



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 PM GMT

PDB ID : 4IRK  
Title : structure of Polymerase-DNA complex, dna  
Authors : Nair, D.T.; Sharma, A.  
Deposited on : 2013-01-14  
Resolution : 2.32 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

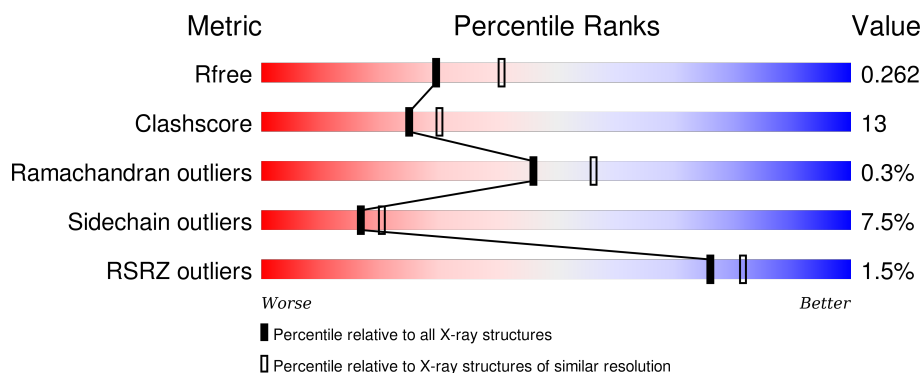
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	342	<div> <div>74%</div> <div>23%</div> <div>•</div> </div>
1	B	342	<div> <div>75%</div> <div>23%</div> <div>•</div> </div>
2	C	18	<div> <div>72%</div> <div>28%</div> </div>
2	F	18	<div> <div>6%</div> <div>67%</div> <div>33%</div> </div>
3	G	17	<div> <div>41%</div> <div>29%</div> <div>12%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	17	

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
4	DCP	A	401	-	-	X	X
4	DCP	B	401	-	-	X	X
5	MG	A	402	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7052 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	B	342	Total	C	N	O	S	0	0	0
			2688	1695	494	485	14			
1	A	342	Total	C	N	O	S	0	0	0
			2688	1695	494	485	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP Q47155
B	1	SER	-	EXPRESSION TAG	UNP Q47155
B	64	ALA	LYS	CONFLICT	UNP Q47155
B	205	ALA	LYS	CONFLICT	UNP Q47155
A	0	GLY	-	EXPRESSION TAG	UNP Q47155
A	1	SER	-	EXPRESSION TAG	UNP Q47155
A	64	ALA	LYS	CONFLICT	UNP Q47155
A	205	ALA	LYS	CONFLICT	UNP Q47155

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			364	174	66	107	17			
2	F	18	Total	C	N	O	P	0	0	0
			364	174	66	107	17			

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

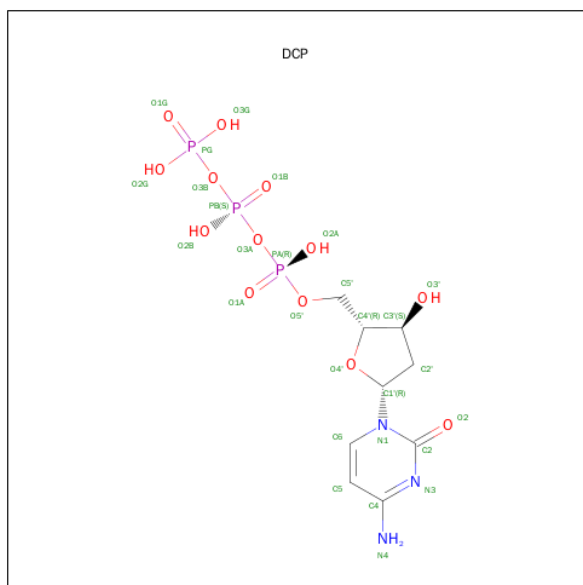
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	14	Total	C	N	O	P	0	0	0
			283	135	54	81	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	14	Total	C	N	O	P	0	0	0
			283	135	54	81	13			

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula:  $C_9H_{16}N_3O_{13}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	96	Total	O	0	0
			96	96		

