



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:04 am GMT

PDB ID : 2XCP  
Title : TERNARY COMPLEX OF SULFOLOBUS SOLFATARICUS DPO4 DNA  
POLYMERASE, 7,8- DIHYDRO-8-OXODEOXYGUANINE MODIFIED  
DNA AND dCTP - MAGNESIUM FORM  
Authors : Irimia, A.; Egli, M.  
Deposited on : 2010-04-24  
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

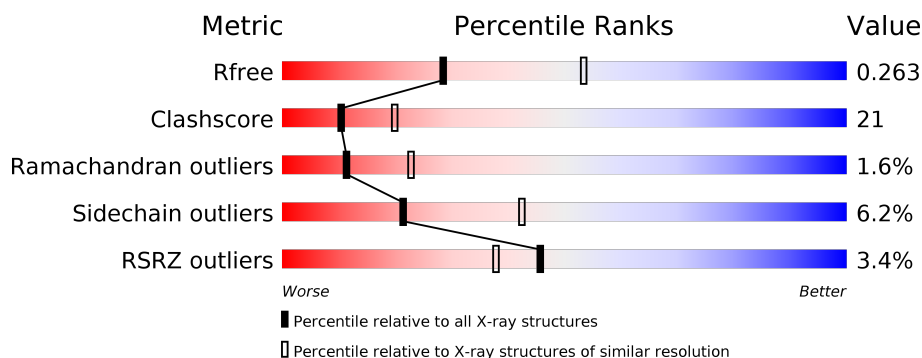
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	358	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 66%, yellow 27%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>66%</span> <span>27%</span> <span>• •</span> </div> </div>
1	B	358	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 57%, yellow 34%, orange 5%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>57%</span> <span>34%</span> <span>5%</span> <span>•</span> </div> </div>
2	E	13	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 46%, yellow 54%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>46%</span> <span>54%</span> </div> </div>
2	P	13	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 69%, yellow 31%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>69%</span> <span>31%</span> </div> </div>
3	F	18	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>11%</span> <span>50%</span> <span>50%</span> </div> </div>
3	T	18	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, green 56%, yellow 44%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>11%</span> <span>56%</span> <span>44%</span> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7158 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	342	Total	C	N	O	S	0	6	1
			2803	1793	488	515	7			
1	B	343	Total	C	N	O	S	0	1	1
			2765	1772	480	506	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
A	0	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
B	0	HIS	-	EXPRESSION TAG	UNP Q97W02

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			271	128	57	74	12			
2	P	13	Total	C	N	O	P	0	0	0
			272	129	57	74	12			

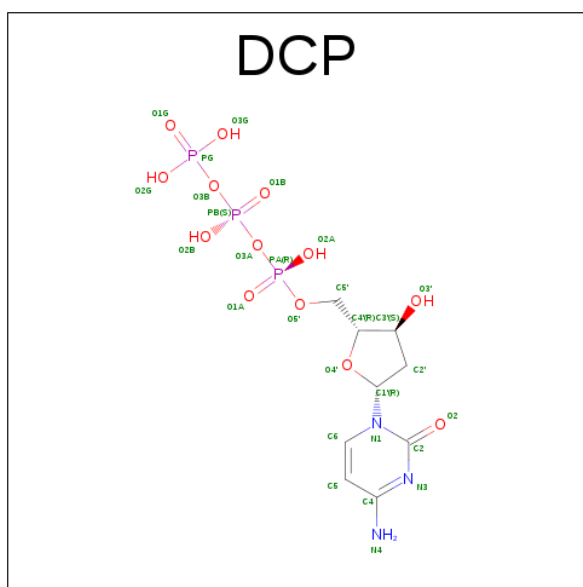
- Molecule 3 is a DNA chain called 5'-D(\*TP\*CP\*AP\*CP\*8OGP\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	18	Total	C	N	O	P	0	0	1
			340	161	58	104	17			
3	T	18	Total	C	N	O	P	0	0	1
			340	161	58	104	17			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
5	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		

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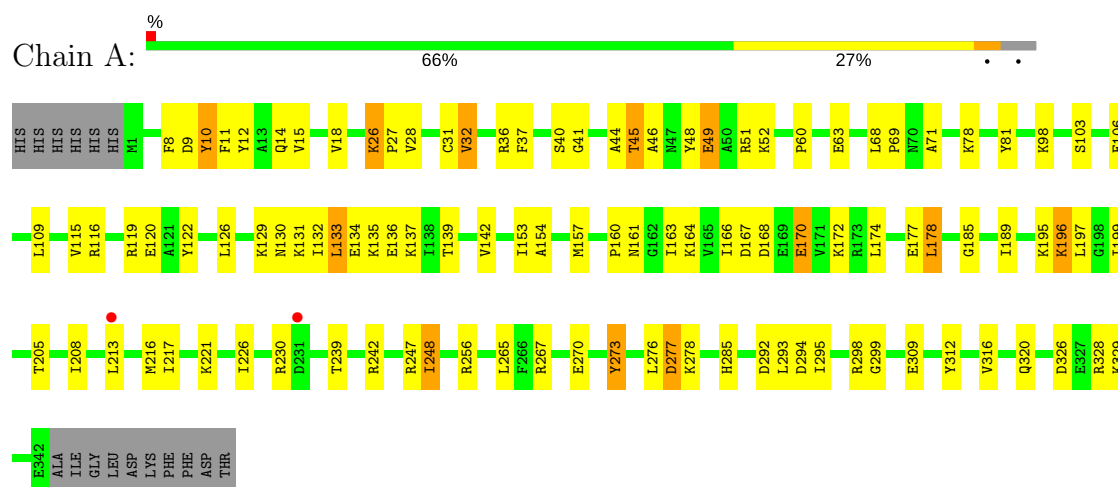
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	90	Total 90	O 90	0	0
6	E	19	Total 19	O 19	0	0
6	F	23	Total 23	O 23	0	0
6	P	18	Total 18	O 18	0	0
6	T	22	Total 22	O 22	0	0

