



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:05 pm BST

PDB ID : 2VS7  
Title : The crystal structure of I-DmoI in complex with DNA and Ca  
Authors : Marcaida, M.J.; Prieto, J.; Redondo, P.; Nadra, A.D.; Alibes, A.; Serrano, L.; Grizot, S.; Duchateau, P.; Paques, F.; Blanco, F.J.; Montoya, G.  
Deposited on : 2008-04-21  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

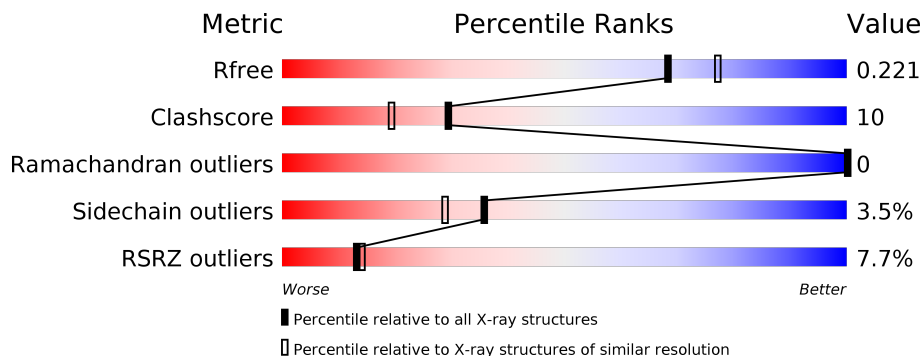
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 respectively. 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	199	 9% 66% 21% • 10%
1	D	199	 7% 73% 20% • •
1	G	199	 11% 71% 17% • 11%
2	B	25	 60% 40%
2	E	25	 40% 48% 12%
2	H	25	 72% 24% •

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Mol	Chain	Length	Quality of chain
3	C	25	
3	F	25	
3	I	25	

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	ACT	D	1197	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8342 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 HOMING ENDONUCLEASE I-DMOI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	Total	C	N	O	S	0	8	0
			1518	984	276	255	3			
1	D	191	Total	C	N	O	S	0	24	0
			1619	1046	294	276	3			
1	G	177	Total	C	N	O	S	0	28	0
			1531	992	280	256	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			
2	E	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			
2	H	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			

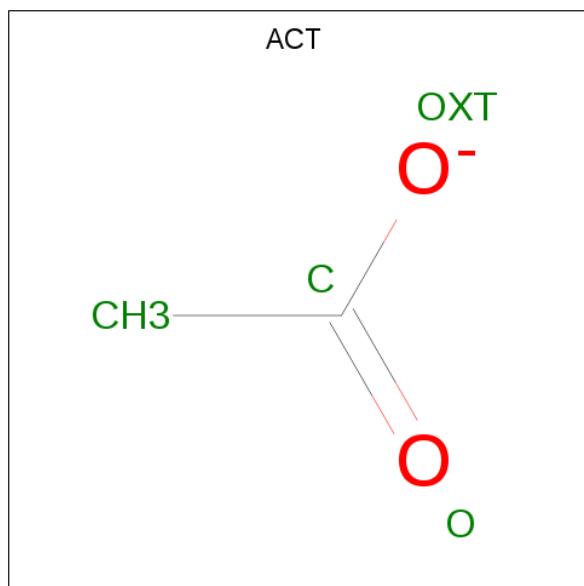
- Molecule 3 is a DNA chain called 5'-D(\*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP \*CP\*TP\*TP\*AP\*CP\*CP\*CP\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			
3	F	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			
3	I	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	132	Total O 132 132	0	0
6	B	53	Total O 53 53	0	0
6	C	45	Total O 45 45	0	0
6	D	128	Total O 128 128	0	0
6	E	33	Total O 33 33	0	0
6	F	44	Total O 44 44	0	0

