



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:46 pm GMT

PDB ID : 4Z20  
Title : Crystal Structure of Meganuclease I-SmaMI Bound to Uncleaveable DNA with a TTGT Central Four  
Authors : Hallinan, J.P.; Stoddard, B.L.  
Deposited on : 2015-03-27  
Resolution : 3.20 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

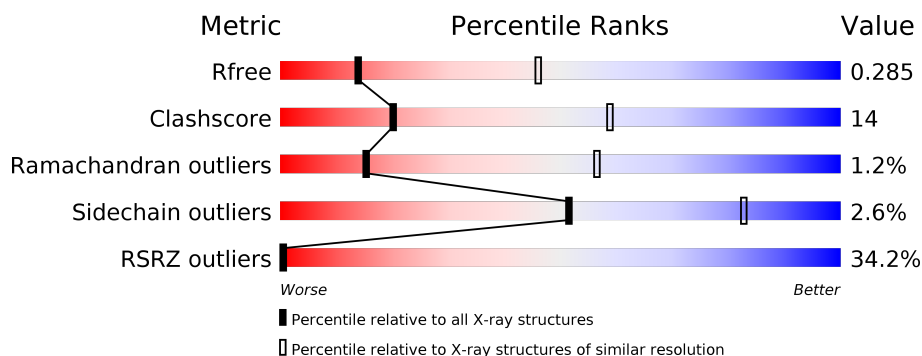
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	303	<div> <div>37%</div> <div>79%</div> <div>17%</div> <div>...</div> </div>
1	D	303	<div> <div>34%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
2	C	26	<div> <div>27%</div> <div>38%</div> <div>58%</div> <div>.</div> </div>
2	F	26	<div> <div>27%</div> <div>46%</div> <div>54%</div> </div>
3	B	26	<div> <div>12%</div> <div>35%</div> <div>62%</div> <div>.</div> </div>
3	E	26	<div> <div>15%</div> <div>42%</div> <div>58%</div> </div>

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	CA	A	401	-	-	-	X
4	CA	D	402	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6503 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 MEGANUCLEASE I-SMAMI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2193	1427	360	398	8			
1	D	291	Total	C	N	O	S	0	0	0
			2147	1400	351	388	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP F7WD42
A	165	ASN	LEU	conflict	UNP F7WD42
A	267	GLN	MET	conflict	UNP F7WD42
D	0	MET	-	initiating methionine	UNP F7WD42
D	165	ASN	LEU	conflict	UNP F7WD42
D	267	GLN	MET	conflict	UNP F7WD42

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	26	Total	C	N	O	P	0	0	0
			522	250	86	160	26			
2	F	26	Total	C	N	O	P	0	0	0
			522	250	86	160	26			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	26	Total	C	N	O	P	0	0	0
			544	256	110	152	26			
3	E	26	Total	C	N	O	P	0	0	0
			544	256	110	152	26			

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

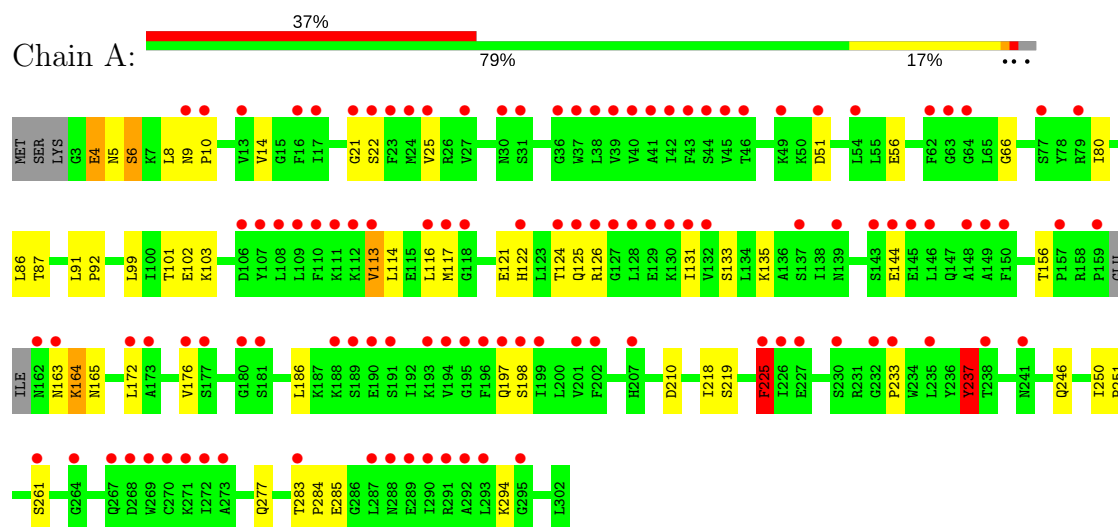
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0
6	C	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	D	4	Total O 4 4	0	0
6	F	2	Total O 2 2	0	0

