



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 12:10 AM JST

PDB ID : 7W5P  
Title : Crystal Structure of the dioxygenase CcTet from Coprinopsis cinerea bound to 12bp N6-methyldeoxyadenine (6mA) containing duplex DNA  
Authors : Mu, Y.J.; Zhang, L.; Zhang, L.  
Deposited on : 2021-11-30  
Resolution : 2.30 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 : 2.27  
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) : 2.27

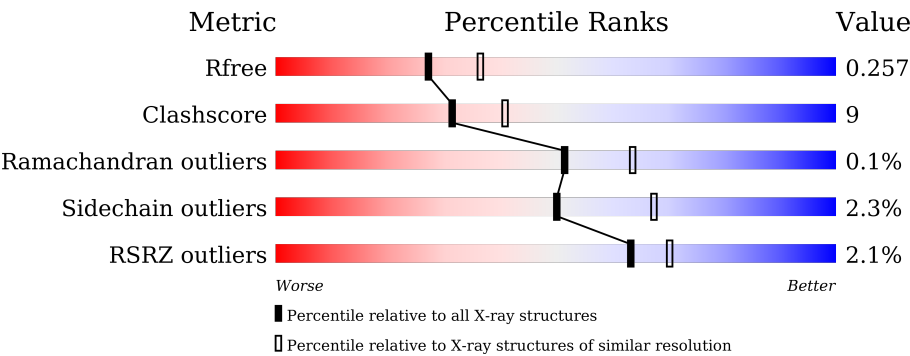
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	430	<div><div>2%</div><div></div><div>73%</div><div>14%</div><div>•</div><div>11%</div></div>
1	D	430	<div><div>2%</div><div></div><div>68%</div><div>17%</div><div>•</div><div>12%</div></div>
1	G	430	<div><div>%</div><div></div><div>73%</div><div>14%</div><div>•</div><div>12%</div></div>
1	H	430	<div><div>2%</div><div></div><div>69%</div><div>15%</div><div>•</div><div>13%</div></div>
2	B	12	<div><div></div><div>67%</div><div>17%</div><div>17%</div></div>
2	E	12	<div><div></div><div>50%</div><div>42%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	12	 33% 67%
3	F	12	 75% 25%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13728 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 CcTet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2992	1912	532	534	14			
1	D	377	Total	C	N	O	S	0	0	0
			2953	1887	524	528	14			
1	G	378	Total	C	N	O	S	0	0	0
			2966	1895	526	531	14			
1	H	372	Total	C	N	O	S	0	0	0
			2917	1867	514	522	14			

- Molecule 2 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			246	117	46	71	12			
2	E	12	Total	C	N	O	P	0	0	0
			246	117	46	71	12			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			249	117	48	72	12			
3	F	12	Total	C	N	O	P	0	0	0
			249	117	48	72	12			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

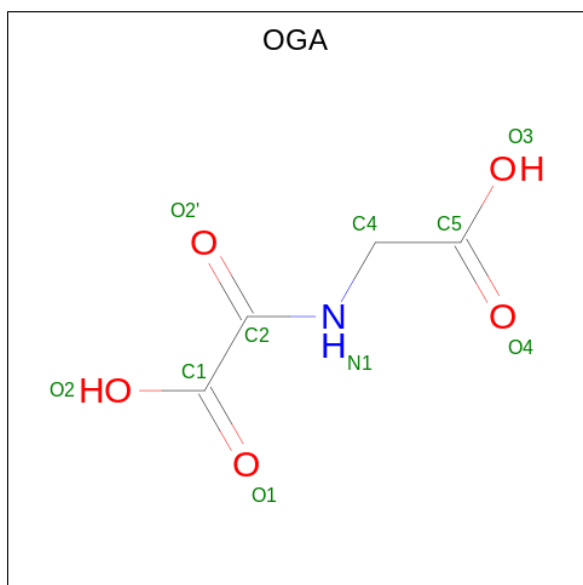
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mn	0	0
			1	1		
4	H	1	Total	Mn	0	0
			1	1		

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula:  $C_4H_5NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		
5	D	1	Total	C	N	O	0	0
			10	4	1	5		
5	G	1	Total	C	N	O	0	0
			10	4	1	5		
5	H	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total	O	0	0
			186	186		
6	B	26	Total	O	0	0
			26	26		
6	C	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	207	Total 207	O 207	0	0
6	E	27	Total 27	O 27	0	0
6	F	24	Total 24	O 24	0	0
6	G	214	Total 214	O 214	0	0
6	H	161	Total 161	O 161	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.79Å 105.20Å 196.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.30 49.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.18-2.30) 99.1 (49.18-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.228 , 0.257 0.228 , 0.257	Depositor DCC
$R_{free}$ test set	4828 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.068 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MN, 6MA, OGA

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	0.57	6/3070 (0.2%)	0.62	6/4176 (0.1%)
1	D	0.75	10/3030 (0.3%)	0.79	11/4123 (0.3%)
1	G	0.63	7/3041 (0.2%)	0.68	6/4135 (0.1%)
1	H	0.63	6/2992 (0.2%)	0.68	9/4070 (0.2%)
2	B	0.78	0/249	1.09	1/379 (0.3%)
2	E	0.73	0/249	1.07	2/379 (0.5%)
3	C	0.71	0/279	1.01	0/429
3	F	0.67	0/279	1.01	0/429