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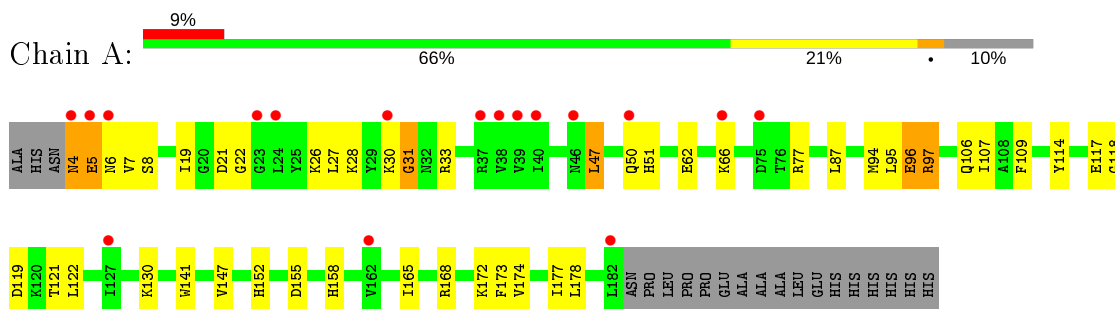
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	G	102	Total 102	O 102	0	0
6	H	46	Total 46	O 46	0	0
6	I	27	Total 27	O 27	0	0

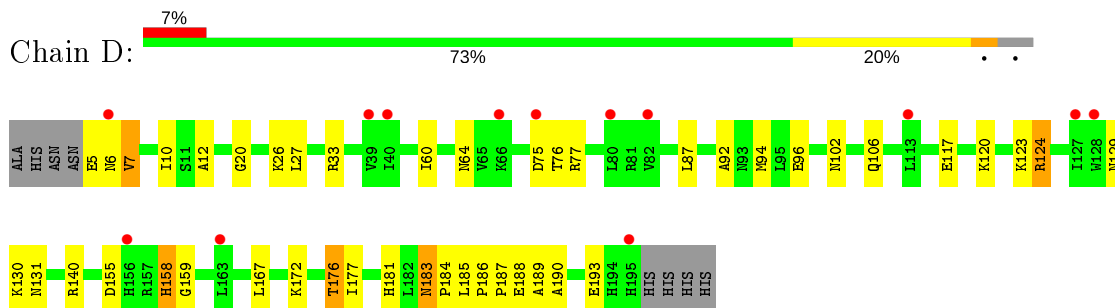
### 3 Residue-property plots [i](#)

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

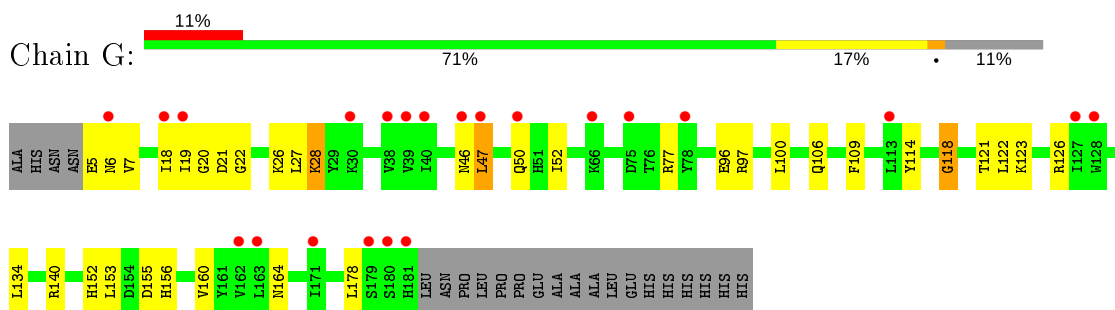
- Molecule 1: HOMING ENDONUCLEASE I-DMOI



- Molecule 1: HOMING ENDONUCLEASE I-DMOI



- Molecule 1: HOMING ENDONUCLEASE I-DMOI



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





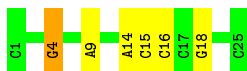
- Molecule 2: 5'-D(\*GP\*CP\*CP\*TP\*TP\*GP\*CP\*CP\*GP\*GP \*GP\*TP\*AP\*AP\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*G)-3'



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



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



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.99Å 70.59Å 106.85Å 90.00° 119.75° 90.00°	Depositor
Resolution (Å)	25.76 – 2.05 25.76 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.4 (25.76-2.05) 95.4 (25.76-2.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.228 0.183 , 0.221	Depositor DCC
$R_{free}$ test set	4178 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,k,-h-l 0.017 for -h-l,k,h 0.013 for -h-l,-k,l 0.012 for h,-k,-h-l 0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, ACT

