



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1N3E  
Title : Crystal structure of I-CreI bound to a palindromic DNA sequence I (palindrome of left side of wildtype DNA target sequence)  
Authors : Chevalier, B.; Turmel, M.; Lemieux, C.; Monnat, R.J.; Stoddard, B.L.  
Deposited on : 2002-10-28  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

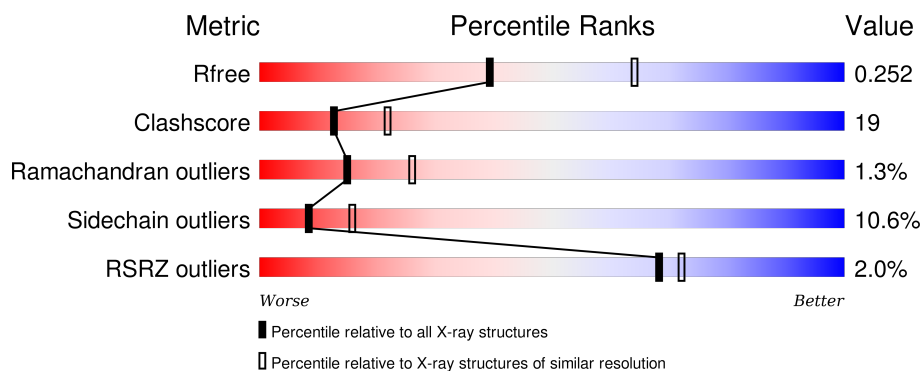
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	14	
1	E	14	
1	I	14	
1	K	14	
2	D	10	

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Mol	Chain	Length	Quality of chain
2	F	10	
2	J	10	
2	L	10	
3	A	163	
3	B	163	
3	G	163	
3	H	163	

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
5	NA	A	495	-	-	-	X
5	NA	G	995	-	-	-	X
5	NA	H	994	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7098 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 DNA chain called 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*CP\*GP\*T  
P\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	E	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	I	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	K	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	F	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	J	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	L	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			

- Molecule 3 is a protein called DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	B	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	G	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	H	151	Total	C	N	O	S	0	0	0
			1226	791	208	226	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	THR	ALA	SEE REMARK 999	UNP P05725
A	110	GLU	TRP	SEE REMARK 999	UNP P05725
A	111	GLN	ARG	SEE REMARK 999	UNP P05725
B	242	THR	ALA	SEE REMARK 999	UNP P05725
B	310	GLU	TRP	SEE REMARK 999	UNP P05725
B	311	GLN	ARG	SEE REMARK 999	UNP P05725
G	542	THR	ALA	SEE REMARK 999	UNP P05725
G	610	GLU	TRP	SEE REMARK 999	UNP P05725
G	611	GLN	ARG	SEE REMARK 999	UNP P05725
H	742	THR	ALA	SEE REMARK 999	UNP P05725
H	810	GLU	TRP	SEE REMARK 999	UNP P05725
H	811	GLN	ARG	SEE REMARK 999	UNP P05725

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total 42	O 42	0	0
6	B	38	Total 38	O 38	0	0
6	C	18	Total 18	O 18	0	0
6	D	9	Total 9	O 9	0	0
6	E	10	Total 10	O 10	0	0
6	F	13	Total 13	O 13	0	0
6	G	41	Total 41	O 41	0	0
6	H	30	Total 30	O 30	0	0
6	I	4	Total 4	O 4	0	0
6	J	9	Total 9	O 9	0	0
6	K	14	Total 14	O 14	0	0
6	L	5	Total 5	O 5	0	0

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

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

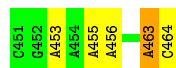
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*CP\*GP\*TP\*AP\*C)-3'

Chain C: 



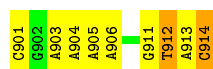
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*CP\*GP\*TP\*AP\*C)-3'

Chain E: 



- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*CP\*GP\*TP\*AP\*C)-3'

Chain I: 

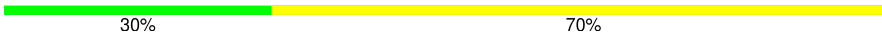


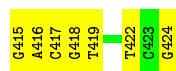
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*TP\*CP\*GP\*TP\*AP\*C)-3'

Chain K: 



- Molecule 2: 5'-D(P\*GP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'

Chain D: 



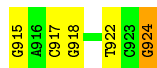
- Molecule 2: 5'-D(P\*GP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'

Chain F: 



- Molecule 2: 5'-D(P\*GP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'