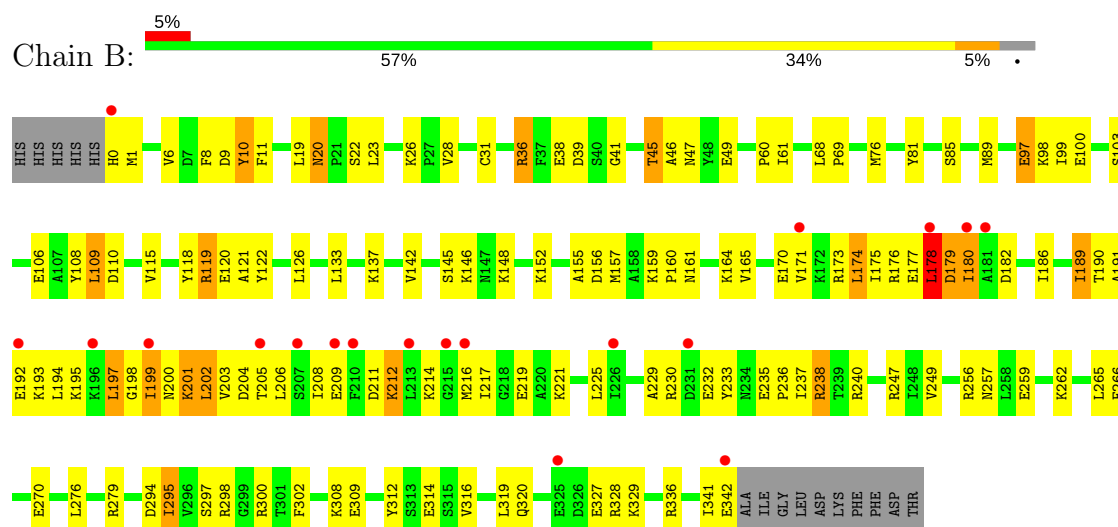
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

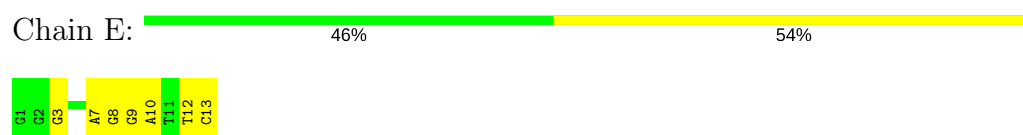
#### • Molecule 1: DNA POLYMERASE IV



#### • Molecule 1: DNA POLYMERASE IV

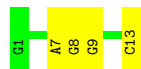


#### • Molecule 2: 5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP \*TP\*DOC)-3'



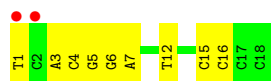
- Molecule 2: 5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP \*TP\*DOC)-3'

Chain P:  69% 31%



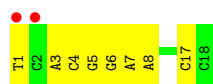
- Molecule 3: 5'-D(\*TP\*CP\*AP\*CP\*8OGP\*GP\*AP\*AP\*TP\*CP\*CP \*TP\*TP\*CP\*CP\*CP\*CP\*CP)-3'

Chain F:  11% 50% 50%



- Molecule 3: 5'-D(\*TP\*CP\*AP\*CP\*8OGP\*GP\*AP\*AP\*TP\*CP\*CP \*TP\*TP\*CP\*CP\*CP\*CP\*CP)-3'

Chain T:  11% 56% 44%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.76Å 100.43Å 105.87Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	49.55 – 2.60 49.55 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.55-2.60) 97.3 (49.55-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.268 0.217 , 0.263	Depositor DCC
$R_{free}$ test set	1874 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.87 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.6408e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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, MG, 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	0.40	0/2843	0.65	0/3817
1	B	0.40	0/2805	0.66	0/3767
2	E	0.66	0/286	0.73	0/442
2	P	0.68	0/287	0.76	0/444
3	F	0.84	1/351 (0.3%)	0.79	0/535
3	T	0.86	1/351 (0.3%)	0.83	0/535
All	All	0.49	2/6923 (0.0%)	0.68	0/9540

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
2	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	DT	O3'-P	-7.64	1.51	1.61
3	T	1	DT	O3'-P	-7.44	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	12	DT	Sidechain