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	0.45	0/1562	0.60	1/2099 (0.0%)
1	D	0.47	0/1665	0.57	1/2241 (0.0%)
1	G	0.45	0/1585	0.59	1/2126 (0.0%)
2	B	0.79	0/572	1.50	11/882 (1.2%)
2	E	0.77	0/572	1.48	8/882 (0.9%)
2	H	0.78	0/572	1.42	7/882 (0.8%)
3	C	0.81	0/570	1.41	5/877 (0.6%)
3	F	0.80	0/570	1.39	6/877 (0.7%)
3	I	0.78	0/570	1.42	5/877 (0.6%)
All	All	0.62	0/8238	1.06	45/11743 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	7
1	D	1	2
1	G	0	4
All	All	3	13

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	9	DA	O4'-C1'-N9	9.34	114.54	108.00
2	H	24	DC	O4'-C1'-N1	8.85	114.19	108.00
2	E	2	DC	O4'-C1'-N1	8.80	114.16	108.00
3	F	18	DG	O4'-C1'-N9	8.47	113.93	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	16	DT	O4'-C1'-N1	-8.33	102.17	108.00
3	C	14	DA	O4'-C1'-N9	-8.00	102.40	108.00
2	E	20	DG	O4'-C1'-N9	7.95	113.56	108.00
3	F	14	DA	O4'-C1'-N9	-7.50	102.75	108.00
3	C	18	DG	O4'-C1'-N9	7.13	112.99	108.00
3	F	9	DA	O4'-C1'-N9	7.12	112.98	108.00
3	C	9	DA	O4'-C1'-N9	6.98	112.88	108.00
2	E	22	DC	O4'-C1'-N1	6.90	112.83	108.00
3	C	4	DG	P-O3'-C3'	6.89	127.97	119.70
3	C	16	DC	P-O5'-C5'	6.84	131.84	120.90
1	A	27	LEU	CA-CB-CG	6.82	130.99	115.30
2	H	10	DG	O4'-C1'-N9	-6.74	103.28	108.00
2	B	21	DG	O4'-C1'-N9	6.62	112.63	108.00
2	B	24	DC	O4'-C1'-N1	6.52	112.56	108.00
2	B	8	DC	O4'-C1'-N1	6.45	112.52	108.00
2	B	1	DG	O4'-C1'-N9	-6.30	103.59	108.00
2	H	18	DC	O4'-C1'-N1	6.21	112.35	108.00
3	I	18	DG	O4'-C1'-N9	6.16	112.31	108.00
2	H	21	DG	O4'-C1'-N9	6.08	112.26	108.00
3	F	2	DG	P-O3'-C3'	6.05	126.96	119.70
2	B	20	DG	O4'-C1'-N9	6.01	112.21	108.00
2	H	24	DC	C1'-O4'-C4'	-5.86	104.24	110.10
2	E	18	DC	O4'-C1'-N1	5.73	112.01	108.00
1	D	27	LEU	CA-CB-CG	5.65	128.29	115.30
2	E	17	DT	C6-C5-C7	-5.61	119.53	122.90
3	F	16	DC	P-O5'-C5'	5.61	129.87	120.90
2	H	24	DC	O4'-C1'-C2'	-5.61	101.41	105.90
2	B	16	DT	O4'-C1'-N1	-5.58	104.09	108.00
3	I	14	DA	O4'-C1'-N9	-5.57	104.10	108.00
2	B	18	DC	O4'-C1'-N1	5.40	111.78	108.00
3	I	3	DC	C1'-O4'-C4'	-5.38	104.72	110.10
2	B	5	DT	N3-C4-O4	5.31	123.08	119.90
2	B	9	DG	O4'-C1'-N9	5.24	111.67	108.00
1	G	27	LEU	CA-CB-CG	5.18	127.22	115.30
3	F	7	DG	P-O3'-C3'	5.17	125.91	119.70
2	B	21	DG	C1'-O4'-C4'	-5.11	104.99	110.10
2	B	5	DT	C5-C4-O4	-5.08	121.34	124.90
2	E	21	DG	O4'-C1'-N9	5.05	111.53	108.00
3	I	13	DT	P-O3'-C3'	5.04	125.75	119.70
2	E	13	DA	P-O3'-C3'	5.04	125.74	119.70
2	H	9	DG	P-O3'-C3'	5.03	125.74	119.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	5	GLU	CA
1	A	97	ARG	CA
1	D	5	GLU	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ASP	Peptide
1	A	30	LYS	Peptide
1	A	31	GLY	Peptide
1	A	4	ASN	Peptide
1	A	5	GLU	Peptide
1	A	96	GLU	Peptide
1	A	97	ARG	Peptide
1	D	123	LYS	Peptide
1	D	158	HIS	Peptide
1	G	118	GLY	Peptide
1	G	21	ASP	Peptide
1	G	47	LEU	Peptide
1	G	6	ASN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	1518	0	1606	41	0
1	D	1619	0	1678	46	0
1	G	1531	0	1602	34	0
2	B	511	0	282	2	0
2	E	511	0	282	8	0
2	H	511	0	282	4	0
3	C	508	0	279	2	0
3	F	508	0	279	4	0
3	I	508	0	279	2	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
5	D	4	0	3	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	132	0	0	8	0
6	B	53	0	0	1	0
6	C	45	0	0	3	0
6	D	128	0	0	6	0
6	E	33	0	0	6	0
6	F	44	0	0	1	0
6	G	102	0	0	6	0
6	H	46	0	0	5	0
6	I	27	0	0	0	0
All	All	8342	0	6572	137	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 10.