Chain J: 50% 40% 10%



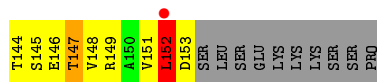
- Molecule 2: 5'-D(P\*GP\*AP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'

Chain L: 50% 40% 10%



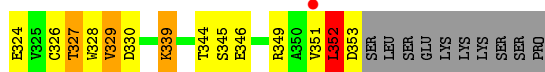
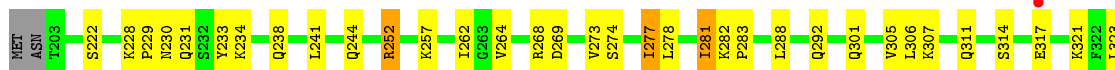
- Molecule 3: DNA endonuclease I-CreI

Chain A: 2% 67% 20% 5% 7%



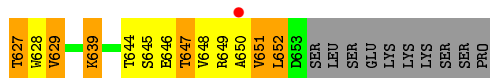
- Molecule 3: DNA endonuclease I-CreI

Chain B: 63% 25% 7%

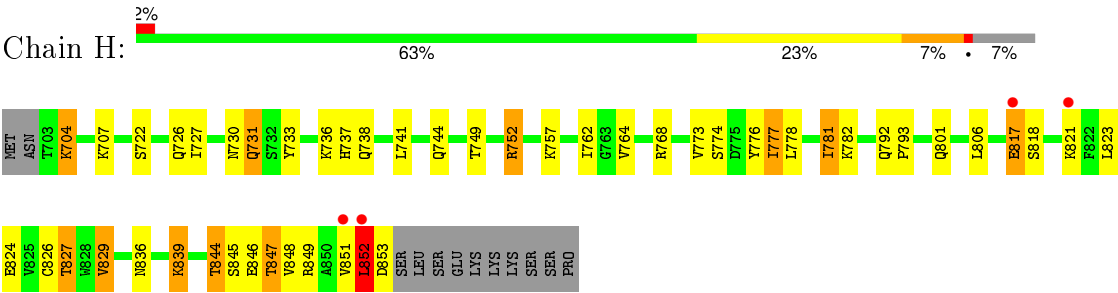


- Molecule 3: DNA endonuclease I-CreI

Chain G: 2% 63% 25% 5% 7%



- Molecule 3: DNA endonuclease I-CreI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.73 Å 68.44 Å 301.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 2.50 46.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.18-2.50) 93.5 (46.18-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.219 , 0.245 0.228 , 0.252	Depositor DCC
$R_{free}$ test set	1598 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.3	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	1 of 32395 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA

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	C	0.50	0/319	0.88	0/490
1	E	0.43	0/319	0.83	0/490
1	I	0.54	0/319	0.95	1/490 (0.2%)
1	K	0.46	0/319	0.86	0/490
2	D	0.72	1/229 (0.4%)	0.96	0/350
2	F	0.78	1/229 (0.4%)	1.00	1/350 (0.3%)
2	J	0.88	1/229 (0.4%)	1.19	1/350 (0.3%)
2	L	0.74	1/229 (0.4%)	0.92	0/350
3	A	0.46	0/1246	0.79	0/1682
3	B	0.47	0/1246	0.81	0/1682
3	G	0.48	0/1246	0.83	0/1682
3	H	0.46	0/1249	0.78	0/1686
All	All	0.52	4/7179 (0.1%)	0.85	3/10092 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	I	0	2
1	K	0	2
2	L	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	915	DG	OP3-P	-8.21	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	415	DG	OP3-P	-7.63	1.51	1.61
2	L	965	DG	OP3-P	-7.47	1.52	1.61
2	F	465	DG	OP3-P	-6.90	1.52	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	924	DG	C5'-C4'-C3'	-8.02	99.66	114.10
2	F	465	DG	OP1-P-OP2	-5.84	110.83	119.60
1	I	912	DT	O4'-C4'-C3'	-5.77	102.19	104.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	410	DC	Sidechain
1	C	413	DA	Sidechain
1	E	463	DA	Sidechain
1	I	903	DA	Sidechain
1	I	914	DC	Sidechain
1	K	963	DA	Sidechain
1	K	964	DC	Sidechain
2	L	968	DG	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	C	284	0	157	4	2
1	E	284	0	157	4	0
1	I	284	0	157	12	0
1	K	284	0	157	5	0
2	D	206	0	115	10	0
2	F	206	0	115	5	0
2	J	206	0	115	6	0
2	L	206	0	115	8	0
3	A	1223	0	1257	55	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1223	0	1257	39	0
3	G	1223	0	1257	58	0
3	H	1226	0	1259	51	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	42	0	0	4	0
6	B	38	0	0	0	0
6	C	18	0	0	0	1
6	D	9	0	0	0	0
6	E	10	0	0	3	0
6	F	13	0	0	1	0
6	G	41	0	0	2	1
6	H	30	0	0	1	3
6	I	4	0	0	1	0
6	J	9	0	0	0	0
6	K	14	0	0	1	0
6	L	5	0	0	2	0
All	All	7098	0	6118	250	4

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 19.