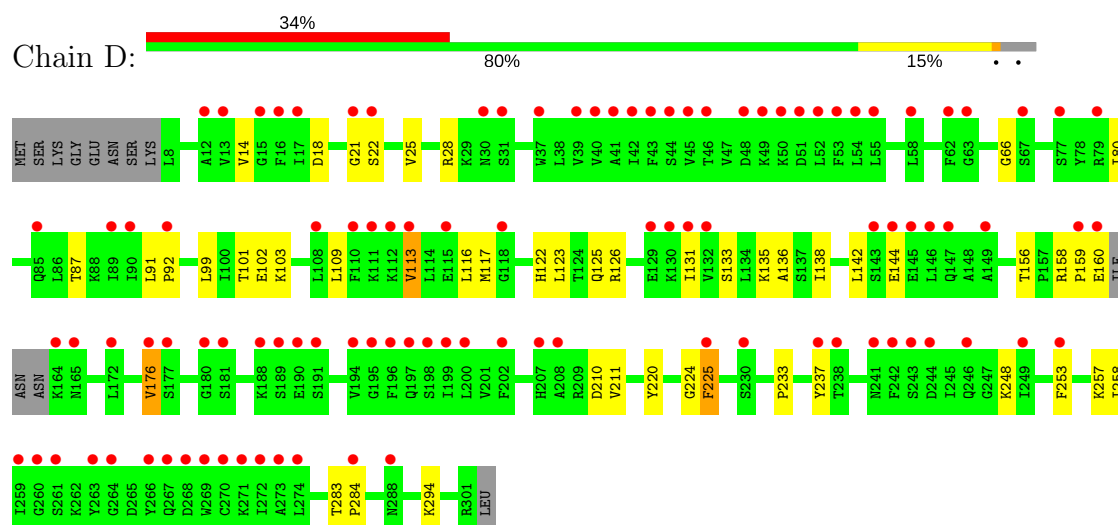
### 3 Residue-property plots [i](#)

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: MEGANUCLEASE I-SMAMI

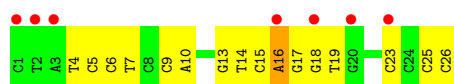


#### • Molecule 1: MEGANUCLEASE I-SMAMI

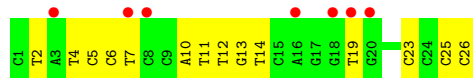


#### • Molecule 2: DNA (26-MER)

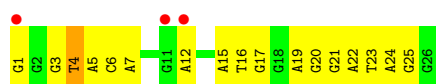




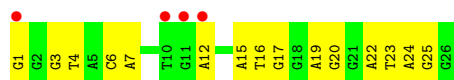
• Molecule 2: DNA (26-MER)



• Molecule 3: DNA (26-MER)