All (137) 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:D:75:ASP:OD1	1:D:76[D]:THR:HG23	1.25	1.25
1:A:94:MET:SD	6:A:2063:HOH:O	2.03	1.16
1:D:94:MET:SD	6:D:2072:HOH:O	2.08	1.09
1:D:26:LYS:NZ	6:D:2014:HOH:O	1.86	1.09
1:G:47:LEU:HD23	1:G:47:LEU:O	1.52	1.06
1:D:6:ASN:O	1:D:10:ILE:HD12	1.61	0.99
1:A:26[A]:LYS:NZ	6:A:2006:HOH:O	2.00	0.94
1:A:4:ASN:N	1:A:5:GLU:CB	2.30	0.94
1:D:186:PRO:HG2	1:D:189:ALA:HB3	1.52	0.92
1:D:183:ASN:HB2	1:D:184:PRO:CD	2.08	0.83
1:D:5:GLU:O	1:D:6:ASN:HB3	1.79	0.81
1:G:96[A]:GLU:OE2	6:G:2051:HOH:O	2.00	0.80
1:G:22:GLY:H	2:H:15:DG:H5''	1.47	0.79
1:D:188:GLU:HB2	5:D:1197:ACT:H2	1.64	0.78
2:E:15:DG:OP2	6:E:2016:HOH:O	2.01	0.78
1:D:181:HIS:HE1	1:D:193:GLU:OE1	1.66	0.77
1:G:26[A]:LYS:NZ	6:G:2012:HOH:O	2.17	0.76
1:D:140:ARG:NH1	6:D:2100:HOH:O	2.19	0.75
3:C:15:DC:OP1	6:C:2031:HOH:O	2.05	0.74
1:G:140:ARG:HD3	6:G:2080:HOH:O	1.87	0.74
2:H:15:DG:OP2	6:H:2023:HOH:O	2.05	0.74
6:E:2016:HOH:O	3:F:15:DC:OP1	2.05	0.74
1:A:5:GLU:CB	1:A:8:SER:H	2.02	0.73
1:D:183:ASN:HB2	1:D:184:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19[B]:ILE:HD11	1:A:95:LEU:HD13	1.74	0.70
6:H:2023:HOH:O	3:I:15:DC:OP1	2.11	0.69
2:E:18:DC:OP1	6:E:2022:HOH:O	2.10	0.68
1:A:121:THR:O	1:A:122:LEU:HB2	1.95	0.67
1:G:46:ASN:O	1:G:47:LEU:CB	2.43	0.66
2:B:15:DG:OP2	6:C:2031:HOH:O	2.12	0.66
1:A:96:GLU:N	1:A:97:ARG:HA	2.09	0.66
1:G:26[B]:LYS:HZ2	1:G:28:LYS:HE2	1.60	0.65
1:G:47:LEU:CD2	1:G:47:LEU:O	2.39	0.65
1:A:117:GLU:OE2	6:C:2031:HOH:O	2.13	0.65
1:A:147:VAL:CG1	1:A:165:ILE:HG23	2.26	0.65
1:A:4:ASN:ND2	1:A:4:ASN:O	2.30	0.65
1:D:129:ASN:HD22	1:D:131:ASN:H	1.43	0.65
1:D:186:PRO:HG2	1:D:189:ALA:CB	2.25	0.64
1:G:97[B]:ARG:NH1	6:G:2053:HOH:O	2.29	0.64
3:I:7:DG:H2"	3:I:8:DG:H5"	1.79	0.64
3:F:2:DG:H2"	3:F:3:DC:H5"	1.80	0.64
1:D:60[A]:ILE:HD11	1:D:87:LEU:HD22	1.80	0.63
1:D:183:ASN:CB	1:D:184:PRO:CD	2.72	0.62
1:A:31:GLY:HA2	1:A:33:ARG:H	1.63	0.62
1:D:181:HIS:CE1	1:D:193:GLU:OE1	2.52	0.61
1:A:22:GLY:H	2:B:15:DG:H5"	1.66	0.61
1:D:188:GLU:HB2	5:D:1197:ACT:CH3	2.31	0.61
1:D:6:ASN:HA	6:D:2123:HOH:O	2.00	0.61
