'-N9	7.25	123.09	115.83
3	E	906[B]	8OG	C2'-C1'-N9	9.53	125.38	115.83
3	E	906[A]	8OG	C2'-C1'-N9	10.34	126.20	115.83
3	E	906[A]	8OG	O4'-C1'-N9	14.74	120.69	108.22
3	E	906[B]	8OG	O4'-C1'-N9	15.42	121.26	108.22
3	J	1906	8OG	O4'-C1'-N9	18.46	123.84	108.22

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	1906	8OG	C4'
3	J	1906	8OG	C1'
3	E	906[A]	8OG	C1'
3	E	906[B]	8OG	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	814[A]	2DA	4	0
2	D	814[B]	2DA	7	0
3	E	906[A]	8OG	2	0
3	E	906[B]	8OG	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	DGT	A	414	5	25,33,33	1.16	3 (12%)	35,52,52	3.35	15 (42%)
4	DGT	B	1414	5	25,33,33	0.95	1 (4%)	35,52,52	3.44	12 (34%)

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	DGT	A	414	5	-	0/18/34/34	0/3/3/3
4	DGT	B	1414	5	-	0/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	414	DGT	C8-N7	-2.68	1.29	1.34
4	A	414	DGT	C2-N1	2.02	1.39	1.35
4	B	1414	DGT	C6-N1	3.30	1.39	1.33
4	A	414	DGT	C6-N1	3.89	1.40	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1414	DGT	C5-C6-N1	-8.60	111.83	123.59
4	A	414	DGT	C5-C6-N1	-8.51	111.95	123.59
4	A	414	DGT	O1G-PG-O3G	-8.15	84.34	110.58
4	B	1414	DGT	O2G-PG-O3G	-8.04	84.71	110.58
4	B	1414	DGT	O1G-PG-O3G	-7.40	86.76	110.58
4	B	1414	DGT	PB-O3B-PG	-6.46	111.02	132.67
4	B	1414	DGT	PA-O3A-PB	-6.40	114.75	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	414	DGT	PB-O3B-PG	-6.35	111.37	132.67
4	A	414	DGT	O2G-PG-O3G	-5.85	91.76	110.58
4	A	414	DGT	C2'-C1'-N9	-5.75	100.18	114.16
4	B	1414	DGT	N3-C2-N1	-3.97	121.40	127.44
4	A	414	DGT	N3-C2-N1	-3.88	121.53	127.44
4	B	1414	DGT	C2'-C1'-N9	-3.46	105.74	114.16
4	A	414	DGT	PA-O3A-PB	-2.78	124.92	132.73
4	A	414	DGT	C6-C5-C4	-2.18	118.29	120.90
4	A	414	DGT	O1B-PB-O3A	2.10	114.60	105.09
4	A	414	DGT	O1B-PB-O3B	2.26	115.36	105.09
4	A	414	DGT	O2G-PG-O3B	2.52	116.51	105.09
4	B	1414	DGT	O4'-C1'-N9	2.55	112.13	107.72
4	B	1414	DGT	O1G-PG-O3B	2.80	117.79	105.09
4	B	1414	DGT	O2G-PG-O1G	2.88	118.34	107.38
4	A	414	DGT	C4-C5-N7	3.22	112.44	109.48
4	A	414	DGT	O1G-PG-O3B	3.30	120.06	105.09
4	B	1414	DGT	O2G-PG-O3B	3.69	121.83	105.09
4	A	414	DGT	O2G-PG-O1G	3.88	122.14	107.38
4	B	1414	DGT	C6-N1-C2	7.40	126.22	115.94
4	A	414	DGT	C6-N1-C2	7.42	126.24	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	414	DGT	4	0
4	B	1414	DGT	5	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	341/341 (100%)	0.81	42 (12%) 5 5	48, 58, 67, 75	0
1	B	341/341 (100%)	1.16	70 (20%) 1 1	49, 64, 74, 81	0
2	D	12/13 (92%)	1.01	4 (33%) 0 1	40, 46, 82, 85	0
2	H	12/13 (92%)	2.16	4 (33%) 0 1	54, 62, 99, 102	0
3	E	17/18 (94%)	0.78	2 (11%) 6 6	43, 58, 72, 75	0
3	J	13/18 (72%)	2.09	5 (38%) 0 0	54, 63, 93, 95	0
All	All	736/744 (98%)	1.02	127 (17%) 2 2	40, 60, 73, 102	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1918	DC	9.4
1	B	1006	VAL	7.2
2	H	1802	DG	7.1
1	B	1004	LEU	6.4
1	B	1005	PHE	5.9
2	H	1804	DT	5.7
2	H	1803	DT	5.7
1	B	1116	ARG	5.1
2	D	802	DG	4.9
1	B	1234	ASN	4.7