All	All	0.65	29/13189 (0.2%)	0.73	35/18120 (0.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	141	PRO	N-CA	12.35	1.68	1.47
1	D	122	GLU	CD-OE2	-12.07	1.12	1.25
1	D	141	PRO	N-CA	11.79	1.67	1.47
1	G	141	PRO	N-CA	11.35	1.66	1.47
1	H	238	LEU	C-N	9.09	1.51	1.34
1	D	122	GLU	CD-OE1	-8.39	1.16	1.25
1	D	113	GLU	CD-OE1	-8.18	1.16	1.25
1	D	113	GLU	CD-OE2	-7.63	1.17	1.25
1	D	145	SER	C-N	7.53	1.48	1.34
1	G	145	SER	C-N	7.41	1.48	1.34
1	H	145	SER	C-N	7.35	1.48	1.34
1	A	137	PHE	C-O	-7.25	1.09	1.23
1	D	142	SER	C-O	-6.51	1.10	1.23
1	D	137	PHE	C-O	-6.42	1.11	1.23
1	G	380	GLU	CD-OE2	-6.12	1.19	1.25
1	H	143	CYS	C-O	-5.90	1.12	1.23
1	G	258	ASP	C-N	-5.75	1.20	1.34
1	A	139	TYR	C-O	-5.70	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	SER	CA-CB	-5.70	1.44	1.52
1	A	201	GLY	C-O	-5.69	1.14	1.23
1	G	142	SER	C-O	-5.67	1.12	1.23
1	A	204	TRP	C-O	-5.62	1.12	1.23
1	A	142	SER	C-O	-5.34	1.13	1.23
1	G	204	TRP	C-O	-5.29	1.13	1.23
1	D	122	GLU	C-O	-5.26	1.13	1.23
1	H	21	LEU	C-O	-5.21	1.13	1.23
1	G	143	CYS	C-O	-5.15	1.13	1.23
1	D	259	ILE	C-N	-5.11	1.24	1.34
1	H	142	SER	C-O	-5.01	1.13	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	LYS	CA-CB-CG	10.30	136.07	113.40
1	D	117	ASP	N-CA-C	9.63	137.00	111.00
1	D	116	SER	C-N-CA	9.11	144.48	121.70
1	D	163	LYS	CB-CG-CD	8.64	134.06	111.60
1	H	286	ARG	CG-CD-NE	-8.21	94.55	111.80
2	B	9	DT	O4'-C1'-N1	7.21	113.05	108.00
1	G	141	PRO	CA-N-CD	-7.21	101.41	111.50
1	A	229	TRP	CA-CB-CG	7.03	127.06	113.70
1	D	163	LYS	CG-CD-CE	-6.90	91.20	111.90
1	H	238	LEU	O-C-N	-6.75	108.28	121.10
1	D	118	HIS	N-CA-CB	-6.71	98.52	110.60
1	H	333	ILE	CG1-CB-CG2	-6.52	97.05	111.40
1	H	238	LEU	CA-C-N	6.50	135.29	117.10
1	D	141	PRO	CA-N-CD	-6.39	102.56	111.50
1	H	159	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	A	174	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	H	24	ASP	CB-CA-C	-6.18	98.03	110.40
1	H	141	PRO	CA-N-CD	-6.06	103.02	111.50
1	H	213	GLN	CA-CB-CG	-6.05	100.10	113.40
1	G	170	LYS	CD-CE-NZ	-6.01	97.88	111.70
1	A	172	ARG	CA-CB-CG	5.84	126.25	113.40
1	D	115	ASN	CB-CA-C	5.82	122.03	110.40
2	E	9	DT	P-O3'-C3'	5.62	126.44	119.70
1	G	174	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	229	TRP	N-CA-CB	-5.42	100.84	110.60
1	H	32	ARG	CG-CD-NE	5.40	123.14	111.80
1	G	106	LYS	CB-CA-C	-5.40	99.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	217	LYS	CB-CG-CD	5.37	125.57	111.60
1	D	396	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	209	ASP	CB-CA-C	-5.30	99.79	110.40
2	E	9	DT	OP1-P-O3'	5.20	116.64	105.20
1	A	205	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	D	229	TRP	N-CA-CB	-5.10	101.42	110.60
1	D	286	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	177	GLU	CB-CA-C	5.01	120.43	110.40

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	2992	0	3009	43	0
1	D	2953	0	2967	66	0
1	G	2966	0	2981	44	0
1	H	2917	0	2930	57	0
2	B	246	0	137	8	0
2	E	246	0	137	8	0
3	C	249	0	135	6	0
3	F	249	0	135	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	10	0	3	0	0
5	D	10	0	3	0	0
5	G	10	0	3	0	0
5	H	10	0	3	0	0
6	A	186	0	0	13	2
6	B	26	0	0	2	0
6	C	21	0	0	1	0
6	D	207	0	0	15	2
6	E	27	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	24	0	0	2	0
6	G	214	0	0	9	3
6	H	161	0	0	9	1
All	All	13728	0	12443	227	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 9.