1:D:172:LYS:O	1:D:176[D]:THR:HB	2.01	0.60
1:D:7:VAL:HG12	6:D:2001:HOH:O	2.03	0.59
1:D:5:GLU:O	1:D:6:ASN:CB	2.48	0.59
1:D:6:ASN:ND2	1:D:6:ASN:O	2.37	0.58
1:A:4:ASN:CG	1:A:4:ASN:O	2.43	0.57
1:G:18:ILE:O	1:G:22:GLY:HA3	2.05	0.57
1:D:12:ALA:HA	1:D:94:MET:CE	2.34	0.56
1:G:126:ARG:HG2	1:G:164:ASN:HD22	1.72	0.55
1:G:46:ASN:HD21	1:G:50[B]:GLN:CD	2.10	0.55
1:A:51:HIS:ND1	6:A:2030:HOH:O	2.33	0.54
1:G:121[D]:THR:C	1:G:123:LYS:H	2.09	0.54
1:D:117:GLU:OE2	6:E:2016:HOH:O	2.19	0.53
1:A:47:LEU:HA	1:A:51:HIS:HD2	1.72	0.53
1:A:19[B]:ILE:HD12	1:A:109:PHE:HE1	1.74	0.53
1:D:155:ASP:O	1:D:159:GLY:HA2	2.09	0.53
3:F:2:DG:OP2	6:F:2003:HOH:O	2.19	0.53
1:D:183:ASN:CB	1:D:184:PRO:HD3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114[D]:TYR:O	1:G:118:GLY:HA3	2.10	0.52
1:A:87:LEU:HD21	6:A:2032:HOH:O	2.09	0.52
1:A:7:VAL:HG21	1:A:62:GLU:HG2	1.90	0.52
1:A:94:MET:O	1:A:97:ARG:HA	2.11	0.51
1:D:20:GLY:O	6:E:2016:HOH:O	2.19	0.51
1:A:152[B]:HIS:NE2	6:A:2102:HOH:O	1.98	0.51
1:G:19[B]:ILE:HD11	1:G:109:PHE:HZ	1.77	0.50
1:A:7:VAL:CG2	1:A:62:GLU:HG2	2.42	0.49
1:A:106:GLN:NE2	6:A:2073:HOH:O	2.43	0.49
1:G:46:ASN:O	1:G:47:LEU:HB3	2.12	0.48
1:A:155:ASP:OD2	1:A:158:HIS:HD2	1.96	0.48
1:A:152[B]:HIS:CD2	6:B:2015:HOH:O	2.67	0.48
1:G:46:ASN:HD21	1:G:50[A]:GLN:HG3	1.79	0.48
2:H:20:DG:H1'	6:H:2030:HOH:O	2.14	0.48
1:G:19[B]:ILE:HD12	1:G:134:LEU:HD21	1.96	0.47
1:G:20:GLY:O	6:H:2023:HOH:O	2.20	0.47
1:A:50[B]:GLN:HG3	1:A:51:HIS:CD2	2.49	0.47
1:A:130:LYS:NZ	6:A:2084:HOH:O	2.38	0.47
1:D:6:ASN:CG	1:D:6:ASN:O	2.51	0.47
1:G:46:ASN:ND2	1:G:50[A]:GLN:HG3	2.30	0.47
1:D:94:MET:HB2	6:D:2072:HOH:O	2.15	0.46
1:G:152[B]:HIS:HD2	6:G:2085:HOH:O	1.98	0.46
1:D:92:ALA:O	1:D:96:GLU:HG3	2.15	0.46
1:D:130:LYS:HE3	1:D:158:HIS:O	2.16	0.46
1:G:155:ASP:HB3	1:G:160:VAL:HB	1.96	0.46
1:D:188:GLU:CB	5:D:1197:ACT:H2	2.42	0.46
1:D:124:ARG:NH2	2:E:6:DG:O6	2.44	0.46
1:D:185:LEU:HB3	1:D:190:ALA:HB2	1.97	0.45
1:A:19[B]:ILE:HD12	1:A:109:PHE:CE1	2.50	0.45
1:A:114:TYR:O	1:A:118:GLY:HA3	2.16	0.45
2:E:8:DC:H2''	2:E:9:DG:C8	2.52	0.45