## 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	2803	0	2936	93	0
1	B	2765	0	2908	148	0
2	E	271	0	144	6	0
2	P	272	0	147	8	0
3	F	340	0	191	12	0
3	T	340	0	191	19	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	28	0	12	7	0
5	B	28	0	12	6	0
6	A	133	0	0	13	0
6	B	90	0	0	6	0
6	E	19	0	0	2	0
6	F	23	0	0	0	0
6	P	18	0	0	1	0
6	T	22	0	0	3	0
All	All	7158	0	6541	277	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 (277) 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:194:LEU:HD21	1:B:217:ILE:HD11	1.34	1.06
3:T:7:DA:H2''	3:T:8:DA:H5'	1.41	1.01
1:B:178:LEU:HG	1:B:179:ASP:H	1.29	0.97
6:A:2129:HOH:O	1:B:45:THR:HG21	1.64	0.96
1:B:209:GLU:H	1:B:212:LYS:HE2	1.34	0.93
1:B:202:LEU:HD22	1:B:229:ALA:HB2	1.51	0.92
3:T:4:DC:O2	3:T:4:DC:H2'	1.71	0.88
1:B:201:LYS:HB3	1:B:203:VAL:HG12	1.57	0.87
1:B:217:ILE:HG22	1:B:221:LYS:HB2	1.55	0.86
1:A:196:LYS:HA	1:A:196:LYS:HE3	1.56	0.86
1:B:178:LEU:CG	1:B:179:ASP:H	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3:DA:H2''	3:F:4:DC:O5'	1.76	0.83
1:A:115:VAL:HG22	1:A:120:GLU:HB3	1.58	0.82
1:B:119:ARG:HH11	1:B:119:ARG:HB3	1.45	0.82
1:B:265:LEU:HD12	1:B:319:LEU:HD22	1.61	0.82
3:T:3:DA:H2''	3:T:4:DC:H5'	1.62	0.81
1:B:103:SER:OG	1:B:106:GLU:HG2	1.81	0.81
1:A:205:THR:HG22	1:A:226:ILE:HD13	1.63	0.80
1:B:202:LEU:O	1:B:205:THR:HG22	1.80	0.80
1:A:139:THR:HB	1:A:161:ASN:HD22	1.45	0.80
1:B:214:LYS:HZ3	1:B:219:GLU:HB2	1.47	0.79
1:B:230:ARG:O	1:B:232:GLU:HG3	1.83	0.78
1:B:214:LYS:NZ	1:B:219:GLU:HB2	1.99	0.77
1:A:256:ARG:HG3	1:A:329:LYS:HG2	1.65	0.77
3:T:7:DA:H2''	3:T:8:DA:C5'	2.15	0.76
1:B:180:ILE:HG21	1:B:194:LEU:HD13	1.67	0.75
1:B:47:ASN:CG	1:B:49:GLU:OE1	2.24	0.75
1:B:197:LEU:HB3	1:B:199:ILE:HG12	1.68	0.73
1:A:205:THR:HG23	1:A:213:LEU:HD11	1.71	0.73
1:A:256:ARG:NH1	1:A:256:ARG:HB3	2.04	0.72
1:B:178:LEU:HG	1:B:179:ASP:N	2.05	0.72
1:B:97:GLU:CD	1:B:97:GLU:H	1.93	0.71
1:B:295:ILE:O	1:B:295:ILE:HD13	1.91	0.71
1:A:131:LYS:HE2	1:A:135:LYS:HE3	1.74	0.70
1:A:45:THR:HG21	5:A:5000:DCP:O1B	1.92	0.69
1:B:194:LEU:HA	6:B:2066:HOH:O	1.93	0.69
1:B:270:GLU:OE2	1:B:308:LYS:HD3	1.94	0.68
1:A:177:GLU:CG	1:A:178:LEU:H	2.07	0.68
1:B:256:ARG:NH1	1:B:256:ARG:HB3	2.09	0.67
1:B:176:ARG:HG3	1:B:177:GLU:OE1	1.94	0.67
3:T:3:DA:H2''	3:T:4:DC:C5'	2.24	0.67
2:E:3:DG:N7	6:E:2004:HOH:O	2.28	0.66
1:A:103:SER:OG	1:A:106:GLU:HG2	1.95	0.66
1:A:130:ASN:O	1:A:134:GLU:HG2	1.95	0.66
1:B:115:VAL:HG13	1:B:120:GLU:HB3	1.78	0.66
3:T:3:DA:H2'	3:T:4:DC:C2	2.30	0.66
1:A:326:ASP:OD1	1:A:328:ARG:HG2	1.95	0.64
1:A:60:PRO:HD2	1:A:63:GLU:HG3	1.80	0.64
1:A:37:PHE:HB2	1:A:40:SER:HB2	1.80	0.63
1:B:178:LEU:CG	1:B:179:ASP:N	2.60	0.63
1:A:51:ARG:HB3	6:A:2019:HOH:O	1.99	0.63
1:B:206:LEU:HD21	1:B:229:ALA:HB1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HB2	1:B:237:ILE:HG23	1.81	0.63
1:B:199:ILE:CD1	1:B:208:ILE:HG13	2.29	0.62
1:A:273:TYR:HA	1:A:276:LEU:HD12	1.82	0.62
1:A:137:LYS:HD3	6:A:2061:HOH:O	2.00	0.61
1:A:205:THR:HG22	1:A:226:ILE:CD1	2.29	0.61
1:B:197:LEU:HB2	6:B:2066:HOH:O	1.98	0.61
3:T:17:DC:H2''	6:T:2020:HOH:O	2.00	0.61
1:B:217:ILE:CG2	1:B:221:LYS:HB2	2.28	0.61
1:A:197:LEU:HD11	1:A:216:MET:HG2	1.83	0.60
3:T:6:DG:H2''	3:T:7:DA:H5''	1.83	0.60
6:A:2130:HOH:O	5:B:5000:DCP:PA	2.60	0.60
1:A:256:ARG:HB3	1:A:256:ARG:HH11	1.64	0.60
6:A:2130:HOH:O	5:B:5000:DCP:O1A	2.16	0.60
1:A:12:TYR:CE1	5:A:5000:DCP:H2'2	2.37	0.60
1:B:256:ARG:HH11	1:B:256:ARG:HB3	1.68	0.59
2:P:7:DA:H2''	2:P:8:DG:C5'	2.32	0.59
1:B:199:ILE:HD13	6:B:2067:HOH:O	2.03	0.59
1:B:20:ASN:ND2	1:B:22:SER:OG	2.35	0.59
6:A:2129:HOH:O	1:B:10:TYR:HA	2.03	0.58
2:P:7:DA:H2''	2:P:8:DG:H5'	1.84	0.58
1:A:199:ILE:HD11	1:A:208:ILE:HG13	1.86	0.58
3:F:6:DG:C2'	3:F:7:DA:H5''	2.33	0.58
1:B:41:GLY:HA2	3:F:5:8OG:H5''	1.85	0.58
1:B:192:GLU:OE1	1:B:195:LYS:HE3	2.03	0.58
1:B:309:GLU:CD	1:B:309:GLU:H	2.06	0.58
1:A:11:PHE:O	1:A:15:VAL:HG23	2.02	0.57
3:F:6:DG:H2''	3:F:7:DA:H5''	1.86	0.57
1:B:295:ILE:C	1:B:295:ILE:HD13	2.24	0.57
1:A:242:ARG:NH2	3:T:8:DA:OP1	2.37	0.57
3:T:6:DG:H2''	3:T:7:DA:C5'	2.34	0.57
1:B:217:ILE:CG2	1:B:221:LYS:CB	2.83	0.56
1:B:180:ILE:HD11	1:B:202:LEU:HA	1.86	0.56
3:T:6:DG:C2'	3:T:7:DA:H5''	2.35	0.56
1:A:298:ARG:HD3	2:P:7:DA:H5'	1.86	0.56
1:A:116:ARG:HB2	1:A:120:GLU:OE2	2.06	0.56