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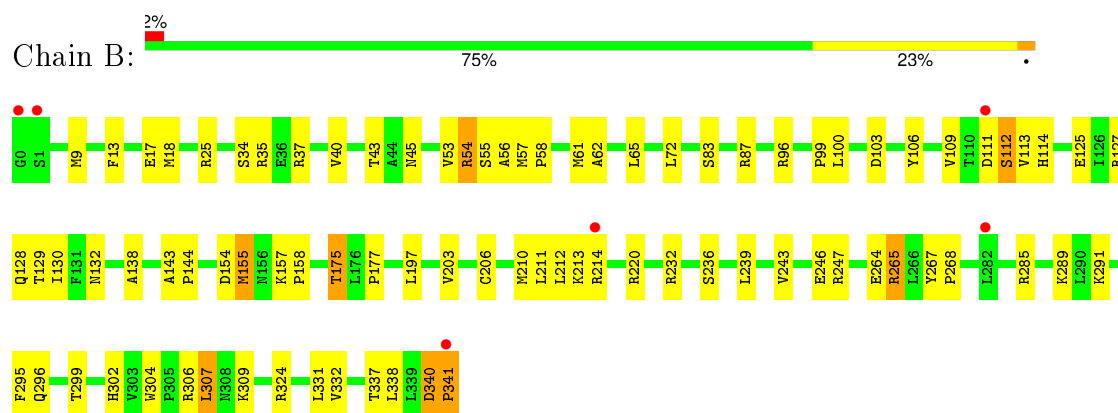
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	18	Total 18	O 18	0	0
6	G	21	Total 21	O 21	0	0
6	A	146	Total 146	O 146	0	0
6	F	24	Total 24	O 24	0	0
6	H	19	Total 19	O 19	0	0

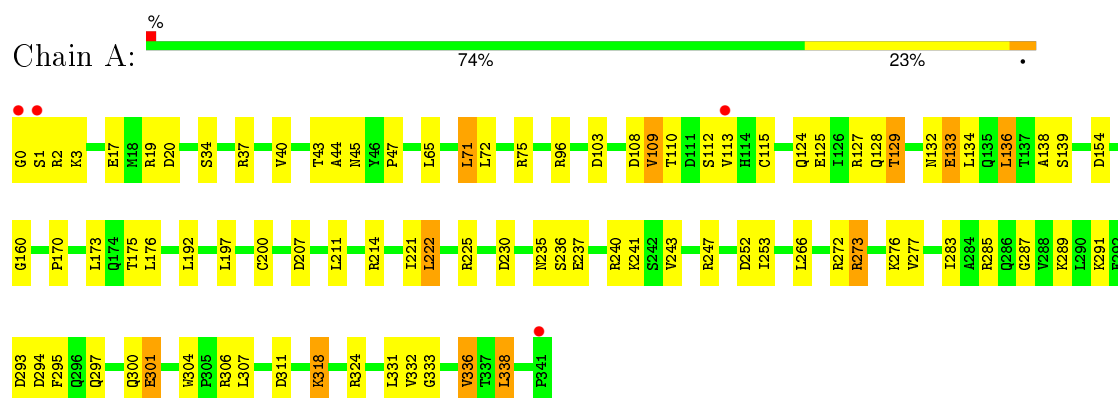
### 3 Residue-property plots

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

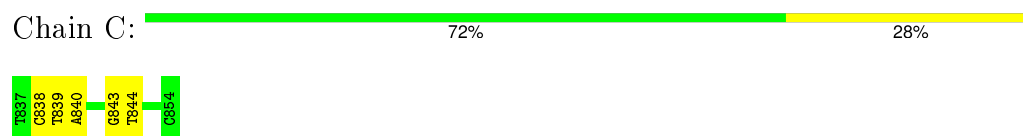
#### • Molecule 1: DNA polymerase IV



#### • Molecule 1: DNA polymerase IV



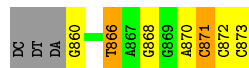
#### • Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*AP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*C)-3')



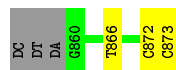
#### • Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*AP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*C)-3')



- Molecule 3: DNA (5'-D(\*CP\*TP\*A\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*(DOC))-3')