• Molecule 3: DNA (26-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.69Å 172.26Å 59.99Å 90.00° 92.36° 90.00°	Depositor
Resolution (Å)	86.13 – 3.20 44.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.13-3.20) 99.2 (44.13-3.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.233 , 0.291 0.229 , 0.285	Depositor DCC
$R_{free}$ test set	752 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 157.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	A	0.66	5/2246 (0.2%)	0.72	4/3051 (0.1%)
1	D	0.70	7/2200 (0.3%)	0.71	2/2994 (0.1%)
2	C	0.40	0/581	0.95	2/892 (0.2%)
2	F	0.39	0/581	0.95	1/892 (0.1%)
3	B	0.47	1/613 (0.2%)	0.83	0/946
3	E	0.40	0/613	0.83	0/946
All	All	0.60	13/6834 (0.2%)	0.78	9/9721 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	PRO	CA-C	9.64	1.72	1.52
1	D	237	TYR	CE1-CZ	-9.47	1.26	1.38
1	A	237	TYR	CE1-CZ	-9.14	1.26	1.38
1	D	160	GLU	N-CA	8.03	1.62	1.46
1	A	237	TYR	CG-CD2	-7.80	1.29	1.39
1	D	237	TYR	CG-CD1	-7.74	1.29	1.39
1	A	237	TYR	CG-CD1	-7.35	1.29	1.39
1	D	237	TYR	CG-CD2	-7.22	1.29	1.39
1	D	237	TYR	CE2-CZ	-6.53	1.30	1.38
1	A	237	TYR	CE2-CZ	-6.46	1.30	1.38
1	D	159	PRO	N-CA	6.03	1.57	1.47
1	A	164	LYS	N-CA	5.48	1.57	1.46
3	B	4	DT	O3'-P	-5.36	1.54	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	PHE	CB-CG-CD2	-7.35	115.66	120.80
2	F	23	DC	C1'-O4'-C4'	-6.53	103.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	23	DC	C1'-O4'-C4'	-6.52	103.58	110.10
1	D	159	PRO	C-N-CA	6.43	137.79	121.70
1	A	163	ASN	N-CA-C	5.82	126.72	111.00
1	A	225	PHE	CB-CG-CD1	5.74	124.82	120.80
1	D	158	ARG	C-N-CD	-5.43	108.64	120.60
1	A	164	LYS	N-CA-C	5.36	125.48	111.00
2	C	16	DA	C1'-O4'-C4'	-5.09	105.01	110.10

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	2193	0	2028	47	0
1	D	2147	0	2000	36	0
2	C	522	0	295	16	0
2	F	522	0	295	15	0
3	B	544	0	291	34	0
3	E	544	0	291	27	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
5	F	6	0	8	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	4	0	0	0	0
6	F	2	0	0	0	0
All	All	6503	0	5224	146	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 14.