All (227) 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:H:141:PRO:N	1:H:141:PRO:CA	1.68	1.36
1:D:167:LEU:HD22	1:D:223:LEU:HD11	1.38	1.05
1:G:234:HIS:HB3	1:G:237:GLN:CD	1.79	1.01
1:H:171:SER:HA	1:H:174:ARG:HE	1.32	0.94
1:D:73:ARG:NE	6:D:602:HOH:O	1.98	0.93
2:E:9:DT:H2''	2:E:10:DA:C8	2.08	0.88
1:G:203:ASN:O	1:G:203:ASN:ND2	2.06	0.87
1:D:56:ILE:O	6:D:601:HOH:O	1.93	0.86
1:G:344:ASN:O	1:G:344:ASN:ND2	2.08	0.85
1:G:234:HIS:HB3	1:G:237:GLN:OE1	1.77	0.84
1:D:99:ASN:ND2	6:D:604:HOH:O	2.11	0.83
1:A:394:GLU:OE1	6:A:601:HOH:O	1.97	0.82
1:A:164:ASP:OD1	1:A:172:ARG:NH1	2.13	0.81
1:H:86:MET:SD	1:H:333:ILE:CG2	2.70	0.80
1:D:167:LEU:CD2	1:D:223:LEU:HD11	2.12	0.79
1:A:162:THR:O	1:A:168:GLN:NE2	2.15	0.79
1:D:20:LEU:HB3	1:D:286:ARG:NH1	1.98	0.78
1:G:182:GLU:N	1:G:182:GLU:OE1	2.17	0.77
1:G:334:GLU:HB3	1:G:407:PRO:HD3	1.66	0.77
1:G:24:ASP:OD2	6:G:601:HOH:O	2.03	0.77
1:H:236:ASN:H	1:H:236:ASN:HD22	1.29	0.77
1:G:203:ASN:HD21	1:G:206:GLU:HB2	1.49	0.77
1:D:320:ASN:HD21	1:D:384:GLU:HA	1.50	0.76
1:A:174:ARG:NH1	1:A:206:GLU:O	2.19	0.76
2:B:9:DT:H2''	2:B:10:DA:N7	2.01	0.76
1:D:17:LEU:HD12	1:D:18:PRO:HD2	1.68	0.76
1:D:33:MET:HE2	1:D:62:TRP:CE2	2.21	0.75
1:H:279:GLU:OE1	6:H:601:HOH:O	2.03	0.75
1:H:236:ASN:H	1:H:236:ASN:ND2	1.80	0.75
3:C:3:DT:OP2	6:C:101:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:5:DG:OP2	6:F:101:HOH:O	2.05	0.74
1:A:232:VAL:O	1:A:234:HIS:HD2	1.71	0.73
1:D:248:PRO:HA	1:D:253:ARG:NH2	2.04	0.73
2:E:9:DT:OP2	6:E:101:HOH:O	2.05	0.73
2:B:10:DA:OP1	6:B:101:HOH:O	2.07	0.72
1:A:135:ILE:O	6:A:603:HOH:O	2.08	0.71
1:G:231:PRO:HG2	1:G:234:HIS:HB2	1.72	0.71
1:D:33:MET:HE1	1:D:62:TRP:CD1	2.26	0.71
1:A:235:GLU:OE2	6:A:604:HOH:O	2.09	0.70
1:H:86:MET:SD	1:H:333:ILE:HG21	2.31	0.70
1:A:334:GLU:HB3	1:A:407:PRO:HD3	1.73	0.70
1:H:174:ARG:HH11	1:H:208:LEU:HD22	1.55	0.70
1:H:177:GLU:O	6:H:602:HOH:O	2.08	0.70
1:G:83:ARG:NH1	6:G:605:HOH:O	2.25	0.69
1:A:398:ASP:OD2	6:A:605:HOH:O	2.11	0.68
1:H:86:MET:CE	1:H:333:ILE:HG21	2.23	0.68
1:D:167:LEU:HD22	1:D:223:LEU:CD1	2.19	0.68
2:B:9:DT:H4'	6:B:101:HOH:O	1.93	0.67
1:H:174:ARG:HD2	1:H:208:LEU:HD21	1.75	0.67
1:D:163:LYS:O	6:D:606:HOH:O	2.14	0.65
1:D:29:VAL:HG21	1:D:51:ILE:HG13	1.78	0.65
1:A:73:ARG:NH2	6:A:613:HOH:O	2.30	0.65
2:E:2:DG:OP2	6:E:102:HOH:O	2.14	0.65
1:G:234:HIS:ND1	1:G:237:GLN:OE1	2.30	0.64
1:H:171:SER:HA	1:H:174:ARG:NE	2.09	0.64