- Molecule 3: DNA (5'-D(\*CP\*TP\*A\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*(DOC))-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.65Å 57.08Å 110.23Å 90.00° 94.92° 90.00°	Depositor
Resolution (Å)	35.18 – 2.32 35.16 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.18-2.32) 99.0 (35.16-2.32)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.209 , 0.262 0.207 , 0.262	Depositor DCC
$R_{free}$ test set	2359 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.1	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	0 of 46490 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.84	1/2739 (0.0%)	1.03	9/3699 (0.2%)
1	B	0.80	0/2739	0.92	3/3699 (0.1%)
2	C	0.59	0/407	0.99	1/626 (0.2%)
2	F	0.60	0/407	0.98	1/626 (0.2%)
3	G	0.67	0/297	0.99	2/457 (0.4%)
3	H	0.67	0/297	0.84	0/457
All	All	0.79	1/6886 (0.0%)	0.97	16/9564 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ARG	CD-NE	6.54	1.57	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	NE-CZ-NH2	-8.75	115.92	120.30
2	C	839	DT	O5'-P-OP1	-7.62	98.84	105.70
1	A	230	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	324	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	324	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	311	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	324	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	230	ASP	CB-CG-OD2	-5.83	113.06	118.30
3	G	871	DC	O5'-P-OP1	-5.79	100.49	105.70
2	F	846	DC	O5'-P-OP2	-5.71	100.56	105.70
1	A	109	VAL	CB-CA-C	5.69	122.21	111.40
1	A	71	LEU	CB-CG-CD2	-5.66	101.39	111.00
1	A	273	ARG	CB-CA-C	5.45	121.30	110.40
1	A	129	THR	N-CA-CB	5.33	120.43	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	866	DT	C1'-O4'-C4'	-5.14	104.96	110.10
1	A	222	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2688	0	2745	77	0
1	B	2688	0	2745	64	0
2	C	364	0	204	5	0
2	F	364	0	204	10	0
3	G	283	0	158	9	0
3	H	283	0	158	4	0
4	A	28	0	12	16	0
4	B	28	0	12	10	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	146	0	0	21	0
6	B	96	0	0	5	0
6	C	18	0	0	0	0
6	F	24	0	0	1	0
6	G	21	0	0	3	0
6	H	19	0	0	0	0
All	All	7052	0	6238	165	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 13.