All (250) 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)
2:D:424:DG:C8	2:J:924:DG:H2''	1.88	1.08
2:D:424:DG:N7	2:J:924:DG:H2''	1.74	1.03
3:G:505:TYR:OH	3:G:562:ILE:HG23	1.59	1.03
1:I:905:DA:H2''	1:I:906:DA:H5'	1.47	0.96
3:G:644:THR:H	3:G:647:THR:CG2	1.80	0.95
3:G:644:THR:HG22	3:G:646:GLU:H	1.32	0.90
3:A:144:THR:H	3:A:147:THR:CG2	1.83	0.89
3:A:144:THR:HG22	3:A:146:GLU:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:644:THR:HG22	3:G:646:GLU:N	1.90	0.86
3:H:844:THR:H	3:H:847:THR:CG2	1.90	0.84
3:B:344:THR:HG22	3:B:346:GLU:H	1.39	0.84
1:E:455:DA:H2''	1:E:456:DA:H5'	1.59	0.84
3:A:118:SER:H	3:A:121:LYS:HE3	1.43	0.84
3:G:623:LEU:CD1	3:G:649:ARG:HG3	2.08	0.83
1:I:912:DT:H6	1:I:912:DT:H5'	1.43	0.82
3:H:844:THR:HG22	3:H:846:GLU:H	1.40	0.82
3:G:649:ARG:O	3:G:652:LEU:HD23	1.80	0.82
3:A:118:SER:OG	3:A:121:LYS:HG3	1.80	0.81
3:A:144:THR:HG22	3:A:146:GLU:N	1.96	0.81
3:H:844:THR:HG22	3:H:846:GLU:N	1.95	0.80
3:G:618:SER:H	3:G:621:LYS:HE3	1.48	0.79
3:H:818:SER:H	3:H:821:LYS:HE3	1.48	0.79
1:K:955:DA:H2''	1:K:956:DA:H5'	1.64	0.79
3:B:344:THR:HG22	3:B:346:GLU:N	1.97	0.78
3:B:311:GLN:HE21	3:B:321:LYS:CE	1.98	0.77
1:C:405:DA:H2''	1:C:406:DA:H5'	1.66	0.77
3:G:644:THR:H	3:G:647:THR:HG21	1.49	0.76
1:I:911:DG:H2''	1:I:912:DT:H5''	1.68	0.76
6:E:1200:HOH:O	3:A:33:TYR:HD2	1.68	0.75
3:A:149:ARG:C	3:A:151:VAL:H	1.91	0.74
3:G:530:ASN:HD22	3:G:533:TYR:HE1	1.33	0.74
3:G:505:TYR:HE2	3:G:562:ILE:HA	1.53	0.73
3:H:844:THR:CG2	3:H:846:GLU:H	2.02	0.72
3:A:144:THR:H	3:A:147:THR:HG21	1.52	0.72
3:G:623:LEU:HD11	3:G:649:ARG:HG3	1.71	0.72
3:G:644:THR:CG2	3:G:646:GLU:H	2.03	0.71
3:H:730:ASN:HD22	3:H:733:TYR:HE1	1.36	0.71
3:H:824:GLU:O	3:H:827:THR:HB	1.91	0.70
3:B:344:THR:CG2	3:B:346:GLU:H	2.06	0.69
1:I:912:DT:C5'	1:I:912:DT:H6	2.05	0.68
3:G:624:GLU:O	3:G:627:THR:HB	1.93	0.68
3:A:144:THR:CG2	3:A:146:GLU:H	2.07	0.68
3:G:505:TYR:CE2	3:G:562:ILE:HA	2.28	0.67
3:H:844:THR:H	3:H:847:THR:HG21	1.58	0.66
3:G:644:THR:H	3:G:647:THR:HG23	1.57	0.66
1:I:912:DT:C6	1:I:912:DT:H5'	2.27	0.65
3:G:618:SER:OG	3:G:621:LYS:HG3	1.96	0.65
2:D:424:DG:C8	2:J:924:DG:C2'	2.75	0.65
3:B:262:ILE:HG22	3:B:264:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:GLN:HE21	3:B:321:LYS:HE2	1.62	0.65
3:A:52:ARG:NH1	3:A:69:ASP:OD2	2.29	0.65
3:H:844:THR:H	3:H:847:THR:HG23	1.62	0.65
3:B:311:GLN:NE2	3:B:321:LYS:NZ	2.45	0.65
3:H:851:VAL:O	3:H:853:ASP:N	2.30	0.64
3:G:651:VAL:CG1	3:G:651:VAL:O	2.46	0.64
3:B:241:LEU:HD12	3:B:281:ILE:HD11	1.80	0.63
3:G:623:LEU:HD11	3:G:649:ARG:CG	2.28	0.62
3:A:124:GLU:O	3:A:127:THR:HB	1.98	0.62
3:A:144:THR:H	3:A:147:THR:HG23	1.62	0.62
3:G:652:LEU:HG	3:G:652:LEU:O	2.00	0.61
3:G:652:LEU:CG	3:G:652:LEU:O	2.49	0.61
3:B:352:LEU:O	3:B:353:ASP:O	2.19	0.61
3:H:730:ASN:HB3	3:H:733:TYR:CD1	2.35	0.61