1:A:100:ARG:HD3	1:H:21:LEU:HD11	1.80	0.64
1:H:203:ASN:N	6:H:611:HOH:O	2.29	0.64
1:H:259:ILE:C	1:H:259:ILE:HD12	2.18	0.64
2:B:9:DT:H2''	2:B:10:DA:C8	2.32	0.64
3:F:12:DG:H8	1:G:18:PRO:HB2	1.61	0.64
1:D:246:LYS:HE3	1:D:297:ASP:OD2	1.98	0.63
1:H:259:ILE:CD1	1:H:259:ILE:O	2.45	0.63
1:D:300:THR:O	1:D:304:ILE:HG12	1.98	0.63
3:C:12:DG:H8	1:H:18:PRO:HB2	1.63	0.63
1:D:17:LEU:HD11	1:D:306:GLU:HG2	1.81	0.63
1:H:141:PRO:N	1:H:141:PRO:C	2.52	0.62
1:D:245:LEU:HB3	1:D:304:ILE:HD12	1.82	0.62
1:D:20:LEU:HB3	1:D:286:ARG:HH12	1.64	0.62
1:G:108:PHE:O	6:G:602:HOH:O	2.16	0.62
1:G:259:ILE:N	1:G:260:PRO:CD	2.63	0.61
1:H:259:ILE:HD12	1:H:259:ILE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:MET:HE3	1:H:333:ILE:HG21	1.81	0.61
1:D:167:LEU:CD2	1:D:223:LEU:CD1	2.76	0.61
1:D:146:PRO:O	6:D:607:HOH:O	2.16	0.61
1:A:106:LYS:NZ	6:A:615:HOH:O	2.33	0.60
1:D:20:LEU:CD2	1:D:286:ARG:HG3	2.32	0.60
2:E:9:DT:H4'	2:E:10:DA:OP1	2.03	0.59
3:F:12:DG:C8	1:G:18:PRO:HB2	2.37	0.59
1:H:174:ARG:HD2	1:H:208:LEU:CD2	2.32	0.59
1:D:33:MET:CE	1:D:62:TRP:CE2	2.86	0.58
1:H:334:GLU:HB3	1:H:407:PRO:HD3	1.85	0.58
1:A:41:ILE:O	6:A:606:HOH:O	2.17	0.58
1:D:33:MET:HE1	1:D:62:TRP:CG	2.38	0.58
1:G:120:VAL:N	6:G:611:HOH:O	2.36	0.58
1:D:393:ARG:NH1	6:D:612:HOH:O	2.22	0.58
1:H:96:ARG:NH2	1:H:201:GLY:O	2.37	0.58
1:H:100:ARG:HD2	6:H:676:HOH:O	2.03	0.57
1:D:232:VAL:O	1:D:234:HIS:HD2	1.87	0.57
1:G:96:ARG:NH2	1:G:201:GLY:O	2.35	0.56
1:A:88:GLU:OE1	6:A:608:HOH:O	2.18	0.56
2:B:8:DC:H2''	2:B:9:DT:C6	2.41	0.56
1:D:115:ASN:ND2	6:D:621:HOH:O	2.39	0.56
1:H:79:PRO:O	6:H:603:HOH:O	2.18	0.56
1:D:20:LEU:HD23	1:D:286:ARG:HG3	1.86	0.56
1:A:105:ALA:O	6:A:607:HOH:O	2.17	0.55
1:H:70:LYS:NZ	6:H:617:HOH:O	2.38	0.55
1:G:86:MET:HG2	1:G:333:ILE:HD11	1.90	0.53
1:D:259:ILE:N	1:D:260:PRO:CD	2.71	0.53
1:G:47:GLU:OE2	6:G:603:HOH:O	2.18	0.53
1:G:159:LEU:HG	1:G:255:PHE:HB2	1.90	0.53
1:G:234:HIS:CB	1:G:237:GLN:OE1	2.51	0.53
3:C:12:DG:C8	1:H:18:PRO:HB2	2.42	0.53
1:H:162:THR:O	1:H:168:GLN:HG3	2.09	0.53
1:D:248:PRO:HA	1:D:253:ARG:HH21	1.73	0.52
1:A:72:TYR:HA	1:A:127:MET:HE3	1.90	0.52
1:G:287:GLU:OE1	6:G:604:HOH:O	2.19	0.52
1:D:22:LEU:HD12	1:D:50:SER:HB3	1.92	0.52
1:D:152:ILE:HD11	1:D:262:ALA:HB1	1.91	0.51
1:D:19:SER:HA	1:D:309:PHE:CE2	2.46	0.51
1:D:20:LEU:HD23	1:D:286:ARG:CG	2.41	0.50
1:D:255:PHE:O	1:D:259:ILE:HG13	2.12	0.50
3:C:10:DT:H2''	3:C:11:DC:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LEU:O	6:D:609:HOH:O	2.19	0.49
