



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G4T  
Title : Mth0212 (WT) in complex with a 7bp dsDNA  
Authors : Lakomek, K.; Dickmanns, A.; Ficner, R.  
Deposited on : 2009-02-04  
Resolution : 2.64 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

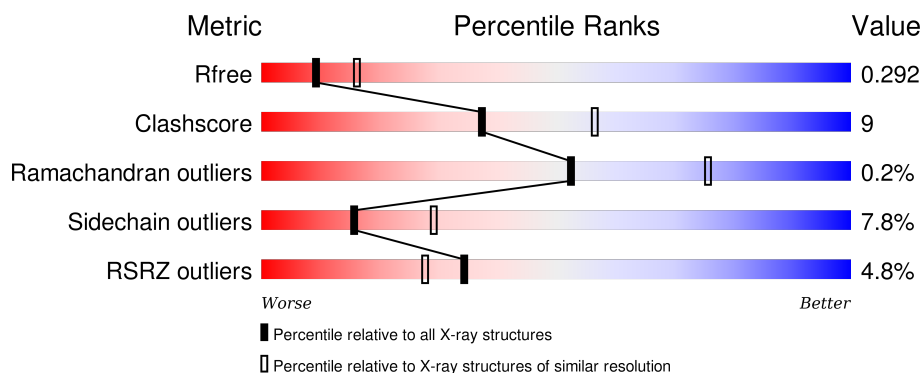
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	265	<div> <div>3%</div> <div>75%</div> <div>18%</div> <div>• •</div> </div>
1	B	265	<div> <div>7%</div> <div>77%</div> <div>16%</div> <div>• •</div> </div>
2	H	9	<div> <div>33%</div> <div>44%</div> <div>22%</div> </div>
3	I	9	<div> <div>11%</div> <div>44%</div> <div>22%</div> <div>22%</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
5	MG	A	267	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4559 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 Exodeoxyribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	1	0
			2122	1362	371	381	8			
1	B	255	Total	C	N	O	S	0	0	0
			2126	1365	372	380	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	ENGINEERED MUTATION	UNP O26314
A	258	LEU	-	EXPRESSION TAG	UNP O26314
A	259	GLU	-	EXPRESSION TAG	UNP O26314
A	260	HIS	-	EXPRESSION TAG	UNP O26314
A	261	HIS	-	EXPRESSION TAG	UNP O26314
A	262	HIS	-	EXPRESSION TAG	UNP O26314
A	263	HIS	-	EXPRESSION TAG	UNP O26314
A	264	HIS	-	EXPRESSION TAG	UNP O26314
A	265	HIS	-	EXPRESSION TAG	UNP O26314
B	2	ALA	THR	ENGINEERED MUTATION	UNP O26314
B	258	LEU	-	EXPRESSION TAG	UNP O26314
B	259	GLU	-	EXPRESSION TAG	UNP O26314
B	260	HIS	-	EXPRESSION TAG	UNP O26314
B	261	HIS	-	EXPRESSION TAG	UNP O26314
B	262	HIS	-	EXPRESSION TAG	UNP O26314
B	263	HIS	-	EXPRESSION TAG	UNP O26314
B	264	HIS	-	EXPRESSION TAG	UNP O26314
B	265	HIS	-	EXPRESSION TAG	UNP O26314

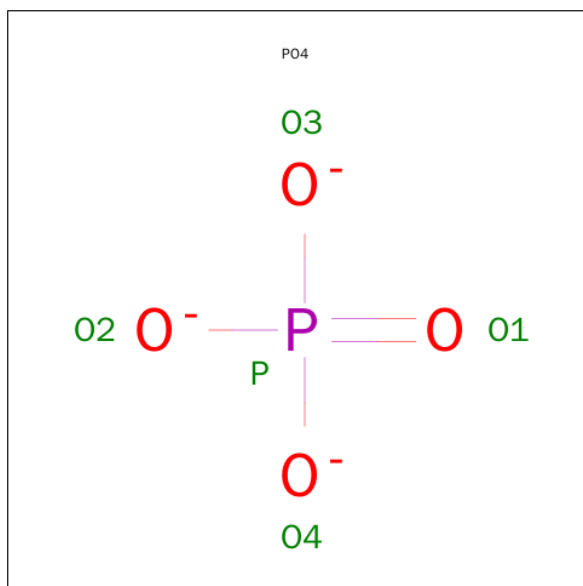
- Molecule 2 is a DNA chain called 5'-D(\*CP\*GP\*TP\*AP\*(UPS)P\*TP\*AP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	H	7	Total	C	N	O	P	S	0	0	0
			139	68	24	40	6	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		