3:F:6:DG:H2''	3:F:7:DA:C5'	2.36	0.56
1:B:189:ILE:HD12	1:B:189:ILE:C	2.26	0.56
1:A:49:GLU:HG3	6:A:2021:HOH:O	2.06	0.56
1:B:217:ILE:HG22	1:B:221:LYS:CB	2.31	0.55
3:F:6:DG:H1'	3:F:7:DA:H5''	1.88	0.55
1:A:153:ILE:O	1:A:157:MET:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG2	1:A:329:LYS:HA	1.88	0.55
5:A:5000:DCP:H6	5:A:5000:DCP:O5'	2.07	0.55
1:A:68:LEU:HB3	1:A:71:ALA:HB2	1.89	0.55
1:B:133:LEU:O	1:B:137:LYS:HD2	2.07	0.54
1:B:203:VAL:HG23	1:B:206:LEU:HD12	1.89	0.54
5:A:5000:DCP:O3A	6:A:2120:HOH:O	2.18	0.54
1:B:38:GLU:O	1:B:39:ASP:OD2	2.25	0.54
1:B:294:ASP:OD1	1:B:328:ARG:NH2	2.39	0.54
1:B:122:TYR:CE2	1:B:126:LEU:HD11	2.42	0.54
1:B:152:LYS:HE2	6:E:2019:HOH:O	2.08	0.54
1:B:0:HIS:CG	1:B:1:MET:H	2.26	0.53
1:B:60:PRO:HB3	3:F:4:DC:H5'	1.91	0.53
1:B:316:VAL:O	1:B:320:GLN:HG3	2.08	0.53
1:B:298:ARG:NH1	2:E:7:DA:H3'	2.23	0.53
1:A:12:TYR:CZ	5:A:5000:DCP:H2'2	2.42	0.53
1:B:300[B]:ARG:HH11	1:B:300[B]:ARG:HG3	1.74	0.53
1:B:20:ASN:HD22	1:B:20:ASN:C	2.11	0.53
1:B:236:PRO:HG2	1:B:238:ARG:HH11	1.74	0.53
1:B:202:LEU:HD21	1:B:225:LEU:O	2.10	0.52
1:B:200:ASN:O	1:B:204:ASP:HB2	2.09	0.52
1:A:131:LYS:HE2	1:A:135:LYS:CE	2.38	0.51
1:B:199:ILE:HD11	1:B:208:ILE:HG13	1.92	0.51
2:E:8:DG:H2''	2:E:9:DG:O5'	2.10	0.51
1:A:142:VAL:O	1:A:163:ILE:HA	2.10	0.51
1:A:9:ASP:O	1:A:10:TYR:C	2.49	0.51
1:A:170:GLU:O	1:A:174:LEU:HG	2.10	0.51
1:B:217:ILE:CG2	1:B:221:LYS:HD2	2.40	0.51
1:A:132:ILE:HB	6:A:2058:HOH:O	2.11	0.51
1:B:97:GLU:CD	1:B:97:GLU:N	2.61	0.51
1:A:239:THR:HA	6:A:2085:HOH:O	2.11	0.51
1:B:68:LEU:N	1:B:69:PRO:HD3	2.25	0.51
1:A:161:ASN:OD1	1:A:161:ASN:O	2.29	0.51
3:T:7:DA:H8	3:T:7:DA:H5'	1.75	0.51
1:B:247:ARG:NH1	1:B:249:VAL:HG12	2.25	0.50
1:B:256:ARG:HG3	1:B:329:LYS:HG2	1.93	0.50
1:A:157:MET:HE3	1:A:164:LYS:NZ	2.26	0.50
1:A:247:ARG:HH11	1:A:247:ARG:HG3	1.75	0.50
1:B:170:GLU:HG2	1:B:170:GLU:O	2.11	0.50
1:B:198:GLY:HA2	6:B:2068:HOH:O	2.11	0.50
1:B:190:THR:O	1:B:194:LEU:HG	2.12	0.50
1:A:41:GLY:HA2	3:T:5:8OG:H5''	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:6:DG:H1'	3:T:7:DA:H5''	1.93	0.49
6:A:2129:HOH:O	5:B:5000:DCP:PB	2.69	0.49
1:A:9:ASP:O	1:A:11:PHE:N	2.45	0.49
1:B:171:VAL:O	1:B:175:ILE:HG13	2.13	0.49
1:B:270:GLU:OE2	1:B:312:TYR:OH	2.29	0.49
1:A:28:VAL:O	1:A:46:ALA:HA	2.13	0.49
3:F:4:DC:C2'	3:F:4:DC:O2	2.59	0.49
1:A:177:GLU:CD	1:A:178:LEU:H	2.15	0.49
1:A:119[A]:ARG:O	1:A:119[A]:ARG:HD3	2.13	0.49
1:B:157:MET:SD	1:B:164:LYS:NZ	2.86	0.49
1:B:202:LEU:CD2	1:B:229:ALA:HB2	2.32	0.49
1:B:28:VAL:HB	1:B:47:ASN:ND2	2.28	0.48
1:A:26:LYS:HB3	1:A:26:LYS:NZ	2.28	0.48
1:B:9:ASP:O	1:B:10:TYR:C	2.51	0.48
1:A:168:ASP:O	1:A:172:LYS:HG2	2.13	0.48
1:A:27:PRO:HG3	1:A:49:GLU:HB3	1.95	0.48
1:B:209:GLU:N	1:B:212:LYS:HE2	2.15	0.48
1:A:12:TYR:CD1	5:A:5000:DCP:H2'2	2.49	0.48
1:A:14:GLN:O	1:A:18:VAL:HG23	2.12	0.48
1:B:159:LYS:HE3	5:B:5000:DCP:O1G	2.13	0.48
2:P:8:DG:H2''	2:P:9:DG:O5'	2.13	0.48
1:B:178:LEU:O	1:B:179:ASP:HB2	2.12	0.48
1:B:197:LEU:HD13	1:B:216:MET:HG3	1.96	0.48
1:B:20:ASN:ND2	1:B:20:ASN:C	2.67	0.48
1:B:300[B]:ARG:HG2	1:B:302:PHE:CE1	2.49	0.48
1:B:99:ILE:HG13	1:B:109:LEU:HD22	1.95	0.48
1:A:285:HIS:CD2	1:A:299:GLY:HA3	2.49	0.47
1:B:189:ILE:HG12	2:E:10:DA:H3'	1.96	0.47
1:A:185:GLY:O	1:A:221:LYS:HE2	2.13	0.47
1:A:312:TYR:O	1:A:316:VAL:HG23	2.14	0.47
1:B:297:SER:O	1:B:298:ARG:NH1	2.43	0.47
1:A:166:ILE:HD13	1:A:174:LEU:HD11	1.96	0.47
1:A:292:ASP:OD2	1:A:294:ASP:HB2	2.14	0.47
1:B:197:LEU:HB3	1:B:199:ILE:CG1	2.43	0.47
1:B:300[A]:ARG:CZ	1:B:314:GLU:OE2	2.63	0.47
1:A:248:ILE:HD13	3:T:6:DG:H2''	1.97	0.47
1:A:136:GLU:O	1:A:137:LYS:HB2	2.15	0.47
1:B:174:LEU:O	1:B:178:LEU:HD22	2.14	0.47
1:A:44:ALA:O	1:A:45:THR:HG23	2.15	0.47
6:B:2071:HOH:O	3:F:12:DT:H5''	2.15	0.47
1:B:178:LEU:CD2	1:B:179:ASP:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:SER:O	1:B:89:MET:HG2	2.15	0.46
1:B:189:ILE:O	1:B:193:LYS:HB2	2.15	0.46
1:B:197:LEU:CD1	1:B:216:MET:HG3	2.46	0.46
1:A:69:PRO:HG3	1:B:309:GLU:HG2	1.97	0.46
1:A:8:PHE:CD1	1:A:8:PHE:N	2.81	0.46
1:B:192:GLU:HA	1:B:195:LYS:HE3	1.97	0.46
1:B:206:LEU:HD21	1:B:229:ALA:CB	2.44	0.46
1:B:47:ASN:OD1	1:B:49:GLU:OE1	2.34	0.46
1:B:193:LYS:NZ	1:B:216:MET:HB3	2.31	0.46
1:B:197:LEU:O	6:B:2067:HOH:O	2.21	0.46
1:B:38:GLU:O	1:B:39:ASP:CG	2.55	0.46