All (165) 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:332:VAL:HA	6:A:632:HOH:O	1.32	1.27
1:B:18:MET:CE	1:B:45:ASN:HD22	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:MET:HE3	1:B:45:ASN:HD22	1.08	1.09
3:G:870:DA:H2''	3:G:871:DC:H5''	1.14	1.09
3:G:870:DA:H2''	3:G:871:DC:C5'	1.84	1.06
1:A:103:ASP:OD2	4:A:401:DCP:H5'2	1.60	1.00
3:G:870:DA:C2'	3:G:871:DC:H5''	1.92	1.00
4:A:401:DCP:HN41	2:F:840:DA:H61	1.09	0.98
1:A:207:ASP:HB3	6:A:635:HOH:O	1.65	0.95
1:B:129:THR:N	6:B:505:HOH:O	1.96	0.95
1:A:235:ASN:O	1:A:236:SER:HB3	1.68	0.92
4:B:401:DCP:HN41	2:C:840:DA:H61	1.14	0.91
1:A:289:LYS:O	6:A:632:HOH:O	1.90	0.90
1:B:103:ASP:CG	4:B:401:DCP:H5'2	1.91	0.90
1:A:103:ASP:OD2	4:A:401:DCP:C5'	2.22	0.87
1:B:18:MET:HE3	1:B:45:ASN:ND2	1.89	0.86
1:B:57:MET:HE3	1:B:62:ALA:HB2	1.63	0.81
1:A:300:GLN:HE22	1:A:318:LYS:NZ	1.80	0.80
1:B:246:GLU:O	1:B:247:ARG:NH1	2.15	0.79
1:A:0:GLY:O	6:A:557:HOH:O	2.01	0.78
1:B:103:ASP:OD2	4:B:401:DCP:H5'2	1.83	0.78
1:B:111:ASP:O	1:B:112:SER:HB2	1.84	0.78
1:A:333:GLY:N	6:A:632:HOH:O	2.14	0.77
1:A:285:ARG:NH1	3:H:866:DT:OP2	2.17	0.77
1:B:35:ARG:HD2	2:C:838:DC:OP1	1.86	0.75
1:B:18:MET:CE	1:B:45:ASN:ND2	2.47	0.75
1:B:53:VAL:HA	1:B:57:MET:CE	2.21	0.71
3:G:860:DG:C5'	6:G:914:HOH:O	2.39	0.70
1:A:129:THR:O	1:A:132:ASN:O	2.10	0.69
1:B:13:PHE:CD2	4:B:401:DCP:H2'2	2.27	0.69
1:B:18:MET:HE1	1:B:45:ASN:HD22	1.58	0.67
3:G:860:DG:H5'	6:G:914:HOH:O	1.95	0.66
1:B:125:GLU:O	1:B:128:GLN:O	2.14	0.66
1:B:34:SER:OG	1:B:37:ARG:HG2	1.95	0.66
1:A:2:ARG:NH2	6:A:609:HOH:O	2.04	0.66
1:A:128:GLN:O	1:A:129:THR:OG1	2.14	0.66
1:B:54:ARG:H	1:B:57:MET:HE2	1.61	0.65
1:B:53:VAL:HA	1:B:57:MET:HE1	1.78	0.65
1:A:43:THR:HG23	4:A:401:DCP:O1B	1.97	0.64
1:A:291:LYS:HB3	1:A:331:LEU:HB3	1.79	0.64
1:A:2:ARG:NH1	6:A:529:HOH:O	2.30	0.64
3:G:868:DG:OP2	6:G:904:HOH:O	2.14	0.64
1:B:154:ASP:OD1	6:B:568:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLY:HA3	1:A:301:GLU:HG2	1.80	0.64
1:B:13:PHE:CE2	4:B:401:DCP:H2'2	2.33	0.63
1:A:127:ARG:HD2	1:A:138:ALA:O	1.97	0.63
1:A:252:ASP:OD1	1:A:293:ASP:HB3	1.99	0.62
1:B:340:ASP:HB3	1:B:341:PRO:HD2	1.82	0.62
1:A:40:VAL:HG13	2:F:840:DA:H5'	1.82	0.62
4:A:401:DCP:H6	4:A:401:DCP:O5'	1.98	0.62
1:A:300:GLN:HE22	1:A:318:LYS:HZ1	1.48	0.62
1:A:235:ASN:O	1:A:236:SER:CB	2.38	0.61
4:B:401:DCP:H6	4:B:401:DCP:O5'	2.00	0.61
1:B:13:PHE:HB2	1:B:43:THR:HG21	1.83	0.61
1:A:207:ASP:CB	6:A:635:HOH:O	2.36	0.60
1:A:332:VAL:CA	6:A:632:HOH:O	2.12	0.60
1:A:240:ARG:NH1	2:F:843:DG:OP1	2.34	0.60
1:A:132:ASN:O	1:A:133:GLU:HB2	2.01	0.60
1:A:170:PRO:HD2	6:A:585:HOH:O	2.01	0.60
1:A:154:ASP:OD1	6:A:508:HOH:O	2.16	0.60
1:B:18:MET:HE2	1:B:25:ARG:HA	1.83	0.59
1:B:103:ASP:OD2	4:B:401:DCP:C5'	2.50	0.59
4:A:401:DCP:H5'1	4:A:401:DCP:PB	2.43	0.59
1:A:175:THR:OG1	6:A:608:HOH:O	2.17	0.59
1:A:173:LEU:O	1:A:200:CYS:HB2	2.03	0.57
1:A:3:LYS:HE2	1:A:110:THR:HA	1.86	0.57
1:A:134:LEU:HB3	1:A:136:LEU:HD22	1.87	0.57
1:B:212:LEU:HD21	1:B:220:ARG:HB2	1.86	0.57
1:A:192:LEU:HD21	1:A:222:LEU:HD21	1.86	0.56
1:A:115:CYS:N	6:A:512:HOH:O	2.07	0.56
1:A:2:ARG:NE	6:A:609:HOH:O	2.33	0.56
4:A:401:DCP:HN41	2:F:840:DA:N6	1.91	0.55
4:A:401:DCP:H5'1	4:A:401:DCP:O2B	2.05	0.55
1:A:103:ASP:OD2	4:A:401:DCP:H5'1	2.07	0.54
1:A:103:ASP:CG	4:A:401:DCP:H5'2	2.26	0.54
1:B:285:ARG:NH1	3:G:866:DT:OP2	2.29	0.54
1:A:276:LYS:NZ	6:A:511:HOH:O	2.29	0.54
1:A:272:ARG:HH12	1:A:273:ARG:HE	1.55	0.53
1:A:2:ARG:CZ	6:A:609:HOH:O	2.52	0.53
3:H:872:DC:H2'	3:H:873:DOC:H6	1.90	0.53
4:B:401:DCP:H5'1	4:B:401:DCP:O2B	2.08	0.53
2:F:850:DG:N7	6:F:905:HOH:O	2.34	0.53
1:A:300:GLN:NE2	1:A:318:LYS:NZ	2.54	0.53
1:B:304:TRP:CD1	1:B:306:ARG:O	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:MET:HE1	1:B:138:ALA:HB2	1.91	0.52