- 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		

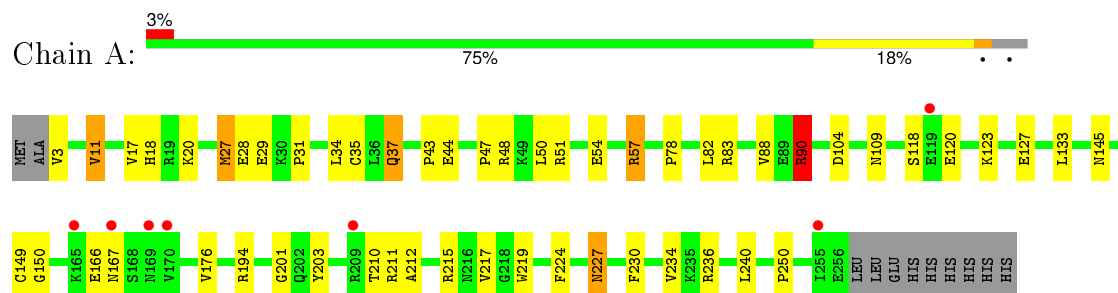
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total 13	O 13	0	0
6	B	2	Total 2	O 2	0	0
6	H	1	Total 1	O 1	0	0

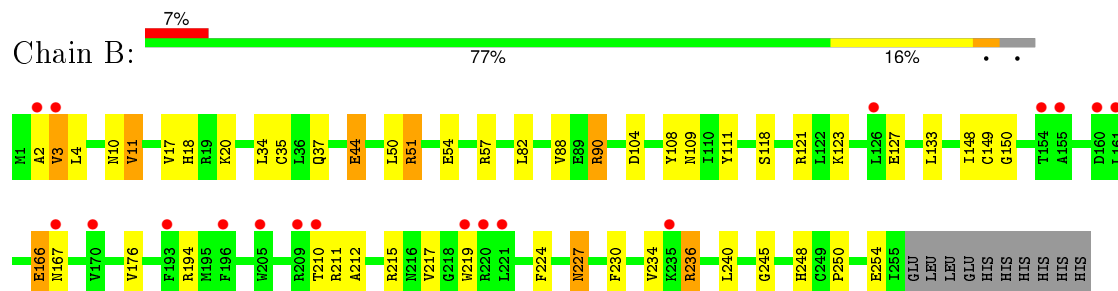
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Exodeoxyribonuclease



- Molecule 1: Exodeoxyribonuclease



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.76Å 79.60Å 99.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 2.64 44.58 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.4 (42.57-2.64) 97.4 (44.58-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.297 0.237 , 0.292	Depositor DCC
$R_{free}$ test set	1212 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.3	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23582 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: PO4, MG, UPS

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	0.51	0/2180	0.70	4/2939 (0.1%)
1	B	0.55	0/2184	0.70	5/2944 (0.2%)
2	H	0.92	0/133	1.65	3/201 (1.5%)
3	I	1.10	0/155	1.86	4/237 (1.7%)
All	All	0.57	0/4652	0.82	16/6321 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ARG	NE-CZ-NH1	-8.93	115.84	120.30
3	I	6	DT	O4'-C1'-N1	8.66	114.06	108.00
3	I	7	DA	P-O3'-C3'	7.91	129.19	119.70
1	A	236	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	236	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	90	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	236	ARG	NE-CZ-NH2	7.07	123.83	120.30
2	H	6	DT	P-O3'-C3'	6.36	127.33	119.70
1	A	90	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	90	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	B	90	ARG	NE-CZ-NH2	-6.16	117.22	120.30
3	I	8	DC	P-O3'-C3'	5.74	126.58	119.70
3	I	6	DT	N3-C2-O2	-5.70	118.88	122.30
1	B	82	LEU	CA-CB-CG	5.39	127.69	115.30
2	H	2	DG	C1'-O4'-C4'	-5.37	104.73	110.10
2	H	6	DT	O4'-C1'-N1	5.35	111.75	108.00