3:G:575:ASP:HB2	3:G:577:ILE:CD1	2.31	0.61
3:A:144:THR:O	3:A:147:THR:HG23	2.00	0.60
6:E:1200:HOH:O	3:A:33:TYR:CD2	2.47	0.60
3:G:505:TYR:OH	3:G:562:ILE:CG2	2.44	0.60
3:G:652:LEU:O	3:G:652:LEU:HD12	2.02	0.60
3:G:644:THR:N	3:G:647:THR:HG23	2.17	0.60
2:D:416:DA:N7	3:A:44:GLN:NE2	2.50	0.60
3:A:151:VAL:O	3:A:153:ASP:N	2.34	0.60
1:I:912:DT:C5'	1:I:912:DT:C6	2.85	0.59
3:H:762:ILE:HG22	3:H:764:VAL:HG12	1.83	0.59
3:A:30:ASN:HB3	3:A:33:TYR:CD1	2.38	0.59
2:F:466:DA:N7	3:B:244:GLN:NE2	2.50	0.59
6:E:1044:HOH:O	3:A:38:GLN:HG3	2.02	0.59
3:B:230:ASN:HB3	3:B:233:TYR:CD1	2.37	0.59
3:H:818:SER:OG	3:H:821:LYS:HG3	2.03	0.58
3:G:651:VAL:O	3:G:651:VAL:HG13	2.03	0.58
1:K:955:DA:C2'	1:K:956:DA:H5'	2.35	0.57
3:A:141:ARG:HD3	6:A:1171:HOH:O	2.05	0.57
1:I:901:DC:H6	1:I:901:DC:HO5'	1.51	0.57
3:A:152:LEU:O	3:A:153:ASP:O	2.23	0.56
3:A:149:ARG:C	3:A:151:VAL:N	2.58	0.56
3:A:118:SER:N	3:A:121:LYS:HE3	2.18	0.56
3:H:776:TYR:O	3:H:777:ILE:HD12	2.06	0.56
3:G:626:CYS:HA	3:G:629:VAL:HG13	1.89	0.55
2:F:467:DC:H2'	2:F:468:DG:H8	1.72	0.55
3:G:562:ILE:HG22	3:G:564:VAL:HG12	1.87	0.55
1:I:911:DG:C2'	1:I:912:DT:H5''	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:324:GLU:O	3:B:327:THR:HB	2.07	0.55
3:A:123:LEU:CD1	3:A:149:ARG:HG3	2.37	0.55
1:I:912:DT:H2'	1:I:913:DA:C8	2.42	0.54
3:B:351:VAL:O	3:B:353:ASP:N	2.41	0.54
3:G:644:THR:N	3:G:647:THR:CG2	2.61	0.54
3:A:144:THR:N	3:A:147:THR:CG2	2.65	0.54
3:G:644:THR:CG2	3:G:645:SER:N	2.70	0.54
3:H:826:CYS:HA	3:H:829:VAL:HG13	1.88	0.54
3:G:644:THR:O	3:G:647:THR:HG23	2.08	0.54
3:H:704:LYS:HG3	3:H:704:LYS:O	2.06	0.54
3:H:844:THR:CG2	3:H:845:SER:N	2.70	0.54
3:B:311:GLN:NE2	3:B:321:LYS:HZ1	2.04	0.54
3:H:817:GLU:HB2	3:H:821:LYS:NZ	2.23	0.53
3:A:31:GLN:H	3:A:31:GLN:NE2	2.06	0.53
1:E:455:DA:C2'	1:E:456:DA:H5'	2.36	0.53
3:A:62:ILE:HG22	3:A:64:VAL:HG12	1.90	0.53
2:L:967:DC:H2'	2:L:968:DG:H8	1.74	0.53
3:A:148:VAL:O	3:A:151:VAL:HB	2.09	0.53
3:H:844:THR:N	3:H:847:THR:HG23	2.23	0.53
3:A:40:SER:HB3	6:A:1222:HOH:O	2.08	0.53
3:A:81:ILE:HG22	3:A:82:LYS:N	2.23	0.52
3:B:252:ARG:NH1	3:B:269:ASP:OD2	2.43	0.52
2:L:967:DC:H2'	2:L:968:DG:C8	2.45	0.52
3:H:741:LEU:HD12	3:H:781:ILE:HD11	1.92	0.52
3:B:314:SER:OG	3:B:321:LYS:NZ	2.43	0.52
6:K:1013:HOH:O	3:G:538:GLN:HG3	2.09	0.52
3:B:323:LEU:HD21	3:B:349:ARG:CD	2.39	0.52
3:G:644:THR:HB	3:G:647:THR:HG22	1.92	0.51
3:G:652:LEU:CD1	3:G:652:LEU:O	2.58	0.51
3:A:117:GLU:HB2	3:A:121:LYS:HZ2	1.74	0.51
3:G:650:ALA:C	3:G:652:LEU:H	2.13	0.51
3:B:349:ARG:O	3:B:352:LEU:HD22	2.10	0.51
3:A:26:GLN:HG3	6:A:1222:HOH:O	2.09	0.51
3:H:737:HIS:CE1	3:H:848:VAL:HG22	2.46	0.51
1:I:905:DA:C2'	1:I:906:DA:H5'	2.31	0.51
3:H:781:ILE:HG22	3:H:782:LYS:N	2.24	0.51
3:H:727:ILE:HG21	3:H:848:VAL:HG21	1.92	0.51