1	A	46	ALA	4.7
3	J	1917	DA	4.6
1	B	1143	GLY	4.5
1	B	1046	ALA	4.5
3	J	1914	DC	4.5
1	A	4	LEU	4.5
2	H	1805	DG	4.1
1	B	1141	THR	4.1
1	B	1035	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	4.1
1	B	1029	VAL	3.9
1	B	1028	VAL	3.9
1	B	1113	ASP	3.8
1	B	1037	PHE	3.8
1	A	6	VAL	3.7
1	B	1109	LEU	3.7
1	A	335	VAL	3.7
1	A	234	ASN	3.6
1	B	1119	ARG	3.6
1	B	1188	ASN	3.6
1	A	28	VAL	3.6
1	B	1111	ILE	3.6
3	J	1913	DT	3.5
1	B	1142	VAL	3.5
1	B	1117	ASP	3.5
1	B	1169	GLU	3.4
3	J	1916	DA	3.4
1	B	1140	VAL	3.4
1	A	284	ILE	3.3
1	B	1107	ALA	3.3
1	B	1284	ILE	3.3
1	B	1324	GLU	3.2
1	B	1259	GLU	3.2
1	A	29	VAL	3.2
1	A	333	ILE	3.2
1	B	1098	LYS	3.2
1	A	149	VAL	3.1
1	A	1	GLY	3.1
1	B	1094	GLU	3.1
1	B	1030	VAL	3.1
1	B	1134	GLU	3.1
1	B	1045	THR	3.1
1	B	1115	VAL	3.1
1	A	261	ILE	3.0
1	B	1001	GLY	3.0
1	B	1038	GLU	3.0
1	B	1334	GLY	3.0
1	A	337	PHE	2.9
1	A	274	TYR	2.9
1	A	210	PHE	2.9
2	D	803	DT	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1097	GLU	2.8
1	B	1288	ALA	2.8
1	B	1225	LEU	2.8
1	B	1112	SER	2.8
1	B	1118	TYR	2.8
1	B	1151	ALA	2.8
1	B	1036	ARG	2.8
1	B	1327	GLU	2.7
1	A	283	ALA	2.7
3	E	916	DA	2.7
1	B	1319	LEU	2.7
1	A	278	LYS	2.7
1	B	1144	ILE	2.7
1	B	1092	LEU	2.7
1	B	1207	SER	2.7
1	B	1210	PHE	2.7
1	B	1123	ASN	2.7
3	E	917	DA	2.6
1	A	107	ALA	2.6
1	A	144	ILE	2.6
1	A	70	ASN	2.6
1	B	1013	ALA	2.6
1	A	334	GLY	2.5
1	A	11	PHE	2.5
1	B	1337	PHE	2.5
1	A	142	VAL	2.5
1	B	1287	VAL	2.5
2	D	804	DT	2.5
1	A	202	LEU	2.5
1	A	47	ASN	2.5
1	B	1238	ARG	2.5
1	B	1012	TYR	2.4
1	B	1047	ASN	2.4
1	B	1230	ARG	2.4
2	D	805	DG	2.4
1	B	1010	TYR	2.4
1	A	285	HIS	2.4
1	A	150	PHE	2.4
1	B	1209	GLU	2.3
1	A	273	TYR	2.3
1	A	116	ARG	2.3
1	A	50	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1159	LYS	2.2
1	B	1320	GLN	2.2
1	B	1278	LYS	2.2
1	A	265	LEU	2.2
1	B	1130	ASN	2.2
1	A	319	LEU	2.2
1	A	287	VAL	2.2
1	A	8	PHE	2.2
1	B	1074	LEU	2.2
1	B	1221	LYS	2.1
1	A	327	GLU	2.1
1	A	286	VAL	2.1
1	B	1254	ASN	2.1
1	A	151	ALA	2.1
1	A	183	VAL	2.1
1	A	88	ILE	2.1
1	A	329	LYS	2.1
1	B	1241	VAL	2.1
1	B	1226	ILE	2.1
1	A	5	PHE	2.1
1	B	1120	GLU	2.1
1	B	1301	THR	2.1
1	B	1158	ALA	2.0
1	B	1331	ARG	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( $\text{\AA}^2$ )	Q<0.9
3	8OG	J	1906	23/24	0.89	0.16	-	57,61,65,66	0
2	2DA	D	814[B]	20/21	0.84	0.29	-	49,51,55,56	20
3	8OG	E	906[A]	23/24	0.92	0.20	-	49,55,60,62	23
2	2DA	D	814[A]	20/21	0.84	0.29	-	54,60,61,63	20
3	8OG	E	906[B]	23/24	0.92	0.20	-	54,57,60,61	23
2	2DA	H	1814	20/21	0.90	0.22	-	57,61,69,70	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( $\text{\AA}^2$ )	Q<0.9
5	CA	B	1417	1/1	0.87	0.23	1.06	69,69,69,69	0
4	DGT	A	414	31/31	0.95	0.18	-0.57	32,38,40,41	0
5	CA	A	415	1/1	0.95	0.19	-0.78	57,57,57,57	0
5	CA	B	1415	1/1	0.93	0.19	-1.22	68,68,68,68	0
4	DGT	B	1414	31/31	0.93	0.16	-1.24	50,53,57,58	0
5	CA	A	417	1/1	0.94	0.13	-1.57	59,59,59,59	0
5	CA	B	1416	1/1	0.85	0.07	-3.53	57,57,57,57	0
5	CA	A	416	1/1	0.96	0.05	-3.97	42,42,42,42	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.