1:B:76:MET:HG3	1:B:81:TYR:HE2	1.81	0.46
3:F:3:DA:C2'	3:F:4:DC:O5'	2.58	0.46
1:A:298:ARG:NH1	2:P:7:DA:H5'	2.31	0.46
1:B:170:GLU:O	1:B:174:LEU:HB2	2.15	0.45
2:P:9:DG:H5'	6:P:2011:HOH:O	2.15	0.45
1:B:115:VAL:HG11	1:B:121:ALA:HB2	1.97	0.45
1:B:145:SER:OG	1:B:146:LYS:N	2.49	0.45
1:A:177:GLU:CG	1:A:178:LEU:N	2.77	0.45
1:B:176:ARG:HA	1:B:203:VAL:HB	1.97	0.45
1:B:100:GLU:CB	1:B:237:ILE:HG23	2.44	0.45
1:B:341:ILE:HG22	1:B:342:GLU:N	2.31	0.45
1:B:8:PHE:N	1:B:8:PHE:CD1	2.80	0.45
1:A:213:LEU:O	1:A:217:ILE:HG12	2.16	0.45
1:A:248:ILE:CD1	3:T:6:DG:H2''	2.46	0.45
1:A:309:GLU:CD	1:A:309:GLU:H	2.20	0.45
1:B:23:LEU:O	1:B:26:LYS:HG2	2.17	0.45
1:A:157:MET:HE2	1:A:166:ILE:HD11	1.98	0.45
1:A:133:LEU:O	1:A:137:LYS:HA	2.17	0.45
1:B:217:ILE:HG21	1:B:221:LYS:HB3	1.98	0.45
1:A:256:ARG:CB	1:A:256:ARG:HH11	2.28	0.44
1:B:28:VAL:O	1:B:46:ALA:HA	2.17	0.44
1:A:247:ARG:HG3	1:A:247:ARG:NH1	2.32	0.44
1:B:298:ARG:HH12	2:E:8:DG:P	2.39	0.44
1:B:31:CYS:HB3	1:B:61:ILE:HD11	1.99	0.44
1:B:179:ASP:O	1:B:180:ILE:HG12	2.17	0.44
1:A:167:ASP:OD1	1:A:170:GLU:HB2	2.17	0.44
1:A:248:ILE:HB	6:T:2006:HOH:O	2.18	0.44
1:B:262:LYS:HE3	1:B:266:PHE:CE2	2.52	0.44
1:B:199:ILE:O	1:B:199:ILE:HG22	2.18	0.44
1:A:293:LEU:HD11	3:T:4:DC:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:6:DG:O6	6:T:2007:HOH:O	2.21	0.43
1:A:270:GLU:HA	1:A:270:GLU:OE1	2.17	0.43
1:B:256:ARG:HH11	1:B:256:ARG:CB	2.31	0.43
1:B:173:ARG:O	1:B:176:ARG:HG2	2.18	0.43
1:B:217:ILE:HG23	1:B:221:LYS:HD2	2.00	0.43
1:A:48:TYR:O	1:A:52:LYS:HG3	2.18	0.43
1:B:164:LYS:HG2	1:B:165:VAL:N	2.34	0.43
1:B:262:LYS:HE3	1:B:266:PHE:CZ	2.54	0.43
1:B:9:ASP:O	1:B:11:PHE:N	2.51	0.43
3:T:7:DA:C8	3:T:7:DA:H5'	2.53	0.43
1:A:177:GLU:HG2	1:A:178:LEU:H	1.82	0.43
1:A:139:THR:HB	1:A:161:ASN:ND2	2.22	0.43
1:B:155:ALA:O	1:B:159:LYS:HG3	2.19	0.43
1:B:197:LEU:CB	1:B:199:ILE:HG12	2.44	0.43
1:B:209:GLU:HB2	1:B:212:LYS:NZ	2.34	0.42
1:B:19:LEU:HD12	1:B:19:LEU:N	2.34	0.42
1:B:209:GLU:HG3	1:B:211:ASP:OD1	2.19	0.42
1:A:277:ASP:HB3	1:A:278:LYS:H	1.65	0.42
1:A:48:TYR:OH	5:A:5000:DCP:O3G	2.31	0.42
1:B:108:TYR:CD2	1:B:148:LYS:HG2	2.53	0.42
1:B:175:ILE:HD13	1:B:229:ALA:HA	2.01	0.42
6:A:2132:HOH:O	5:B:5000:DCP:PA	2.78	0.42
1:B:98:LYS:HB2	1:B:110:ASP:HB3	2.00	0.42
1:A:122:TYR:CE2	1:A:126:LEU:HD11	2.55	0.42
1:B:180:ILE:C	1:B:182:ASP:H	2.23	0.42
1:B:209:GLU:HB2	1:B:212:LYS:HZ1	1.85	0.42
1:A:298:ARG:HD3	2:P:7:DA:C5'	2.47	0.42
1:B:191:ALA:HA	1:B:194:LEU:HD12	2.02	0.42
5:B:5000:DCP:C6	2:E:13:DOC:H2''	2.50	0.42
1:A:278:LYS:HA	1:A:278:LYS:HZ2	1.84	0.42
1:B:233:TYR:OH	1:B:235:GLU:HB2	2.20	0.42
3:F:15:DC:H2''	3:F:16:DC:OP2	2.19	0.42
1:A:9:ASP:C	1:A:11:PHE:N	2.71	0.42
1:A:205:THR:CG2	1:A:226:ILE:HD13	2.41	0.42
1:B:199:ILE:HD12	1:B:208:ILE:HG13	2.00	0.42
3:F:6:DG:C1'	3:F:7:DA:H5''	2.50	0.42
1:A:78:LYS:HA	1:A:81:TYR:CD2	2.54	0.41
1:B:118:TYR:HB3	1:B:165:VAL:HG11	2.00	0.41
1:B:276:LEU:O	1:B:279:ARG:HB2	2.19	0.41
1:B:308:LYS:HG2	1:B:312:TYR:CE2	2.55	0.41
1:B:186:ILE:HG13	1:B:225:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:OE1	2:P:13:DOC:H5'	2.20	0.41
1:A:166:ILE:HD13	1:A:174:LEU:CD1	2.49	0.41
1:B:203:VAL:C	1:B:205:THR:H	2.23	0.41
1:B:256:ARG:NE	1:B:327:GLU:O	2.52	0.41
1:B:208:ILE:HG23	1:B:212:LYS:HD2	2.03	0.41
1:B:257:ASN:OD1	1:B:259:GLU:N	2.53	0.41
1:B:200:ASN:O	1:B:201:LYS:O	2.38	0.41
1:B:208:ILE:HG22	1:B:209:GLU:N	2.36	0.41
1:B:45:THR:HG22	1:B:46:ALA:H	1.86	0.41
1:A:129:LYS:O	1:A:133:LEU:HB2	2.21	0.40
1:A:139:THR:CB	1:A:161:ASN:HD22	2.24	0.40
1:B:160:PRO:O	1:B:161:ASN:C	2.60	0.40
1:A:166:ILE:HG23	1:A:170:GLU:HB3	2.04	0.40
1:A:32:VAL:HG22	1:A:32:VAL:O	2.21	0.40
1:A:154:ALA:HB2	1:A:166:ILE:HD12	2.02	0.40
1:B:6:VAL:HG22	1:B:142:VAL:HG22	2.04	0.40
1:A:157:MET:CE	1:A:166:ILE:HD11	2.51	0.40
6:A:2129:HOH:O	1:B:10:TYR:C	2.60	0.40
1:B:193:LYS:HZ3	1:B:216:MET:HB3	1.86	0.40
1:B:49:GLU:H	1:B:49:GLU:CD	2.25	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	346/358 (97%)	330 (95%)	14 (4%)	2 (1%)	28	53
1	B	342/358 (96%)	303 (89%)	30 (9%)	9 (3%)	6	10
All	All	688/716 (96%)	633 (92%)	44 (6%)	11 (2%)	11	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	B	178	LEU
1	B	179	ASP
1	B	201	LYS
1	A	10	TYR
1	B	10	TYR
1	B	199	ILE
1	B	36	ARG
1	B	174	LEU
1	B	180	ILE
1	B	240	ARG