1:D:107:GLU:OE2	6:D:610:HOH:O	2.20	0.49
1:D:224:THR:HG21	1:D:229:TRP:CZ2	2.48	0.49
1:D:329:THR:HA	1:D:372:LYS:HD3	1.94	0.49
1:D:76:TYR:HB2	1:D:128:ILE:HD13	1.95	0.49
1:D:334:GLU:HB3	1:D:407:PRO:HD3	1.95	0.49
1:H:123:ILE:HG12	1:H:360:THR:OG1	2.13	0.49
1:H:160:ALA:HB1	1:H:219:THR:H	1.79	0.48
1:H:259:ILE:HD13	1:H:263:SER:OG	2.13	0.48
1:D:288:LEU:O	1:D:298:HIS:HE1	1.97	0.48
1:G:259:ILE:HG13	1:G:259:ILE:O	2.12	0.48
1:A:406:TYR:CG	1:A:407:PRO:HD2	2.47	0.48
1:H:82:ALA:HB2	1:H:136:LEU:HD21	1.95	0.48
1:D:271:ALA:O	1:D:275:GLN:HG3	2.13	0.48
1:G:132:GLU:HB3	6:G:606:HOH:O	2.13	0.48
1:A:174:ARG:NH2	1:A:206:GLU:HB2	2.30	0.47
2:E:8:DC:H2"	2:E:9:DT:C5	2.49	0.47
2:E:9:DT:H2"	2:E:10:DA:N7	2.30	0.47
1:D:20:LEU:CB	1:D:286:ARG:NH1	2.74	0.47
1:H:20:LEU:HA	1:H:23:ILE:HG12	1.96	0.47
1:D:320:ASN:ND2	6:D:623:HOH:O	2.44	0.47
1:A:407:PRO:HB3	6:A:603:HOH:O	2.15	0.46
1:D:313:SER:HB2	1:D:392:TRP:HA	1.97	0.46
1:G:158:THR:O	1:G:162:THR:HG23	2.16	0.46
1:A:275:GLN:O	1:A:279:GLU:HG3	2.15	0.46
1:A:92:ARG:NH1	6:A:629:HOH:O	2.49	0.46
1:D:163:LYS:HB3	1:D:164:ASP:CG	2.36	0.46
1:H:259:ILE:C	1:H:259:ILE:CD1	2.83	0.46
1:D:212:ARG:NH2	6:D:628:HOH:O	2.49	0.46
3:F:12:DG:C4	1:G:22:LEU:HD12	2.51	0.46
1:D:170:LYS:HE3	6:D:639:HOH:O	2.17	0.45
1:G:217:LYS:H	1:G:384:GLU:CD	2.19	0.45
1:A:163:LYS:O	1:A:168:GLN:OE1	2.35	0.45
1:H:136:LEU:HD23	1:H:370:LEU:HD12	1.97	0.45
1:G:351:VAL:O	1:G:376:HIS:HA	2.17	0.45
1:H:160:ALA:HB1	1:H:219:THR:N	2.32	0.45
1:A:224:THR:HG21	1:A:229:TRP:CZ2	2.52	0.45
1:A:334:GLU:CB	1:A:407:PRO:HD3	2.43	0.44
1:D:225:PHE:HB3	1:D:245:LEU:HD11	2.00	0.44
1:G:278:PHE:CD1	1:G:311:PRO:HG3	2.52	0.44
1:A:217:LYS:HE2	1:A:384:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LYS:HE3	1:G:222:VAL:O	2.18	0.44
1:H:209:ASP:OD1	1:H:209:ASP:N	2.51	0.44
1:D:230:TRP:CZ3	1:D:395:ARG:HB3	2.53	0.44
1:D:396:LEU:HA	1:D:396:LEU:HD23	1.46	0.44
1:G:259:ILE:N	1:G:260:PRO:HD2	2.33	0.44
1:H:345:TYR:HE2	1:H:348:GLY:HA3	1.82	0.44
1:G:73:ARG:NH1	6:G:622:HOH:O	2.51	0.44
1:G:100:ARG:O	1:G:104:MET:HG2	2.18	0.44
1:A:176:GLY:N	6:A:618:HOH:O	2.40	0.44
1:D:294:LEU:O	6:D:611:HOH:O	2.20	0.44
1:D:229:TRP:HD1	2:E:8:DC:OP1	2.01	0.43
1:G:292:SER:HA	1:G:298:HIS:CE1	2.53	0.43
1:H:100:ARG:O	1:H:104:MET:HG2	2.18	0.43
1:A:38:ARG:NH2	1:A:413:SER:OG	2.48	0.43
1:A:86:MET:SD	1:A:373:LEU:HD12	2.58	0.43