1:D:186:PRO:HB2	5:D:1197:ACT:CH3	2.46	0.45
1:D:33:ARG:NH1	2:E:21:DG:O6	2.49	0.45
2:E:19:DC:H2'	2:E:20:DG:C8	2.52	0.45
1:G:19[B]:ILE:HD11	1:G:109:PHE:CZ	2.52	0.45
1:G:46:ASN:O	1:G:47:LEU:HB2	2.16	0.44
1:D:176[D]:THR:HG22	1:D:177:ILE:HG13	2.00	0.44
1:A:174:VAL:HG22	1:A:178[B]:LEU:HD12	1.99	0.44
1:D:33:ARG:HD2	3:F:4:DG:O6	2.17	0.44
2:E:11:DG:H2''	2:E:12:DT:H71	1.99	0.44
1:A:147:VAL:HG11	1:A:165:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PRO:HB2	5:D:1197:ACT:H3	2.00	0.43
2:E:15:DG:H5'	6:E:2019:HOH:O	2.16	0.43
1:D:12:ALA:HA	1:D:94:MET:HE1	2.00	0.43
1:G:153:LEU:HD23	1:G:156:HIS:CE1	2.53	0.43
1:A:107:ILE:HG12	1:A:177:ILE:HD13	2.00	0.43
1:A:114:TYR:CE2	1:A:119:ASP:O	2.71	0.42
1:A:19[A]:ILE:HD11	1:A:95:LEU:HD22	2.00	0.42
1:A:106:GLN:HG2	1:A:141:TRP:CD2	2.55	0.42
1:A:165:ILE:HD13	1:A:173:PHE:CE1	2.55	0.42
1:G:5:GLU:C	1:G:7:VAL:H	2.22	0.42
1:G:46:ASN:ND2	1:G:50[A]:GLN:CG	2.83	0.41
1:D:102:ASN:O	1:D:106:GLN:HG3	2.21	0.41
2:H:24:DC:OP2	6:H:2037:HOH:O	2.22	0.41
1:D:186:PRO:HA	1:D:187:PRO:HD3	1.89	0.41
1:G:19[B]:ILE:CD1	1:G:109:PHE:HZ	2.32	0.41
1:A:94:MET:HB2	6:A:2063:HOH:O	2.20	0.41
1:D:158:HIS:H	1:D:159:GLY:HA2	1.86	0.41
1:D:124:ARG:HA	1:D:167:LEU:HD21	2.02	0.41
1:D:185:LEU:HA	1:D:186:PRO:HD2	1.56	0.41
1:G:19[B]:ILE:CD1	1:G:134:LEU:HD21	2.50	0.41
1:A:28:LYS:HD3	1:A:28:LYS:HA	1.87	0.41
1:G:5:GLU:N	6:G:2001:HOH:O	2.54	0.41
1:A:172:LYS:HE3	1:A:172:LYS:HB2	1.93	0.40
1:A:33:ARG:HD2	3:C:4:DG:O6	2.21	0.40
1:G:19[B]:ILE:HD12	1:G:134:LEU:CD2	2.51	0.40
1:G:121[D]:THR:C	1:G:123:LYS:N	2.72	0.40
1:A:121:THR:O	1:A:122:LEU:CB	2.65	0.40
1:G:47:LEU:O	1:G:52:ILE:HG13	2.21	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	185/199 (93%)	181 (98%)	4 (2%)	0	100	100
1	D	196/199 (98%)	188 (96%)	8 (4%)	0	100	100
1	G	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
All	All	567/597 (95%)	550 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/178 (93%)	160 (96%)	6 (4%)	35	28
1	D	178/178 (100%)	170 (96%)	8 (4%)	27	20
1	G	168/178 (94%)	163 (97%)	5 (3%)	41	34
All	All	512/534 (96%)	493 (96%)	19 (4%)	36	27