1:A:113:VAL:HG22	1:A:113:VAL:O	2.09	0.52
1:A:43:THR:OG1	4:A:401:DCP:C2'	2.58	0.52
3:G:870:DA:H2''	3:G:871:DC:H5'	1.86	0.51
1:A:300:GLN:NE2	6:A:604:HOH:O	2.43	0.51
1:B:203:VAL:O	1:B:206:CYS:HB2	2.11	0.51
2:C:843:DG:H2''	2:C:844:DT:H5'	1.93	0.51
1:B:53:VAL:HA	1:B:57:MET:HE2	1.92	0.50
1:B:55:SER:O	1:B:56:ALA:HB3	2.11	0.50
1:A:43:THR:HG22	1:A:44:ALA:N	2.27	0.50
1:A:207:ASP:CG	6:A:635:HOH:O	2.49	0.50
1:B:128:GLN:HA	6:B:505:HOH:O	2.11	0.50
1:A:294:ASP:O	1:A:295:PHE:HB2	2.12	0.50
1:B:103:ASP:OD1	4:B:401:DCP:H5'2	2.10	0.49
1:B:57:MET:HE3	1:B:62:ALA:CB	2.38	0.49
1:B:57:MET:HG3	1:B:61:MET:HE3	1.95	0.49
1:B:127:ARG:HD2	1:B:138:ALA:O	2.13	0.48
1:B:9:MET:CE	1:B:130:ILE:HD13	2.44	0.48
1:A:43:THR:OG1	4:A:401:DCP:C3'	2.61	0.48
1:B:13:PHE:HB2	1:B:43:THR:CG2	2.41	0.48
1:A:129:THR:O	1:A:133:GLU:HB2	2.13	0.48
1:B:337:THR:OG1	6:B:581:HOH:O	2.20	0.48
1:A:17:GLU:HG3	1:A:72:LEU:HD23	1.96	0.47
1:B:83:SER:O	1:B:87:ARG:HG3	2.14	0.47
2:F:838:DC:H1'	2:F:839:DT:C6	2.50	0.47
1:A:96:ARG:NH2	6:A:550:HOH:O	2.48	0.47
3:H:872:DC:H2'	3:H:873:DOC:C6	2.45	0.47
1:A:235:ASN:OD1	1:A:237:GLU:N	2.35	0.47
1:B:175:THR:O	1:B:177:PRO:HD3	2.15	0.47
4:A:401:DCP:H3'	4:A:401:DCP:O1B	2.15	0.46
1:B:57:MET:SD	1:B:61:MET:HG2	2.55	0.46
1:A:272:ARG:NH1	1:A:273:ARG:HE	2.13	0.46
1:A:43:THR:HG1	4:A:401:DCP:C3'	2.29	0.46
1:B:267:TYR:OH	1:B:307:LEU:HD13	2.16	0.46
4:A:401:DCP:N3	2:F:840:DA:N1	2.64	0.46
1:B:265:ARG:O	1:B:268:PRO:HD2	2.16	0.45
1:A:283:ILE:HD12	1:A:336:VAL:HG22	1.98	0.45
1:A:34:SER:HA	1:A:71:LEU:CD2	2.46	0.45
1:A:272:ARG:NH2	6:A:622:HOH:O	2.50	0.45
1:A:295:PHE:CE2	2:F:839:DT:C5	3.05	0.45
1:B:9:MET:HE3	1:B:130:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HB3	6:B:595:HOH:O	2.17	0.44
1:A:132:ASN:O	1:A:133:GLU:CB	2.63	0.44
1:B:17:GLU:HG3	1:B:72:LEU:HD23	1.99	0.44
1:B:264:GLU:OE1	1:B:309:LYS:NZ	2.45	0.44
1:A:221:ILE:O	1:A:225:ARG:HG2	2.18	0.44
1:A:37:ARG:HB3	1:A:37:ARG:HH11	1.82	0.44
1:A:20:ASP:OD2	1:A:75:ARG:NH2	2.41	0.44
1:B:340:ASP:CB	1:B:341:PRO:HD2	2.43	0.44
1:A:139:SER:HA	1:A:160:GLY:O	2.18	0.44
1:B:157:LYS:HB3	1:B:157:LYS:HE2	1.81	0.43
1:A:295:PHE:CE2	2:F:839:DT:C4	3.06	0.43
1:B:18:MET:HE2	1:B:25:ARG:O	2.19	0.43
1:A:45:ASN:CG	1:A:47:PRO:HD2	2.38	0.43
1:B:40:VAL:HG13	2:C:840:DA:H5'	2.00	0.43
1:B:58:PRO:HD2	1:B:61:MET:HE2	2.01	0.43
1:B:100:LEU:HD11	1:B:106:TYR:CE1	2.53	0.43
1:B:129:THR:O	1:B:132:ASN:O	2.36	0.43
1:B:103:ASP:CG	4:B:401:DCP:C5'	2.78	0.43
1:B:40:VAL:HG21	2:C:840:DA:C5	2.54	0.43
1:A:124:GLN:OE1	1:A:127:ARG:NH2	2.51	0.43
3:G:872:DC:H2''	3:G:873:DOC:H5''	2.01	0.43
1:A:318:LYS:HE2	1:A:318:LYS:HB3	1.53	0.42
1:B:157:LYS:HB2	1:B:158:PRO:HA	2.00	0.42
1:B:291:LYS:HB3	1:B:331:LEU:HB3	2.00	0.42
4:A:401:DCP:C6	3:H:873:DOC:H2'	2.49	0.42
1:A:40:VAL:HG21	2:F:840:DA:C5	2.54	0.42
1:A:125:GLU:O	1:A:128:GLN:O	2.38	0.42
1:A:19:ARG:NH1	6:A:589:HOH:O	2.31	0.42
1:B:18:MET:HE1	1:B:45:ASN:ND2	2.27	0.42
1:A:241:LYS:O	1:A:338:LEU:HB2	2.19	0.42
1:B:143:ALA:HB1	1:B:144:PRO:CD	2.50	0.42
1:B:155:MET:HB2	1:B:155:MET:HE3	1.48	0.42
1:B:87:ARG:CZ	1:B:99:PRO:HB3	2.51	0.41
1:A:108:ASP:C	1:A:108:ASP:OD1	2.59	0.41
1:B:289:LYS:HB2	1:B:299:THR:HG22	2.03	0.41
1:A:37:ARG:NH1	1:A:37:ARG:HB3	2.36	0.41
1:A:289:LYS:HD2	1:A:297:GLN:OE1	2.21	0.40
1:A:300:GLN:NE2	1:A:318:LYS:HZ3	2.18	0.40
1:A:34:SER:HA	1:A:71:LEU:HD21	2.03	0.40
1:A:304:TRP:NE1	1:A:306:ARG:O	2.55	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	340/342 (99%)	323 (95%)	16 (5%)	1 (0%)	46	56
1	B	340/342 (99%)	326 (96%)	13 (4%)	1 (0%)	46	56
All	All	680/684 (99%)	649 (95%)	29 (4%)	2 (0%)	46	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	SER
1	A	133	GLU