1:D:351:VAL:O	1:D:376:HIS:HA	2.18	0.43
1:H:69:GLU:OE2	6:H:604:HOH:O	2.21	0.43
1:H:230:TRP:HB3	1:H:235:GLU:HG2	2.00	0.43
1:A:391:PHE:HB3	2:B:6:6MA:H13	2.01	0.43
1:H:104:MET:HB2	6:H:624:HOH:O	2.17	0.43
1:D:20:LEU:HD21	1:D:286:ARG:HG3	2.00	0.43
1:A:225:PHE:HB3	1:A:245:LEU:HD11	2.00	0.43
1:D:178:ARG:HA	1:D:178:ARG:HD2	1.84	0.43
1:D:224:THR:HG21	1:D:229:TRP:HZ2	1.83	0.43
1:D:271:ALA:HB2	1:D:278:PHE:CG	2.54	0.43
1:A:20:LEU:HA	1:A:23:ILE:HG12	2.01	0.43
1:A:90:THR:OG1	1:A:93:GLN:HB2	2.19	0.43
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.93	0.42
3:C:6:DC:H2'	3:C:7:DG:C5	2.54	0.42
1:G:288:LEU:O	1:G:298:HIS:HE1	2.02	0.42
1:H:76:TYR:HB2	1:H:128:ILE:HD13	2.01	0.42
1:H:332:PRO:HB3	1:H:394:GLU:HB2	1.99	0.42
1:A:393:ARG:HH22	2:B:6:6MA:H8	1.84	0.42
1:H:211:PHE:O	1:H:213:GLN:HG2	2.20	0.42
1:A:172:ARG:O	1:A:175:GLU:HB3	2.18	0.42
1:D:33:MET:CE	1:D:62:TRP:NE1	2.82	0.42
1:D:46:THR:N	6:D:603:HOH:O	1.98	0.42
1:A:22:LEU:HD23	1:A:50:SER:HB2	2.02	0.42
1:H:45:HIS:NE2	1:H:51:ILE:HB	2.34	0.42
1:H:220:PRO:HA	1:H:319:VAL:O	2.20	0.42
1:G:297:ASP:N	6:G:623:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:TYR:CG	1:G:407:PRO:HD2	2.55	0.42
1:D:92:ARG:NE	6:D:631:HOH:O	2.53	0.42
1:G:60:ALA:CB	1:G:148:ILE:HD12	2.50	0.42
1:G:159:LEU:HD12	1:G:255:PHE:CD1	2.55	0.42
1:H:230:TRP:CB	1:H:235:GLU:HG2	2.50	0.42
1:H:122:GLU:HA	6:H:616:HOH:O	2.20	0.42
1:A:313:SER:HB2	1:A:392:TRP:HA	2.02	0.41
1:D:20:LEU:HD23	1:D:286:ARG:NH1	2.35	0.41
1:H:157:GLY:O	1:H:161:THR:OG1	2.25	0.41
1:A:393:ARG:HH22	2:B:6:6MA:C8	2.33	0.41
1:G:340:VAL:HG22	1:G:366:VAL:HG22	2.02	0.41
1:H:99:ASN:O	1:H:103:VAL:HG23	2.19	0.41
1:H:167:LEU:HG	1:H:223:LEU:HD11	2.02	0.41
3:C:1:DC:H2'	3:C:2:DG:C8	2.55	0.41
1:D:303:LYS:HD3	1:D:303:LYS:HA	1.80	0.41
1:G:174:ARG:CD	1:G:208:LEU:HG	2.50	0.41
1:H:90:THR:OG1	1:H:93:GLN:HB2	2.20	0.41
1:A:351:VAL:O	1:A:376:HIS:HA	2.20	0.41
1:A:408:SER:HA	6:A:611:HOH:O	2.20	0.41
1:G:120:VAL:HG12	1:G:121:GLN:H	1.84	0.41
1:G:234:HIS:HB3	1:G:237:GLN:NE2	2.29	0.41
1:H:278:PHE:CD1	1:H:311:PRO:HG3	2.56	0.41
1:D:22:LEU:HD12	1:D:50:SER:CB	2.50	0.41
1:H:351:VAL:O	1:H:376:HIS:HA	2.21	0.41
1:D:29:VAL:O	1:D:33:MET:HG3	2.21	0.41
1:H:114:LEU:HD23	1:H:357:ARG:CZ	2.51	0.41
1:A:20:LEU:HD12	1:A:286:ARG:HG3	2.03	0.40
2:E:12:DG:OP2	6:E:103:HOH:O	2.22	0.40
1:A:86:MET:SD	1:A:89:LEU:HD12	2.62	0.40
3:F:6:DC:OP2	6:F:102:HOH:O	2.22	0.40
1:G:332:PRO:HB3	1:G:394:GLU:HB2	2.02	0.40