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	47	LEU
1	A	66	LYS
1	A	77	ARG
1	A	168[A]	ARG
1	A	168[B]	ARG
1	D	7	VAL
1	D	64[A]	ASN
1	D	64[B]	ASN
1	D	77	ARG
1	D	120	LYS
1	D	124	ARG
1	D	176[D]	THR
1	D	183	ASN
1	G	28	LYS

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Mol	Chain	Res	Type
1	G	77	ARG
1	G	100	LEU
1	G	122	LEU
1	G	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	51	HIS
1	A	106	GLN
1	A	158	HIS
1	D	6	ASN
1	D	42	GLN
1	D	50	GLN
1	D	93	ASN
1	D	129	ASN
1	D	158	HIS
1	D	181	HIS
1	G	46	ASN
1	G	106	GLN
1	G	156	HIS
1	G	164	ASN

### 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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ACT	D	1197	-	1,3,3	1.15	0	0,3,3	0.00	-

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1197	ACT	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	179/199 (89%)	0.34	17 (9%) 8 9	26, 41, 60, 74	0
1	D	191/199 (95%)	0.30	13 (6%) 17 18	25, 41, 55, 66	0
1	G	177/199 (88%)	0.42	22 (12%) 4 3	28, 40, 60, 73	0
2	B	25/25 (100%)	-0.57	0 100 100	36, 46, 58, 60	0
2	E	25/25 (100%)	-0.60	0 100 100	34, 52, 67, 76	0
2	H	25/25 (100%)	-0.57	0 100 100	37, 53, 59, 60	0
3	C	25/25 (100%)	-0.40	0 100 100	33, 50, 65, 71	0
3	F	25/25 (100%)	-0.18	2 (8%) 12 13	35, 46, 80, 82	0
3	I	25/25 (100%)	-0.19	0 100 100	34, 49, 70, 76	0
All	All	697/747 (93%)	0.18	54 (7%) 13 14	25, 42, 64, 82	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156[A]	HIS	5.6
1	G	181	HIS	4.6
1	A	6	ASN	4.2
1	A	75	ASP	4.1
1	G	46	ASN	3.7
1	G	6	ASN	3.5
1	A	39	VAL	3.3
1	A	4	ASN	3.3
1	G	18	ILE	3.2
1	G	127	ILE	3.0
1	D	127	ILE	2.9
1	G	50[A]	GLN	2.8
1	A	40	ILE	2.7
1	D	82	VAL	2.7
1	G	38	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	128[D]	TRP	2.7
1	G	113	LEU	2.7
1	G	171	ILE	2.7
1	G	47	LEU	2.7
1	A	50[A]	GLN	2.6
1	A	38	VAL	2.5
1	D	6	ASN	2.5
1	D	163	LEU	2.5
1	A	24	LEU	2.4
1	D	195	HIS	2.4
1	G	30	LYS	2.4
1	A	37	ARG	2.4
1	G	163	LEU	2.4
1	A	46[A]	ASN	2.3
1	G	39	VAL	2.3
1	G	66[A]	LYS	2.3
1	D	128[D]	TRP	2.3
3	F	24	DG	2.2
1	A	23	GLY	2.2
1	G	40	ILE	2.2
1	D	66[A]	LYS	2.2
1	G	179	SER	2.2
1	A	5	GLU	2.1
1	G	78[D]	TYR	2.1
1	G	75[A]	ASP	2.1
1	D	40	ILE	2.1
1	D	75	ASP	2.1
1	A	127	ILE	2.1
1	D	113	LEU	2.1
1	A	30	LYS	2.1
1	A	66	LYS	2.1
1	A	182	LEU	2.1
1	A	162	VAL	2.1
1	G	162	VAL	2.1
1	G	19[A]	ILE	2.0
1	D	39	VAL	2.0
3	F	23	DG	2.0
1	G	180	SER	2.0
1	D	80	LEU	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	D	1197	4/4	0.89	0.19	20,20,20,20	0
4	CA	A	1183	1/1	0.99	0.04	35,35,35,35	0
4	CA	G	1182	1/1	1.00	0.04	35,35,35,35	0
4	CA	D	1196	1/1	1.00	0.09	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.