3:A:144:THR:N	3:A:147:THR:HG23	2.24	0.51
3:H:722:SER:HB3	3:H:744:GLN:HG2	1.92	0.51
3:G:530:ASN:HB3	3:G:533:TYR:CD1	2.47	0.50
3:A:144:THR:HB	3:A:147:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:966:DA:N7	3:H:744:GLN:NE2	2.59	0.50
3:A:151:VAL:O	3:A:152:LEU:C	2.49	0.50
2:D:417:DC:H4'	2:D:417:DC:OP1	2.12	0.50
3:A:31:GLN:H	3:A:31:GLN:HE21	1.59	0.50
3:H:849:ARG:C	3:H:851:VAL:H	2.15	0.49
3:H:730:ASN:HB3	3:H:733:TYR:HD1	1.77	0.49
1:C:405:DA:C2'	1:C:406:DA:H5'	2.37	0.49
1:C:401:DC:H2''	1:C:402:DG:O5'	2.12	0.49
3:B:311:GLN:HG3	3:B:321:LYS:HZ3	1.77	0.49
2:D:417:DC:H2'	2:D:418:DG:C8	2.48	0.49
3:H:818:SER:N	3:H:821:LYS:HE3	2.24	0.49
3:B:230:ASN:HB3	3:B:233:TYR:CE1	2.48	0.49
2:L:967:DC:H2''	2:L:968:DG:H5'	1.95	0.49
3:A:41:LEU:HD12	3:A:81:ILE:HD11	1.95	0.49
3:A:144:THR:CG2	3:A:145:SER:N	2.75	0.49
3:A:40:SER:CB	6:A:1222:HOH:O	2.61	0.48
3:B:344:THR:CG2	3:B:345:SER:N	2.76	0.48
1:K:951:DC:H2''	1:K:952:DG:O5'	2.12	0.48
3:B:233:TYR:CE2	3:B:238:GLN:HB2	2.49	0.48
3:H:817:GLU:HB2	3:H:821:LYS:HZ2	1.77	0.48
3:A:30:ASN:HB3	3:A:33:TYR:CE1	2.48	0.48
1:K:963:DA:H1'	1:K:964:DC:O4'	2.13	0.48
2:F:465:DG:OP2	6:F:1229:HOH:O	2.18	0.48
3:G:530:ASN:ND2	3:G:533:TYR:CE1	2.81	0.48
3:G:552:ARG:NH1	3:G:569:ASP:OD2	2.46	0.48
2:F:467:DC:H2'	2:F:468:DG:C8	2.49	0.48
2:L:967:DC:H1'	6:L:1201:HOH:O	2.13	0.47
3:G:508:GLU:HG3	6:G:1217:HOH:O	2.14	0.47
2:D:417:DC:H2'	2:D:418:DG:H8	1.78	0.47
3:A:117:GLU:HB2	3:A:121:LYS:NZ	2.30	0.47
6:G:1155:HOH:O	3:H:707:LYS:HE2	2.15	0.47
2:L:967:DC:H2''	6:L:1201:HOH:O	2.15	0.47
3:G:541:LEU:HD12	3:G:581:ILE:HD11	1.97	0.47
3:H:823:LEU:CD1	3:H:849:ARG:HG3	2.45	0.47
3:G:537:HIS:CE1	3:G:648:VAL:HG22	2.50	0.47
3:H:733:TYR:CE2	3:H:738:GLN:HB2	2.49	0.47
3:B:230:ASN:HB3	3:B:233:TYR:HD1	1.80	0.46
3:A:27:ILE:HG21	3:A:148:VAL:HG21	1.98	0.46
1:I:904:DA:H5'	6:I:1213:HOH:O	2.13	0.46
3:H:844:THR:HB	3:H:847:THR:CG2	2.45	0.46
3:G:588:LEU:O	3:G:592:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:537:HIS:ND1	3:G:648:VAL:HG22	2.31	0.46
3:B:282:LYS:HB3	3:B:283:PRO:CD	2.45	0.46
3:B:326:CYS:HA	3:B:329:VAL:HG13	1.97	0.46
3:B:323:LEU:HD21	3:B:349:ARG:HG3	1.97	0.46
3:A:31:GLN:N	3:A:31:GLN:NE2	2.64	0.46
3:A:139:LYS:HE2	3:A:139:LYS:HB2	1.67	0.46
3:G:618:SER:HG	3:G:621:LYS:HG3	1.81	0.46
2:D:422:DT:H5'	2:D:422:DT:H6	1.80	0.46
3:H:730:ASN:HB3	3:H:733:TYR:CE1	2.52	0.45
3:A:30:ASN:HB3	3:A:33:TYR:HD1	1.80	0.45
3:G:528:LYS:O	3:G:538:GLN:N	2.42	0.45
3:B:244:GLN:HB2	3:B:277:ILE:CD1	2.46	0.45
3:B:307:LYS:HE2	3:B:328:TRP:CH2	2.52	0.45
3:G:623:LEU:HD11	3:G:649:ARG:CD	2.46	0.45
3:H:844:THR:HB	3:H:847:THR:HG22	1.99	0.45
3:G:527:ILE:HG21	3:G:648:VAL:HG21	1.99	0.45
2:J:917:DC:H2'	2:J:918:DG:C8	2.51	0.45
3:A:27:ILE:HG21	3:A:148:VAL:CG2	2.46	0.44
3:B:323:LEU:CD2	3:B:349:ARG:HG3	2.48	0.44