1:H:232:VAL:O	1:H:232:VAL:HG13	2.20	0.40
1:A:345:TYR:CZ	1:A:363:PRO:HD3	2.56	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:A:758:HOH:O	6:G:757:HOH:O[4_565]	1.97	0.23
6:A:783:HOH:O	6:G:801:HOH:O[4_555]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:787:HOH:O	6:G:814:HOH:O[3_454]	2.07	0.13
6:D:803:HOH:O	6:H:757:HOH:O[3_454]	2.11	0.09

## 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	377/430 (88%)	366 (97%)	11 (3%)	0	100	100
1	D	373/430 (87%)	358 (96%)	14 (4%)	1 (0%)	41	50
1	G	372/430 (86%)	362 (97%)	10 (3%)	0	100	100
1	H	366/430 (85%)	355 (97%)	11 (3%)	0	100	100
All	All	1488/1720 (86%)	1441 (97%)	46 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS

### 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	318/362 (88%)	314 (99%)	4 (1%)	69	82
1	D	314/362 (87%)	304 (97%)	10 (3%)	39	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	315/362 (87%)	308 (98%)	7 (2%)	52 69
1	H	310/362 (86%)	302 (97%)	8 (3%)	46 63
All	All	1257/1448 (87%)	1228 (98%)	29 (2%)	50 67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LYS
1	A	117	ASP
1	A	159	LEU
1	A	209	ASP
1	D	116	SER
1	D	163	LYS
1	D	167	LEU
1	D	175	GLU
1	D	209	ASP
1	D	229	TRP
1	D	290	SER
1	D	296	LYS
1	D	299	SER
1	D	303	LYS
1	G	175	GLU
1	G	178	ARG
1	G	180	ARG
1	G	203	ASN
1	G	299	SER
1	G	344	ASN
1	G	380	GLU
1	H	21	LEU
1	H	24	ASP
1	H	100	ARG
1	H	142	SER
1	H	236	ASN
1	H	237	GLN
1	H	238	LEU
1	H	254	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	234	HIS
1	A	275	GLN
1	D	48	ASN
1	D	99	ASN
1	D	115	ASN
1	D	121	GLN
1	D	234	HIS
1	D	320	ASN
1	D	356	ASN
1	G	35	GLN
1	G	99	ASN
1	G	203	ASN
1	H	48	ASN
1	H	236	ASN
1	H	237	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	6MA	B	6	2	18,24,25	2.20	3 (16%)	15,34,37	3.89	3 (20%)
2	6MA	E	6	2	18,24,25	2.18	4 (22%)	15,34,37	4.14	3 (20%)

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	6MA	B	6	2	-	0/5/23/24	0/3/3/3
2	6MA	E	6	2	-	0/5/23/24	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	6MA	C6-N1	6.80	1.43	1.34
2	E	6	6MA	C6-N1	6.75	1.43	1.34
2	B	6	6MA	C4-N3	-3.27	1.31	1.35
2	E	6	6MA	C4-N3	-3.12	1.31	1.35
2	B	6	6MA	C1'-N9	-2.55	1.41	1.49
2	E	6	6MA	C1'-N9	-2.51	1.42	1.49
2	E	6	6MA	O4'-C4'	-2.11	1.40	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	6MA	C1-N6-C6	-15.35	109.65	122.87
2	B	6	6MA	C1-N6-C6	-14.33	110.53	122.87
2	E	6	6MA	C2'-C1'-N9	-2.66	108.14	114.27