All (146) 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:165:ASN:OD1	1:D:248:LYS:CE	1.72	1.37
1:A:165:ASN:OD1	1:D:248:LYS:HE2	1.41	1.18
1:A:165:ASN:OD1	1:D:248:LYS:HE3	1.38	1.08
3:B:15:DA:H2''	3:B:16:DT:H5''	1.36	1.06
1:A:225:PHE:CE2	3:B:6:DC:H5''	1.91	1.05
1:A:225:PHE:HE2	3:B:6:DC:H5''	1.20	1.05
3:E:15:DA:H2''	3:E:16:DT:H5''	1.37	1.04
1:A:164:LYS:NZ	1:A:210:ASP:OD1	1.97	0.96
2:C:25:DC:N3	3:B:1:DG:N2	2.19	0.89
1:D:225:PHE:HE2	3:E:6:DC:H3'	1.44	0.82
1:A:225:PHE:CD1	1:A:225:PHE:N	2.47	0.81
3:E:20:DG:H8	3:E:20:DG:H5''	1.49	0.77
1:A:225:PHE:HD1	1:A:225:PHE:N	1.83	0.77
2:C:25:DC:H2''	2:C:26:DC:O5'	1.85	0.75
1:D:225:PHE:CD1	1:D:225:PHE:N	2.54	0.74
1:D:225:PHE:HD1	1:D:225:PHE:N	1.84	0.74
1:D:225:PHE:CE2	3:E:6:DC:H3'	2.23	0.73
3:B:24:DA:H1'	3:B:25:DG:H5''	1.72	0.70
2:F:25:DC:H2''	2:F:26:DC:O5'	1.91	0.70
3:B:24:DA:H1'	3:B:25:DG:C5'	2.24	0.68
3:E:24:DA:H1'	3:E:25:DG:H5''	1.75	0.68
1:A:246:GLN:NE2	1:A:277:GLN:OE1	2.26	0.67
3:E:24:DA:H1'	3:E:25:DG:C5'	2.26	0.66
2:C:19:DT:H5''	2:C:19:DT:H6	1.60	0.66
1:D:101:THR:HG22	1:D:102:GLU:N	2.11	0.65
2:F:19:DT:H5''	2:F:19:DT:H6	1.61	0.65
1:A:101:THR:HG22	1:A:102:GLU:N	2.13	0.64
3:B:20:DG:H5''	3:B:20:DG:H8	1.62	0.64
1:A:283:THR:HG21	1:A:285:GLU:HG2	1.80	0.62
3:E:20:DG:C8	3:E:20:DG:H5''	2.33	0.62
2:C:25:DC:C2	3:B:1:DG:N2	2.66	0.62
2:C:5:DC:N3	3:B:21:DG:C6	2.68	0.62
1:A:21:GLY:O	1:A:103:LYS:NZ	2.32	0.62
1:A:225:PHE:CZ	3:B:6:DC:H5''	2.36	0.61
3:E:20:DG:H8	3:E:20:DG:C5'	2.14	0.61
2:C:5:DC:C4	3:B:21:DG:O6	2.53	0.61
2:C:6:DC:H2''	2:C:7:DT:O5'	2.01	0.60
3:E:19:DA:H2'	3:E:20:DG:H5''	1.82	0.60
1:A:283:THR:CG2	1:A:285:GLU:HG2	2.32	0.59
3:B:6:DC:H2''	3:B:7:DA:H5'	1.84	0.59
2:F:6:DC:H2''	2:F:7:DT:O5'	2.02	0.58
1:D:225:PHE:HE2	3:E:6:DC:C3'	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:6:DC:H2''	3:E:7:DA:H5'	1.86	0.57
1:A:237:TYR:C	1:A:237:TYR:CD1	2.79	0.57
1:D:224:GLY:C	1:D:225:PHE:HD1	2.08	0.57
1:A:101:THR:HG22	1:A:102:GLU:H	1.70	0.56
3:B:19:DA:H2'	3:B:20:DG:H5''	1.87	0.56
1:D:101:THR:HG22	1:D:102:GLU:H	1.71	0.55
1:D:117:MET:HA	1:D:122:HIS:ND1	2.22	0.55
1:A:5:ASN:OD1	1:A:6:SER:N	2.40	0.55