3:B:307:LYS:HE2	3:B:328:TRP:CZ2	2.52	0.44
3:B:288:LEU:O	3:B:292:GLN:HB2	2.17	0.44
3:H:839:LYS:HB2	3:H:839:LYS:HE2	1.66	0.44
2:J:917:DC:H2'	2:J:918:DG:H8	1.82	0.44
3:H:792:GLN:HB3	3:H:793:PRO:HD3	1.98	0.44
3:A:22:SER:HB3	3:A:44:GLN:HG2	1.98	0.44
3:G:552:ARG:NH1	3:G:569:ASP:OD1	2.51	0.44
2:D:422:DT:H5'	2:D:422:DT:C6	2.53	0.44
3:G:644:THR:HB	3:G:647:THR:CG2	2.48	0.44
3:H:730:ASN:ND2	3:H:733:TYR:CE1	2.85	0.44
3:B:339:LYS:HE2	3:B:339:LYS:HB2	1.76	0.44
3:B:241:LEU:HD22	3:B:305:VAL:HG13	2.00	0.43
3:B:351:VAL:O	3:B:352:LEU:C	2.57	0.43
3:G:528:LYS:HA	3:G:529:PRO:HD2	1.88	0.43
3:H:836:ASN:O	6:H:1204:HOH:O	2.21	0.43
3:B:273:VAL:CG1	3:B:274:SER:N	2.82	0.43
3:G:639:LYS:HB2	3:G:639:LYS:HE2	1.61	0.43
3:A:126:CYS:HA	3:A:129:VAL:HG13	2.01	0.43
3:H:817:GLU:CB	3:H:821:LYS:NZ	2.82	0.43
3:A:52:ARG:NH1	3:A:69:ASP:CG	2.73	0.43
3:G:533:TYR:CZ	3:G:538:GLN:HB2	2.54	0.42
3:G:530:ASN:ND2	3:G:533:TYR:HE1	2.09	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:81:ILE:CG2	3:A:82:LYS:N	2.82	0.42
3:H:749:THR:O	3:H:752:ARG:HB3	2.19	0.42
3:H:737:HIS:ND1	3:H:848:VAL:HG22	2.34	0.42
2:L:972:DT:H5'	2:L:972:DT:H6	1.83	0.42
3:A:123:LEU:HD11	3:A:149:ARG:CD	2.50	0.42
3:B:228:LYS:HA	3:B:229:PRO:HD2	1.86	0.42
3:G:504:LYS:HA	3:G:590:GLN:HE22	1.85	0.42
1:C:413:DA:H1'	1:C:414:DC:O4'	2.19	0.42
3:G:527:ILE:HG21	3:G:648:VAL:CG2	2.50	0.42
3:G:592:GLN:HB3	3:G:593:PRO:HD3	2.01	0.42
3:H:849:ARG:O	3:H:852:LEU:HD22	2.20	0.42
3:A:144:THR:HB	3:A:147:THR:CG2	2.49	0.42
3:A:146:GLU:OE2	3:A:149:ARG:NH2	2.54	0.41
3:H:823:LEU:HD11	3:H:849:ARG:HD3	2.03	0.41
1:K:962:DT:H2''	1:K:963:DA:C8	2.55	0.41
3:H:844:THR:HG23	3:H:845:SER:N	2.34	0.41
3:A:52:ARG:NH1	3:A:69:ASP:OD1	2.54	0.41
3:H:852:LEU:O	3:H:853:ASP:O	2.39	0.41
3:B:222:SER:HB3	3:B:244:GLN:HG2	2.02	0.41
3:A:82:LYS:HB3	3:A:83:PRO:CD	2.51	0.41
3:G:581:ILE:HG22	3:G:582:LYS:N	2.35	0.41
1:I:913:DA:H1'	1:I:914:DC:O4'	2.20	0.41
3:G:530:ASN:HB3	3:G:533:TYR:CE1	2.55	0.41
3:H:731:GLN:HA	3:H:736:LYS:HD2	2.03	0.41
3:H:731:GLN:NE2	3:H:731:GLN:H	2.19	0.41
3:B:311:GLN:NE2	3:B:321:LYS:CE	2.73	0.40
2:F:467:DC:H2''	2:F:468:DG:H5'	2.02	0.40
2:D:418:DG:H2''	2:D:419:DT:H5'	2.02	0.40
1:E:453:DA:P	3:A:116:LYS:HE2	2.61	0.40
2:L:966:DA:H2''	2:L:967:DC:O5'	2.21	0.40
2:J:922:DT:H6	2:J:922:DT:H5'	1.86	0.40
3:B:330:ASP:OD2	3:B:345:SER:HB3	2.21	0.40
3:G:627:THR:HG22	3:G:628:TRP:CD1	2.56	0.40
3:H:844:THR:O	3:H:847:THR:HG23	2.22	0.40
3:H:733:TYR:CZ	3:H:738:GLN:HB2	2.56	0.40
3:H:773:VAL:CG1	3:H:774:SER:N	2.84	0.40
1:E:463:DA:H1'	1:E:464:DC:O4'	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1216:HOH:O	6:H:1231:HOH:O[3_756]	1.81	0.39
1:C:407:DC:O3'	6:H:1231:HOH:O[3_756]	1.99	0.21
1:C:408:DG:OP1	6:H:1231:HOH:O[3_756]	2.12	0.08
3:A:7:LYS:NZ	6:G:1217:HOH:O[3_656]	2.12	0.08