### 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	306/315 (97%)	283 (92%)	23 (8%)	16	31
1	B	302/315 (96%)	287 (95%)	15 (5%)	28	53
All	All	608/630 (96%)	570 (94%)	38 (6%)	21	42

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	31	CYS
1	A	32	VAL
1	A	36	ARG
1	A	45	THR
1	A	49	GLU
1	A	98	LYS
1	A	109	LEU
1	A	133	LEU
1	A	160	PRO
1	A	170	GLU
1	A	189	ILE
1	A	195	LYS

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Mol	Chain	Res	Type
1	A	196	LYS
1	A	230	ARG
1	A	248	ILE
1	A	265	LEU
1	A	267	ARG
1	A	273	TYR
1	A	277	ASP
1	A	295	ILE
1	A	320[A]	GLN
1	A	320[B]	GLN
1	B	20	ASN
1	B	36	ARG
1	B	45	THR
1	B	97	GLU
1	B	109	LEU
1	B	119	ARG
1	B	156	ASP
1	B	178	LEU
1	B	189	ILE
1	B	197	LEU
1	B	202	LEU
1	B	212	LYS
1	B	238	ARG
1	B	295	ILE
1	B	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	20	ASN
1	B	130	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	E	13	3,2	13,19,20	1.44	2 (15%)	12,26,29	2.38	3 (25%)
3	8OG	F	5	3	17,25,26	1.44	2 (11%)	22,37,40	1.75	5 (22%)
2	DOC	P	13	3,2	13,19,20	1.41	2 (15%)	12,26,29	1.27	1 (8%)
3	8OG	T	5	3	17,25,26	1.32	2 (11%)	22,37,40	2.21	6 (27%)