3:B:3:DG:H2''	3:B:4:DT:O5'	2.07	0.55
1:A:116:LEU:HD23	1:A:131:ILE:HG13	1.90	0.54
1:A:197:GLN:HE22	3:B:5:DA:H62	1.55	0.54
1:A:225:PHE:CE2	3:B:6:DC:C5'	2.81	0.54
1:A:121:GLU:O	1:A:124:THR:HB	2.08	0.54
1:A:283:THR:HG22	1:A:284:PRO:HD2	1.89	0.54
3:E:20:DG:C8	3:E:20:DG:C5'	2.90	0.53
3:B:19:DA:H2''	3:B:20:DG:OP1	2.08	0.53
1:D:21:GLY:O	1:D:103:LYS:NZ	2.35	0.53
3:E:19:DA:H2''	3:E:20:DG:OP1	2.08	0.53
1:A:225:PHE:CE2	3:B:6:DC:H3'	2.44	0.53
1:A:25:VAL:O	1:A:135:LYS:HD2	2.09	0.52
1:D:225:PHE:CE2	3:E:6:DC:H5''	2.44	0.52
3:E:15:DA:H2''	3:E:16:DT:C5'	2.25	0.52
3:E:25:DG:H5'	3:E:25:DG:C8	2.44	0.52
2:F:25:DC:C2	3:E:1:DG:N2	2.77	0.52
3:B:25:DG:H5'	3:B:25:DG:C8	2.44	0.52
1:A:86:LEU:HB3	1:A:114:LEU:HD21	1.92	0.52
3:E:16:DT:H2''	3:E:17:DG:C5'	2.40	0.52
1:D:113:VAL:CG1	1:D:131:ILE:HG23	2.40	0.51
3:B:23:DT:H4'	3:B:24:DA:OP1	2.09	0.51
1:D:116:LEU:HD23	1:D:131:ILE:HG13	1.92	0.51
3:B:20:DG:H8	3:B:20:DG:C5'	2.24	0.50
1:D:283:THR:CG2	1:D:284:PRO:HD2	2.42	0.50
1:A:283:THR:CG2	1:A:284:PRO:HD2	2.41	0.50
1:D:109:LEU:HB3	1:D:138:ILE:HD11	1.94	0.50
3:B:16:DT:H2''	3:B:17:DG:C5'	2.42	0.49
1:A:66:GLY:HA3	1:A:80:ILE:HD13	1.93	0.49
3:B:15:DA:H2''	3:B:16:DT:C5'	2.26	0.49
1:A:124:THR:HG22	1:A:125:GLN:N	2.28	0.49
1:D:25:VAL:O	1:D:135:LYS:HD2	2.12	0.49
3:E:23:DT:H4'	3:E:24:DA:OP1	2.12	0.49
1:D:136:ALA:HB2	1:D:142:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG1	1:A:131:ILE:HG23	2.42	0.49
2:C:6:DC:H2'	2:C:7:DT:C6	2.48	0.49
1:D:283:THR:HG22	1:D:284:PRO:HD2	1.95	0.49
3:E:3:DG:H2''	3:E:4:DT:O5'	2.12	0.49
2:C:5:DC:N3	3:B:21:DG:O6	2.46	0.48
1:D:123:LEU:CD2	2:F:2:DT:H3'	2.43	0.48
3:B:20:DG:H5''	3:B:20:DG:C8	2.45	0.48
1:D:66:GLY:HA3	1:D:80:ILE:HD13	1.96	0.48
1:D:87:THR:HG23	1:D:91:LEU:HD12	1.97	0.47
1:D:176:VAL:HG12	1:D:258:ILE:CD1	2.45	0.47
1:D:14:VAL:HG13	1:D:99:LEU:HD23	1.98	0.46
1:A:133:SER:HB3	1:A:156:THR:HG23	1.97	0.46
1:A:9:ASN:O	1:A:10:PRO:C	2.54	0.46
2:F:14:DT:H6	2:F:14:DT:H5''	1.80	0.46
2:C:14:DT:H5''	2:C:14:DT:H6	1.81	0.46
1:A:4:GLU:HA	1:A:56:GLU:HB3	1.98	0.46
1:A:117:MET:HA	1:A:122:HIS:ND1	2.31	0.45
3:B:23:DT:H2'	3:B:24:DA:C8	2.51	0.45
2:C:13:DG:C6	3:B:12:DA:N6	2.85	0.45