2	B	6	6MA	C2'-C1'-N9	-2.56	108.36	114.27
2	E	6	6MA	O3'-C3'-C4'	2.10	118.14	110.10
2	B	6	6MA	O3'-C3'-C4'	2.09	118.08	110.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	6MA	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	OGA	G	502	4	3,9,9	0.87	0	4,11,11	1.14	0
5	OGA	H	502	4	3,9,9	0.95	0	4,11,11	1.11	0
5	OGA	D	502	4	3,9,9	0.95	0	4,11,11	1.10	0
5	OGA	A	502	4	3,9,9	0.94	0	4,11,11	1.09	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	OGA	G	502	4	-	0/3/9/9	-
5	OGA	H	502	4	-	0/3/9/9	-
5	OGA	D	502	4	-	0/3/9/9	-
5	OGA	A	502	4	-	0/3/9/9	-

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	381/430 (88%)	-0.11	10 (2%) 56 63	14, 29, 54, 83	0
1	D	377/430 (87%)	-0.02	10 (2%) 54 62	14, 32, 55, 77	0
1	G	378/430 (87%)	-0.23	3 (0%) 86 89	12, 29, 56, 72	0
1	H	372/430 (86%)	-0.07	9 (2%) 59 66	15, 35, 59, 77	0
2	B	11/12 (91%)	-0.32	0 100 100	23, 33, 58, 59	0
2	E	11/12 (91%)	-0.06	0 100 100	25, 34, 70, 71	0
3	C	12/12 (100%)	-0.11	0 100 100	24, 33, 71, 114	0
3	F	12/12 (100%)	-0.18	0 100 100	24, 38, 86, 123	0
All	All	1554/1768 (87%)	-0.11	32 (2%) 63 70	12, 31, 58, 123	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	116	SER	5.6
1	H	213	GLN	5.1
1	A	179	ALA	4.7
1	H	232	VAL	4.7
1	D	116	SER	4.7
1	D	163	LYS	4.6
1	H	120	VAL	4.3
1	A	415	THR	4.3
1	A	215	ALA	4.1
1	H	215	ALA	3.9
1	D	413	SER	3.5
1	D	117	ASP	3.2
1	H	161	THR	3.0
1	A	180	ARG	3.0
1	H	233	GLY	2.9
1	A	119	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	215	ALA	2.7
1	H	163	LYS	2.6
1	A	163	LYS	2.6
1	A	176	GLY	2.5
1	G	180	ARG	2.5
1	H	333	ILE	2.5
1	D	20	LEU	2.3
1	G	179	ALA	2.3
1	H	234	HIS	2.3
1	A	254	MET	2.2
1	D	118	HIS	2.2
1	A	413	SER	2.1
1	D	304	ILE	2.1
1	D	19	SER	2.1
1	D	172	ARG	2.0
1	A	175	GLU	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. 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(Å <sup>2</sup> )	Q<0.9
2	6MA	B	6	22/23	0.97	0.09	13,24,33,36	0
2	6MA	E	6	22/23	0.97	0.10	16,23,27,44	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	OGA	D	502	10/10	0.96	0.09	19,23,28,29	0
5	OGA	G	502	10/10	0.97	0.10	14,22,24,27	0
5	OGA	H	502	10/10	0.97	0.11	22,27,30,31	0
5	OGA	A	502	10/10	0.98	0.09	17,21,25,25	0
4	MN	G	501	1/1	0.99	0.10	24,24,24,24	0
4	MN	H	501	1/1	0.99	0.13	32,32,32,32	0
4	MN	D	501	1/1	0.99	0.16	26,26,26,26	0
4	MN	A	501	1/1	1.00	0.19	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.