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	E	13	3,2	-	0/3/18/19	0/2/2/2
3	8OG	F	5	3	-	0/3/21/22	0/3/3/3
2	DOC	P	13	3,2	-	0/3/18/19	0/2/2/2
3	8OG	T	5	3	-	0/3/21/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	13	DOC	C4-N3	2.85	1.40	1.35
3	T	5	8OG	C2-N1	2.94	1.40	1.35
2	E	13	DOC	C4-N3	2.95	1.40	1.35
3	F	5	8OG	C2-N1	3.06	1.40	1.35
2	P	13	DOC	C6-N1	3.43	1.40	1.35
2	E	13	DOC	C6-N1	3.47	1.40	1.35
3	T	5	8OG	C6-N1	3.82	1.40	1.33
3	F	5	8OG	C6-N1	4.47	1.41	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	N3-C2-N1	-5.83	118.94	127.46
2	E	13	DOC	C3'-C2'-C1'	-5.69	96.36	102.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	8OG	N3-C2-N1	-4.15	121.40	127.46
2	E	13	DOC	O4'-C1'-C2'	-3.53	102.84	106.67
3	F	5	8OG	C5-C6-N1	-3.08	119.09	123.48
3	T	5	8OG	C5-C6-N1	-2.74	119.58	123.48
2	P	13	DOC	C2'-C3'-C4'	-2.63	97.73	102.69
3	T	5	8OG	C6-C5-C4	-2.22	118.63	120.84
3	F	5	8OG	C6-C5-C4	-2.15	118.71	120.84
3	F	5	8OG	O4'-C1'-N9	2.13	110.14	108.15
3	T	5	8OG	N2-C2-N1	2.40	121.07	117.24
3	T	5	8OG	C6-N1-C2	2.40	119.52	116.06
2	E	13	DOC	O4'-C1'-N1	3.19	113.16	107.78
3	F	5	8OG	C2-N3-C4	3.94	119.77	115.16
3	T	5	8OG	C2-N3-C4	6.19	122.39	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	13	DOC	1	0
3	F	5	8OG	1	0
2	P	13	DOC	1	0
3	T	5	8OG	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
5	DCP	A	5000	4	23,29,29	1.40	3 (13%)	25,45,45	0.95	1 (4%)
5	DCP	B	5000	4	23,29,29	1.40	3 (13%)	25,45,45	0.94	1 (4%)