3:E:22:DA:H2'	3:E:23:DT:H71	1.99	0.45
1:A:225:PHE:CZ	3:B:6:DC:C5'	3.00	0.45
1:D:28:ARG:NH2	3:E:20:DG:C8	2.84	0.45
2:C:4:DT:H2''	2:C:5:DC:O5'	2.16	0.45
3:B:21:DG:H2'	3:B:22:DA:C8	2.52	0.44
1:A:14:VAL:HG13	1:A:99:LEU:HD23	1.99	0.44
3:B:21:DG:C6	3:B:22:DA:C6	3.05	0.44
2:F:6:DC:H2'	2:F:7:DT:C6	2.52	0.44
1:A:125:GLN:HG3	1:A:126:ARG:N	2.32	0.44
1:A:87:THR:HG23	1:A:91:LEU:HD12	1.99	0.44
3:B:20:DG:C8	3:B:20:DG:C5'	3.00	0.44
2:F:25:DC:N3	3:E:1:DG:N2	2.47	0.43
1:A:218:ILE:CD1	1:A:225:PHE:HA	2.48	0.43
1:A:225:PHE:HZ	3:B:6:DC:O5'	2.01	0.43
1:A:218:ILE:HD11	1:A:225:PHE:HA	2.00	0.43
1:D:133:SER:HB3	1:D:156:THR:HG23	2.01	0.43
2:F:4:DT:H2''	2:F:5:DC:O5'	2.18	0.43
1:A:250:ILE:N	1:A:251:PRO:HD2	2.34	0.43
1:A:91:LEU:HB2	1:A:92:PRO:HD3	2.01	0.43
1:D:123:LEU:HD21	2:F:2:DT:H3'	1.99	0.43
2:F:10:DA:H2'	2:F:10:DA:O5'	2.19	0.43
3:E:15:DA:C2'	3:E:16:DT:H5''	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:176:VAL:HB	2.19	0.42
1:D:109:LEU:HD23	1:D:138:ILE:HG13	2.01	0.42
2:C:9:DC:H2''	2:C:10:DA:C8	2.54	0.42
2:C:17:DG:C4	2:C:18:DG:C8	3.07	0.42
1:D:210:ASP:O	1:D:211:VAL:C	2.58	0.42
1:A:186:LEU:HD23	1:A:198:SER:HA	2.02	0.42
1:D:125:GLN:HG3	1:D:126:ARG:N	2.33	0.41
1:D:253:PHE:O	1:D:257:LYS:HA	2.21	0.41
2:F:11:DT:H2''	2:F:12:DT:O5'	2.19	0.41
2:F:4:DT:C2	2:F:5:DC:C6	3.07	0.41
2:F:25:DC:C2'	2:F:26:DC:O5'	2.66	0.41
1:A:51:ASP:OD1	1:A:261:SER:N	2.52	0.41
2:C:15:DC:H2''	2:C:16:DA:O4'	2.21	0.41
2:C:25:DC:C2'	2:C:26:DC:O5'	2.62	0.41
3:E:23:DT:H2'	3:E:24:DA:C8	2.56	0.41
1:A:219:SER:HB2	1:D:220:TYR:O	2.20	0.41
1:D:91:LEU:HB2	1:D:92:PRO:HD3	2.02	0.41
1:A:86:LEU:CB	1:A:114:LEU:HD21	2.50	0.40
2:F:13:DG:C6	3:E:12:DA:N6	2.89	0.40
3:B:16:DT:H2''	3:B:17:DG:O4'	2.20	0.40
1:D:225:PHE:CE2	3:E:6:DC:C5'	3.04	0.40
3:B:24:DA:H2''	3:B:25:DG:OP2	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	294/303 (97%)	265 (90%)	24 (8%)	5 (2%)	11	48
1	D	287/303 (95%)	263 (92%)	22 (8%)	2 (1%)	25	68
All	All	581/606 (96%)	528 (91%)	46 (8%)	7 (1%)	15	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	6	SER
1	A	8	LEU
1	A	144	GLU
1	D	144	GLU
1	A	233	PRO
1	D	233	PRO