### 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	286/286 (100%)	267 (93%)	19 (7%)	21	26
1	B	286/286 (100%)	262 (92%)	24 (8%)	14	16
All	All	572/572 (100%)	529 (92%)	43 (8%)	17	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	ARG
1	B	65	LEU
1	B	109	VAL
1	B	113	VAL

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Mol	Chain	Res	Type
1	B	114	HIS
1	B	155	MET
1	B	175	THR
1	B	197	LEU
1	B	210	MET
1	B	211	LEU
1	B	213	LYS
1	B	214	ARG
1	B	236	SER
1	B	239	LEU
1	B	243	VAL
1	B	265	ARG
1	B	295	PHE
1	B	296	GLN
1	B	302	HIS
1	B	307	LEU
1	B	332	VAL
1	B	338	LEU
1	B	340	ASP
1	B	341	PRO
1	A	1	SER
1	A	65	LEU
1	A	109	VAL
1	A	112	SER
1	A	136	LEU
1	A	176	LEU
1	A	197	LEU
1	A	211	LEU
1	A	214	ARG
1	A	243	VAL
1	A	247	ARG
1	A	253	ILE
1	A	266	LEU
1	A	277	VAL
1	A	301	GLU
1	A	307	LEU
1	A	318	LYS
1	A	336	VAL
1	A	338	LEU