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
5	DCP	A	5000	4	-	0/18/34/34	0/2/2/2
5	DCP	B	5000	4	-	0/18/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5000	DCP	C4-N3	2.90	1.40	1.35
5	B	5000	DCP	C4-N3	2.91	1.40	1.35
5	B	5000	DCP	PG-O1G	3.13	1.61	1.50
5	A	5000	DCP	PG-O1G	3.21	1.61	1.50
5	A	5000	DCP	C6-N1	3.44	1.40	1.35
5	B	5000	DCP	C6-N1	3.50	1.40	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5000	DCP	C2'-C3'-C4'	-2.31	97.81	102.73
5	B	5000	DCP	C2'-C3'-C4'	-2.12	98.21	102.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5000	DCP	7	0
5	B	5000	DCP	6	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	342/358 (95%)	-0.00	2 (0%) 89 88	24, 42, 61, 76	15 (4%)
1	B	343/358 (95%)	0.23	19 (5%) 26 19	23, 45, 92, 115	15 (4%)
2	E	12/13 (92%)	-0.40	0 100 100	43, 51, 61, 65	0
2	P	12/13 (92%)	-0.20	0 100 100	38, 46, 59, 61	0
3	F	17/18 (94%)	0.52	2 (11%) 5 3	32, 52, 122, 124	0
3	T	17/18 (94%)	0.97	2 (11%) 5 3	31, 49, 130, 136	0
All	All	743/778 (95%)	0.13	25 (3%) 46 38	23, 45, 85, 136	30 (4%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	1	DT	17.1
1	B	196	LYS	5.3
1	B	210	PHE	5.0
3	F	1	DT	4.5
1	B	226	ILE	4.3
1	B	199	ILE	4.1
1	B	180	ILE	4.1
3	F	2	DC	4.0
1	B	178	LEU	3.5
1	B	213	LEU	3.5
1	B	205	THR	3.2
1	B	181	ALA	3.1
1	B	216	MET	3.1
1	B	209	GLU	3.1
1	B	0	HIS	2.9
3	T	2	DC	2.9
1	B	192	GLU	2.7
1	B	215	GLY	2.6
1	A	231	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	SER	2.4
1	B	171	VAL	2.3
1	B	325	GLU	2.2
1	B	231	ASP	2.2
1	A	213	LEU	2.1
1	B	342	GLU	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
3	8OG	F	5	23/24	0.98	0.18	-	25,31,42,45	0
2	DOC	E	13	18/19	0.95	0.18	-	41,47,49,50	0
3	8OG	T	5	23/24	0.98	0.17	-	28,31,43,45	0
2	DOC	P	13	18/19	0.94	0.20	-	41,47,54,55	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
5	DCP	A	5000	28/28	0.97	0.18	0.16	21,28,39,42	0
5	DCP	B	5000	28/28	0.97	0.16	-0.37	25,28,33,37	0
4	MG	B	1005	1/1	0.89	0.16	-0.72	48,48,48,48	0
4	MG	A	1000	1/1	0.97	0.09	-3.92	27,27,27,27	0
4	MG	B	1001	1/1	0.88	0.12	-5.31	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	1004	1/1	0.91	0.10	-	31,31,31,31	0
4	MG	B	1003	1/1	0.96	0.15	-	55,55,55,55	0
4	MG	A	1002	1/1	0.80	0.18	-	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.