### 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	209/267 (78%)	204 (98%)	5 (2%)	54	84
1	D	209/267 (78%)	203 (97%)	6 (3%)	48	80
All	All	418/534 (78%)	407 (97%)	11 (3%)	51	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	113	VAL
1	A	225	PHE
1	A	237	TYR
1	A	294	LYS
1	D	18	ASP
1	D	22	SER
1	D	113	VAL
1	D	176	VAL
1	D	225	PHE
1	D	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	267	GLN

### 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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	GOL	C	101	-	5,5,5	0.20	0	5,5,5	0.19	0
5	GOL	D	401	-	5,5,5	0.29	0	5,5,5	0.24	0
5	GOL	F	101	-	5,5,5	0.18	0	5,5,5	0.15	0

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	GOL	C	101	-	-	0/4/4/4	0/0/0/0
5	GOL	D	401	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	101	-	-	0/4/4/4	0/0/0/0

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	A	298/303 (98%)	2.06	113 (37%) <b>0</b> <b>0</b>	138, 186, 253, 290	0
1	D	291/303 (96%)	1.99	103 (35%) <b>0</b> <b>0</b>	147, 190, 257, 280	0
2	C	26/26 (100%)	1.54	7 (26%) <b>1</b> <b>1</b>	167, 206, 235, 276	0
2	F	26/26 (100%)	1.62	7 (26%) <b>1</b> <b>1</b>	167, 206, 225, 248	0
3	B	26/26 (100%)	1.20	3 (11%) <b>5</b> <b>3</b>	186, 216, 309, 324	0
3	E	26/26 (100%)	1.23	4 (15%) <b>2</b> <b>1</b>	178, 216, 271, 298	0
All	All	693/710 (97%)	1.93	237 (34%) <b>0</b> <b>0</b>	138, 192, 260, 324	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	SER	14.4
1	A	195	GLY	13.5
1	D	51	ASP	12.7
1	A	190	GLU	11.5
1	A	41	ALA	10.8
1	D	189	SER	10.7
1	A	40	VAL	10.7
1	A	194	VAL	10.2
1	D	270	CYS	9.5
1	D	43	PHE	9.5
1	D	41	ALA	9.0
1	D	190	GLU	9.0
1	D	54	LEU	8.9
1	D	40	VAL	8.7
1	A	43	PHE	8.6
1	A	144	GLU	8.4
1	D	195	GLY	7.8
1	D	143	SER	7.3
1	A	44	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	31	SER	6.8
1	A	163	ASN	6.8
1	D	17	ILE	6.5
1	D	165	ASN	6.5
1	D	160	GLU	6.5
1	D	30	ASN	6.4
1	D	149	ALA	6.3
1	A	143	SER	6.3
1	D	44	SER	6.1
1	D	13	VAL	6.1
1	A	45	VAL	6.0
1	A	124	THR	5.9
1	D	145	GLU	5.8
1	A	145	GLU	5.6
1	A	225	PHE	5.5
1	A	39	VAL	5.4
1	D	267	GLN	5.3
1	A	196	PHE	5.3
1	A	146	LEU	5.3
1	A	17	ILE	5.2
1	A	198	SER	5.2
1	D	144	GLU	5.2
1	A	54	LEU	5.0
1	D	172	LEU	4.9
1	A	108	LEU	4.8
1	A	172	LEU	4.8
1	D	176	VAL	4.8
1	A	42	ILE	4.7
1	D	63	GLY	4.7
1	D	52	LEU	4.7
1	A	292	ALA	4.7
1	D	198	SER	4.6
1	D	273	ALA	4.5
1	A	63	GLY	4.5
1	D	111	LYS	4.5
1	D	146	LEU	4.5
1	A	162	ASN	4.5
1	D	15	GLY	4.3
1	D	225	PHE	4.3
1	A	51	ASP	4.3
1	A	132	VAL	4.3
1	A	270	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	ARG	4.2
1	A	150	PHE	4.2
1	A	106	ASP	4.2
1	A	233	PRO	4.1
1	A	230	SER	4.1
1	D	42	ILE	4.1
1	D	112	LYS	4.1
1	D	196	PHE	4.1
1	A	181	SER	4.1
1	A	25	VAL	4.1
1	A	23	PHE	4.0
1	A	176	VAL	4.0
1	A	62	PHE	4.0
1	A	149	ALA	4.0
1	D	207	HIS	3.9
1	D	202	PHE	3.9
1	D	159	PRO	3.9
1	D	268	ASP	3.9
1	D	45	VAL	3.8
1	A	24	MET	3.8
2	C	3	DA	3.8
1	A	232	GLY	3.7
1	A	110	PHE	3.7
1	A	283	THR	3.7
1	D	271	LYS	3.7
1	D	39	VAL	3.6
1	D	113	VAL	3.6