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	2122	0	2058	38	0
1	B	2126	0	2069	34	0
2	H	139	0	80	6	0
3	I	139	0	81	4	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	I	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	13	0	0	1	0
6	B	2	0	0	0	0
6	H	1	0	0	0	0
All	All	4559	0	4288	81	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 9.

All (81) 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:H:5:UPS:P	2:H:5:UPS:S1P	1.49	1.47
1:B:51:ARG:HB2	1:B:51:ARG:HH11	1.05	1.13
1:A:35:CYS:HB3	1:A:109:ASN:ND2	1.63	1.11
1:A:210:THR:HB	1:A:215:ARG:HH22	1.15	1.05
1:B:210:THR:HB	1:B:215:ARG:HH22	1.19	1.05
1:A:35:CYS:HB3	1:A:109:ASN:HD22	1.29	0.98
1:A:35:CYS:CB	1:A:109:ASN:HD22	1.78	0.97
1:B:51:ARG:CB	1:B:51:ARG:HH11	1.81	0.94
1:A:210:THR:HB	1:A:215:ARG:NH2	1.83	0.93
1:A:18:HIS:HD2	1:A:50:LEU:HG	1.35	0.92
1:B:210:THR:HB	1:B:215:ARG:NH2	1.86	0.90
1:A:35:CYS:CB	1:A:109:ASN:ND2	2.35	0.87
1:B:51:ARG:NH1	1:B:51:ARG:HB2	1.89	0.85
1:A:90:ARG:NH1	1:A:127:GLU:OE1	2.12	0.81
1:B:37:GLN:NE2	1:B:150:GLY:HA2	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:OD1	1:A:230:PHE:HD1	1.66	0.76
1:A:57:ARG:HH21	1:A:57:ARG:HG2	1.49	0.74
1:B:18:HIS:HD2	1:B:50:LEU:HG	1.53	0.74
1:B:2:ALA:O	1:B:3:VAL:HG22	1.90	0.72
1:A:227:ASN:HD21	1:A:230:PHE:HB2	1.56	0.71
2:H:4:DA:C3'	2:H:5:UPS:S1P	2.78	0.71
1:A:27[A]:MET:HG2	1:A:28:GLU:N	2.08	0.68
2:H:4:DA:O3'	2:H:5:UPS:S1P	2.50	0.67
2:H:5:UPS:O5'	2:H:5:UPS:S1P	2.49	0.66
1:B:227:ASN:HD21	1:B:230:PHE:HB2	1.59	0.66
1:A:18:HIS:CD2	1:A:50:LEU:HG	2.26	0.65
1:B:236:ARG:NH2	1:B:254:GLU:OE1	2.30	0.65
1:A:166:GLU:N	1:A:166:GLU:OE2	2.22	0.62
1:B:11:VAL:HG22	1:B:17:VAL:HG11	1.81	0.62
1:A:35:CYS:HB3	1:A:109:ASN:HD21	1.62	0.61
1:B:166:GLU:N	1:B:166:GLU:OE2	2.23	0.61
1:B:35:CYS:HB3	1:B:109:ASN:ND2	2.16	0.59
1:A:149:CYS:HB3	1:A:224:PHE:CE2	2.40	0.57
1:B:123:LYS:HE3	1:B:127:GLU:OE2	2.05	0.57
1:A:83:ARG:NH1	6:A:278:HOH:O	2.37	0.56
1:A:145:ASN:OD1	1:A:230:PHE:CD1	2.54	0.56
1:B:18:HIS:HD2	1:B:50:LEU:CG	2.18	0.56
3:I:3:DT:H5'	4:I:10:PO4:P	2.47	0.55
1:B:227:ASN:ND2	1:B:230:PHE:HB2	2.22	0.55