## 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	
3	A	149/163 (91%)	137 (92%)	9 (6%)	3 (2%)	9	15
3	B	149/163 (91%)	141 (95%)	6 (4%)	2 (1%)	15	26
3	G	149/163 (91%)	139 (93%)	9 (6%)	1 (1%)	26	46
3	H	149/163 (91%)	139 (93%)	8 (5%)	2 (1%)	15	26
All	All	596/652 (91%)	556 (93%)	32 (5%)	8 (1%)	15	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	852	LEU
3	A	152	LEU
3	B	352	LEU
3	G	617	GLU
3	B	317	GLU
3	A	117	GLU
3	H	817	GLU
3	A	30	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	136/150 (91%)	123 (90%)	13 (10%)	10	19
3	B	136/150 (91%)	122 (90%)	14 (10%)	9	17
3	G	136/150 (91%)	122 (90%)	14 (10%)	9	17
3	H	137/150 (91%)	120 (88%)	17 (12%)	6	11
All	All	545/600 (91%)	487 (89%)	58 (11%)	8	16

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	30	ASN
3	A	31	GLN
3	A	52	ARG
3	A	68	ARG
3	A	78	LEU
3	A	81	ILE
3	A	101	GLN
3	A	106	LEU
3	A	127	THR
3	A	129	VAL
3	A	139	LYS
3	A	147	THR
3	A	152	LEU
3	B	231	GLN
3	B	234	LYS
3	B	252	ARG
3	B	257	LYS
3	B	268	ARG
3	B	277	ILE
3	B	278	LEU
3	B	281	ILE
3	B	301	GLN
3	B	306	LEU
3	B	327	THR
3	B	329	VAL
3	B	339	LYS
3	B	352	LEU
3	G	531	GLN
3	G	552	ARG
3	G	557	LYS