1	A	287	LEU	3.6
1	A	30	ASN	3.6
1	A	9	ASN	3.6
1	D	288	ASN	3.6
1	A	180	GLY	3.5
1	A	21	GLY	3.5
1	A	272	ILE	3.5
1	D	199	ILE	3.5
1	D	53	PHE	3.5
1	D	16	PHE	3.4
1	A	288	ASN	3.4
1	D	49	LYS	3.4
1	D	261	SER	3.3
1	D	62	PHE	3.3
2	C	18	DG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	PRO	3.3
1	A	128	LEU	3.3
1	A	273	ALA	3.3
2	C	2	DT	3.3
1	D	230	SER	3.2
1	A	267	GLN	3.2
1	A	157	PRO	3.2
2	F	3	DA	3.1
1	A	241	ASN	3.1
2	F	7	DT	3.1
1	A	268	ASP	3.1
1	A	290	ILE	3.1
1	D	55	LEU	3.1
1	D	191	SER	3.1
1	D	194	VAL	3.1
1	D	48	ASP	3.0
1	A	131	ILE	3.0
1	A	238	THR	3.0
1	A	202	PHE	3.0
1	A	199	ILE	3.0
1	D	67	SER	3.0
2	F	20	DG	3.0
1	A	129	GLU	3.0
1	A	159	PRO	3.0
1	A	13	VAL	2.9
1	D	264	GLY	2.9
1	D	115	GLU	2.9
1	A	113	VAL	2.9
1	A	207	HIS	2.9
1	A	197	GLN	2.9
1	A	107	TYR	2.8
1	D	50	LYS	2.8
1	D	77	SER	2.8
2	F	16	DA	2.8
1	D	249	ILE	2.8
1	A	111	LYS	2.7
1	A	46	THR	2.7
1	A	22	SER	2.7
1	D	118	GLY	2.7
1	A	191	SER	2.7
1	A	193	LYS	2.7
1	A	109	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	197	GLN	2.7
1	D	37	TRP	2.7
1	D	263	TYR	2.7
1	A	293	LEU	2.7
1	A	118	GLY	2.7
1	D	177	SER	2.6
1	D	272	ILE	2.6
3	B	12	DA	2.6
3	B	1	DG	2.6
1	D	147	GLN	2.6
1	D	21	GLY	2.6
1	D	132	VAL	2.6
1	D	130	LYS	2.6
3	E	12	DA	2.6
1	A	37	TRP	2.6
1	D	259	ILE	2.6
1	D	241	ASN	2.6
1	D	180	GLY	2.6
1	A	36	GLY	2.5
1	D	238	THR	2.5
1	D	164	LYS	2.5
1	A	112	LYS	2.5
1	D	237	TYR	2.5
1	A	269	TRP	2.5
1	A	16	PHE	2.5
1	D	85	GLN	2.5
1	A	295	GLY	2.5
1	D	12	ALA	2.5
1	D	253	PHE	2.5
1	D	129	GLU	2.5
1	D	181	SER	2.5
1	D	58	LEU	2.4
2	F	18	DG	2.4
1	A	64	GLY	2.4
1	D	246	GLN	2.4
1	A	148	ALA	2.4
1	D	284	PRO	2.4
1	A	122	HIS	2.4
1	A	188	LYS	2.4
1	A	264	GLY	2.4
1	D	269	TRP	2.4
3	B	11	DG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	271	LYS	2.3
1	D	22	SER	2.3
1	A	27	VAL	2.3
1	A	130	LYS	2.3
1	A	173	ALA	2.3
1	D	46	THR	2.3
1	A	31	SER	2.3
3	E	11	DG	2.3
1	D	243	SER	2.3
2	F	8	DC	2.3
1	D	110	PHE	2.3
1	A	227	GLU	2.2
2	C	1	DC	2.2
1	A	127	GLY	2.2
1	A	126	ARG	2.2
1	A	139	ASN	2.2
1	D	208	ALA	2.2
1	A	261	SER	2.2
1	A	49	LYS	2.2
2	C	23	DC	2.2
3	E	10	DT	2.2
2	F	19	DT	2.2
1	A	226	ILE	2.2
1	D	89	ILE	2.2
3	E	1	DG	2.2
1	D	108	LEU	2.2
1	D	200	LEU	2.2
1	A	117	MET	2.1
1	A	201	VAL	2.1
1	A	177	SER	2.1
2	C	16	DA	2.1
1	D	92	PRO	2.1
1	D	79	ARG	2.1
2	C	20	DG	2.1
1	A	235	LEU	2.1
1	A	289	GLU	2.1
1	A	116	LEU	2.1
1	A	137	SER	2.1
1	D	131	ILE	2.1
1	A	125	GLN	2.1
1	D	242	PHE	2.1
1	D	244	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	79	ARG	2.0
1	A	38	LEU	2.0
1	D	260	GLY	2.0
1	D	188	LYS	2.0
1	D	266	TYR	2.0
1	D	90	ILE	2.0
1	A	77	SER	2.0
1	D	274	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. 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
4	CA	A	401	1/1	-0.12	1.05	21.75	439,439,439,439	0
4	CA	D	402	1/1	0.85	0.45	3.97	438,438,438,438	0
5	GOL	D	401	6/6	-0.06	2.07	-	439,439,439,439	0
5	GOL	C	101	6/6	0.27	1.08	-	420,421,421,421	0
5	GOL	F	101	6/6	0.22	0.92	-	420,420,420,420	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.