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

Mol	Chain	Res	Type
1	B	45	ASN
1	B	116	HIS
1	A	300	GLN

### 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	$\# Z  > 2$
3	DOC	G	873	3,2	11,19,20	0.76	0	14,26,29	1.32	2 (14%)
3	DOC	H	873	3,2	11,19,20	0.82	0	14,26,29	1.04	1 (7%)

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	DOC	G	873	3,2	-	0/3/18/19	0/2/2/2
3	DOC	H	873	3,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	873	DOC	C3'-C2'-C1'	2.30	105.28	102.71
3	H	873	DOC	C2-N3-C4	3.03	119.89	115.61
3	G	873	DOC	C2-N3-C4	3.07	119.95	115.61

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
3	G	873	DOC	1	0
3	H	873	DOC	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	DCP	A	401	5	21,29,29	0.94	1 (4%)	33,45,45	1.89	11 (33%)
4	DCP	B	401	5	21,29,29	0.49	0	33,45,45	1.58	6 (18%)

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	DCP	A	401	5	-	0/18/34/34	0/2/2/2
4	DCP	B	401	5	-	0/18/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	DCP	O3'-C3'	2.38	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	DCP	C5-C4-N4	-3.42	116.07	121.31
4	B	401	DCP	C2'-C1'-N1	-2.40	108.32	114.16
4	A	401	DCP	C6-N1-C2	-2.09	117.89	121.28
4	B	401	DCP	C3'-C2'-C1'	2.04	107.29	102.40
4	B	401	DCP	O2B-PB-O3A	2.23	115.20	105.09
4	A	401	DCP	O3G-PG-O1G	2.24	117.78	110.58
4	A	401	DCP	O4'-C4'-C3'	2.37	111.62	105.67
4	B	401	DCP	N4-C4-N3	2.46	120.98	116.50
4	A	401	DCP	O2B-PB-O3A	2.67	117.22	105.09
4	A	401	DCP	C2-N3-C4	2.74	119.48	115.61
4	A	401	DCP	C3'-C2'-C1'	2.92	109.41	102.40
4	A	401	DCP	O5'-C5'-C4'	3.12	120.61	109.12
4	A	401	DCP	N4-C4-N3	3.17	122.28	116.50
4	A	401	DCP	O3'-C3'-C2'	3.24	121.48	110.74
4	B	401	DCP	C2-N3-C4	3.83	121.02	115.61
4	B	401	DCP	O4'-C1'-N1	4.63	115.73	107.72
4	A	401	DCP	O4'-C1'-N1	4.71	115.86	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	DCP	16	0
4	B	401	DCP	10	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	342/342 (100%)	-0.17	4 (1%) 81 85	17, 31, 55, 86	0
1	B	342/342 (100%)	-0.24	6 (1%) 71 78	18, 34, 54, 86	0
2	C	18/18 (100%)	-0.44	0 100 100	24, 40, 70, 79	0
2	F	18/18 (100%)	-0.30	1 (5%) 28 36	18, 32, 79, 87	0
3	G	13/17 (76%)	-0.61	0 100 100	27, 33, 44, 44	0
3	H	13/17 (76%)	-0.26	0 100 100	21, 27, 65, 78	0
All	All	746/754 (98%)	-0.22	11 (1%) 76 82	17, 33, 57, 87	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	GLY	6.4
1	B	341	PRO	4.8
1	A	113	VAL	3.8
2	F	837	DT	3.0
1	A	0	GLY	2.9
1	A	341	PRO	2.8
1	B	282	LEU	2.8
1	B	1	SER	2.7
1	A	1	SER	2.4
1	B	214	ARG	2.4
1	B	111	ASP	2.3

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

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	DOC	G	873	18/19	0.97	0.11	-	29,37,42,43	0
3	DOC	H	873	18/19	0.98	0.12	-	21,23,25,26	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
4	DCP	B	401	28/28	0.79	0.27	5.53	38,68,82,83	0
4	DCP	A	401	28/28	0.78	0.25	3.99	32,54,71,74	0
5	MG	A	402	1/1	0.82	0.21	2.51	73,73,73,73	0
5	MG	B	402	1/1	0.82	0.08	-	46,46,46,46	0

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

There are no such residues in this entry.