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Mol	Chain	Res	Type
3	G	568	ARG
3	G	578	LEU
3	G	581	ILE
3	G	601	GLN
3	G	606	LEU
3	G	627	THR
3	G	629	VAL
3	G	639	LYS
3	G	647	THR
3	G	651	VAL
3	G	652	LEU
3	H	704	LYS
3	H	726	GLN
3	H	731	GLN
3	H	752	ARG
3	H	757	LYS
3	H	768	ARG
3	H	777	ILE
3	H	778	LEU
3	H	781	ILE
3	H	801	GLN
3	H	806	LEU
3	H	827	THR
3	H	829	VAL
3	H	839	LYS
3	H	844	THR
3	H	847	THR
3	H	852	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	30	ASN
3	A	31	GLN
3	A	37	HIS
3	B	231	GLN
3	B	250	GLN
3	B	311	GLN
3	G	531	GLN
3	G	599	GLN
3	H	730	ASN
3	H	731	GLN

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Mol	Chain	Res	Type
3	H	737	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	C	14/14 (100%)	-0.57	0 100 100	24, 36, 45, 57	0
1	E	14/14 (100%)	-0.54	0 100 100	25, 45, 52, 55	0
1	I	14/14 (100%)	-0.35	0 100 100	33, 50, 55, 61	0
1	K	14/14 (100%)	-0.60	0 100 100	30, 40, 48, 50	0
2	D	10/10 (100%)	-0.42	0 100 100	29, 48, 60, 61	0
2	F	10/10 (100%)	-0.50	0 100 100	21, 32, 44, 51	0
2	J	10/10 (100%)	-0.29	0 100 100	27, 41, 50, 53	0
2	L	10/10 (100%)	-0.11	0 100 100	30, 53, 65, 66	0
3	A	151/163 (92%)	-0.02	4 (2%) 59 63	19, 39, 73, 82	0
3	B	151/163 (92%)	-0.14	2 (1%) 79 82	17, 31, 65, 76	0
3	G	151/163 (92%)	-0.04	4 (2%) 59 63	21, 35, 72, 83	0
3	H	151/163 (92%)	0.07	4 (2%) 59 63	21, 44, 72, 88	0
All	All	700/748 (93%)	-0.09	14 (2%) 68 72	17, 39, 71, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	505	TYR	4.2
3	G	617	GLU	3.3
3	A	117	GLU	3.0
3	B	351	VAL	3.0
3	G	623	LEU	2.7
3	H	851	VAL	2.6
3	G	650	ALA	2.5
3	A	30	ASN	2.4
3	A	3	THR	2.3
3	H	817	GLU	2.2
3	H	852	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	152	LEU	2.0
3	B	317	GLU	2.0
3	H	821	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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	NA	G	995	1/1	0.81	0.28	8.94	38,38,38,38	0
5	NA	H	994	1/1	0.94	0.38	8.56	49,49,49,49	0
5	NA	A	495	1/1	0.94	0.22	2.99	34,34,34,34	0
4	CA	F	491	1/1	0.95	0.12	-0.04	29,29,29,29	0
5	NA	B	494	1/1	0.94	0.13	-0.54	24,24,24,24	0
4	CA	L	992	1/1	0.99	0.12	-0.63	28,28,28,28	0
4	CA	D	493	1/1	0.99	0.11	-1.06	18,18,18,18	0
4	CA	C	492	1/1	0.99	0.09	-1.73	27,27,27,27	0
4	CA	I	993	1/1	0.98	0.09	-2.06	30,30,30,30	0
4	CA	J	991	1/1	0.99	0.10	-2.24	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.