1:A:227:ASN:ND2	1:A:230:PHE:HB2	2.20	0.54
1:A:18:HIS:HD2	1:A:50:LEU:CG	2.14	0.53
1:B:18:HIS:CD2	1:B:50:LEU:HG	2.39	0.53
3:I:7:DA:H2''	3:I:8:DC:C5'	2.39	0.53
1:B:35:CYS:CB	1:B:109:ASN:ND2	2.72	0.53
1:A:43:PRO:O	1:A:51:ARG:HD3	2.09	0.52
1:A:123:LYS:HE3	1:A:127:GLU:OE2	2.09	0.52
1:B:240:LEU:HB2	1:B:250:PRO:HG2	1.93	0.51
1:A:47:PRO:HD2	1:A:50:LEU:HD12	1.93	0.50
1:B:149:CYS:HB3	1:B:224:PHE:CE2	2.45	0.50
1:B:240:LEU:N	1:B:240:LEU:HD12	2.27	0.50
2:H:4:DA:C2'	2:H:5:UPS:S1P	3.00	0.49
1:A:227:ASN:HD22	1:A:227:ASN:C	2.17	0.47
1:A:118:SER:OG	1:A:120:GLU:HG2	2.15	0.46
1:B:167:ASN:ND2	1:B:219:TRP:CZ2	2.81	0.46
1:A:11:VAL:HG22	1:A:17:VAL:HG11	1.96	0.46
2:H:4:DA:H3'	2:H:5:UPS:S1P	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:CYS:HB3	1:A:224:PHE:CD2	2.51	0.45
1:A:210:THR:OG1	1:A:212:ALA:HB2	2.15	0.45
1:A:57:ARG:HD3	1:A:78:PRO:HG3	1.99	0.45
1:A:167:ASN:ND2	1:A:219:TRP:CZ2	2.85	0.45
1:B:108:TYR:HB2	1:B:148:ILE:HA	1.98	0.44
1:B:10:ASN:HB3	1:B:248:HIS:CG	2.52	0.44
1:A:20:LYS:NZ	3:I:5:DC:OP1	2.49	0.44
1:A:240:LEU:HB2	1:A:250:PRO:HG2	1.99	0.44
1:B:44:GLU:H	1:B:44:GLU:CD	2.21	0.43
1:B:215:ARG:HB3	1:B:217:VAL:HG23	2.01	0.43
1:B:37:GLN:HB3	1:B:111:TYR:HB2	2.00	0.43
1:A:194:ARG:HD3	1:A:194:ARG:HA	1.86	0.43
1:B:194:ARG:HA	1:B:194:ARG:HD3	1.86	0.42
1:A:215:ARG:HB3	1:A:217:VAL:HG23	2.01	0.42
3:I:3:DT:H2''	3:I:4:DA:H5'	2.01	0.42
1:B:227:ASN:C	1:B:227:ASN:HD22	2.22	0.42
1:A:201:GLY:HA2	1:A:203:TYR:CZ	2.54	0.42
1:A:57:ARG:HG2	1:A:57:ARG:NH2	2.26	0.41
1:A:37:GLN:NE2	1:A:150:GLY:HA2	2.35	0.41
1:B:149:CYS:HB3	1:B:224:PHE:CD2	2.56	0.40
1:B:51:ARG:CG	1:B:51:ARG:HH11	2.33	0.40
1:B:20:LYS:HD3	1:B:245:GLY:HA2	2.02	0.40
1:B:121:ARG:HD2	1:B:121:ARG:HA	1.85	0.40
1:B:210:THR:OG1	1:B:212:ALA:HB2	2.20	0.40
1:A:29:GLU:O	1:A:31:PRO:HD3	2.21	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	252/265 (95%)	246 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	253/265 (96%)	247 (98%)	5 (2%)	1 (0%)	39	63
All	All	505/530 (95%)	493 (98%)	11 (2%)	1 (0%)	52	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	VAL

### 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	225/235 (96%)	207 (92%)	18 (8%)	15	28
1	B	225/235 (96%)	208 (92%)	17 (8%)	16	30
All	All	450/470 (96%)	415 (92%)	35 (8%)	16	29

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	11	VAL
1	A	27[A]	MET
1	A	34	LEU
1	A	37	GLN
1	A	44	GLU
1	A	48	ARG
1	A	54	GLU
1	A	57	ARG
1	A	82	LEU
1	A	88	VAL
1	A	90	ARG
1	A	104	ASP
1	A	133	LEU
1	A	176	VAL

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	227	ASN
1	A	234	VAL
1	B	4	LEU
1	B	11	VAL
1	B	34	LEU
1	B	44	GLU
1	B	51	ARG
1	B	54	GLU
1	B	57	ARG
1	B	88	VAL
1	B	90	ARG
1	B	104	ASP
1	B	118	SER
1	B	133	LEU
1	B	166	GLU
1	B	176	VAL
1	B	211	ARG
1	B	227	ASN
1	B	234	VAL

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

Mol	Chain	Res	Type
1	A	18	HIS
1	A	145	ASN
1	B	18	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	UPS	H	5	2	11,20,21	1.20	1 (9%)	17,28,31	3.16	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UPS	H	5	2	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	5	UPS	C4-N3	2.89	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	UPS	C5-C4-N3	-3.17	114.99	123.12
2	H	5	UPS	C4-N3-C2	12.39	126.42	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	5	UPS	6	0

## 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	$\# Z  > 2$
4	PO4	A	266	5	4,4,4	0.39	0	6,6,6	0.31	0
4	PO4	B	266	5	4,4,4	0.38	0	6,6,6	0.27	0
4	PO4	I	10	-	4,4,4	0.44	0	6,6,6	0.28	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
4	PO4	A	266	5	-	0/0/0/0	0/0/0/0
4	PO4	B	266	5	-	0/0/0/0	0/0/0/0
4	PO4	I	10	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	10	PO4	1	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	254/265 (95%)	0.37	7 (2%) 56 50	48, 65, 78, 84	1 (0%)
1	B	255/265 (96%)	0.33	18 (7%) 19 13	50, 70, 85, 90	0
2	H	6/9 (66%)	-0.17	0 100 100	65, 69, 85, 98	0
3	I	7/9 (77%)	-0.07	0 100 100	60, 67, 76, 86	0
All	All	522/548 (95%)	0.34	25 (4%) 34 28	48, 67, 83, 98	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	5.0
1	B	170	VAL	4.8
1	A	167	ASN	4.4
1	A	209	ARG	3.9
1	A	170	VAL	3.8
1	A	165	LYS	3.5
1	B	161	LEU	3.2
1	B	154	THR	3.1
1	B	219	TRP	2.9
1	B	193	PHE	2.8
1	B	220	ARG	2.8
1	B	167	ASN	2.7
1	B	3	VAL	2.6
1	A	169	ASN	2.6
1	B	221	LEU	2.5
1	B	2	ALA	2.4
1	B	235	LYS	2.4
1	B	210	THR	2.4
1	B	209	ARG	2.2
1	A	119	GLU	2.2
1	A	255	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	196	PHE	2.2
1	B	205	TRP	2.2
1	B	160	ASP	2.1
1	B	126	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	UPS	H	5	19/20	0.95	0.13	-	60,68,69,69	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	267	1/1	0.89	0.46	9.65	77,77,77,77	0
5	MG	B	267	1/1	0.91	0.27	1.54	80,80,80,80	0
4	PO4	B	266	5/5	0.94	0.16	-0.82	74,75,76,78	0
4	PO4	A	266	5/5	0.94	0.13	-1.75	59,63,64,66	0
4	PO4	I	10	5/5	0.66	0.77	-	164,165,165,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.