



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 03:49 PM GMT

PDB ID : 4GOM
Title : Crystal Structure of E. coli DNA Adenine Methyltransferase in Complex with Aza-SAM
Authors : Harmer, J.E.; Roach, P.L.
Deposited on : 2012-08-20
Resolution : 2.45 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

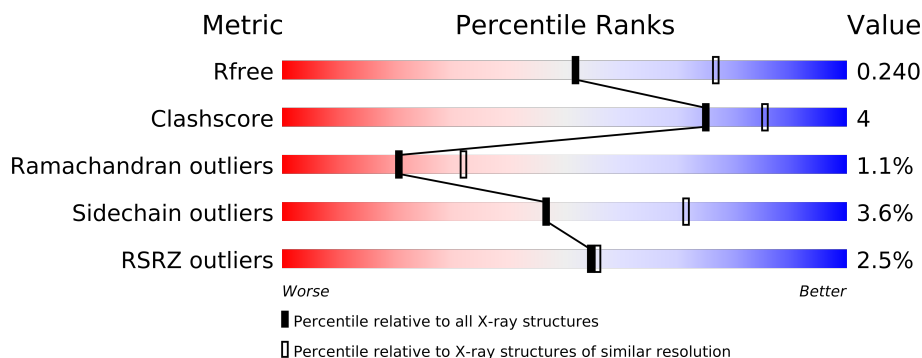
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.45 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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	D	278	
1	E	278	
1	F	278	

2 Entry composition i

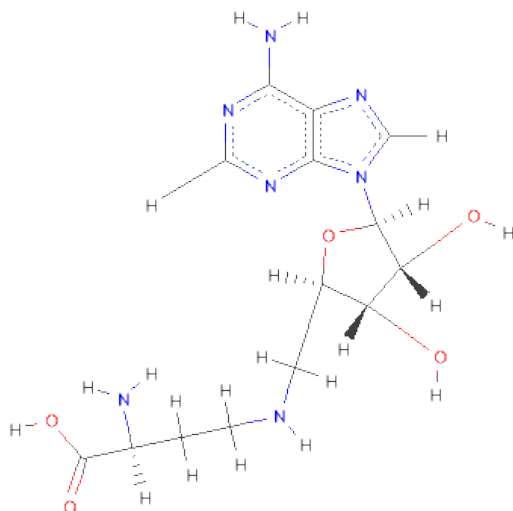
There are 3 unique types of molecules in this entry. The entry contains 6065 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA adenine methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	243	Total	C	N	O	S	0	0	0
			1954	1266	325	355	8			
1	E	244	Total	C	N	O	S	0	0	0
			1941	1256	325	352	8			
1	F	244	Total	C	N	O	S	3	0	0
			1961	1271	328	354	8			

- Molecule 2 is 5'-{[(3S)-3-AMINO-3-CARBOXYPROPYL]AMINO}-5'-DEOXYADENOSIN E (three-letter code: 0Y0) (formula: C₁₄H₂₁N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			26	14	7	5		
2	E	1	Total	C	N	O	0	0
			26	14	7	5		
2	F	1	Total	C	N	O	0	0
			26	14	7	5		

- Molecule 3 is water.

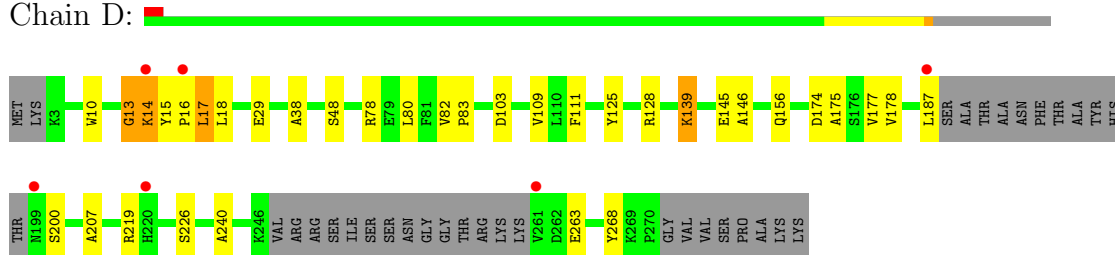
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	66	Total 66	O 66	0	0
3	E	33	Total 33	O 33	0	0
3	F	32	Total 32	O 32	0	0

3 Residue-property plots

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

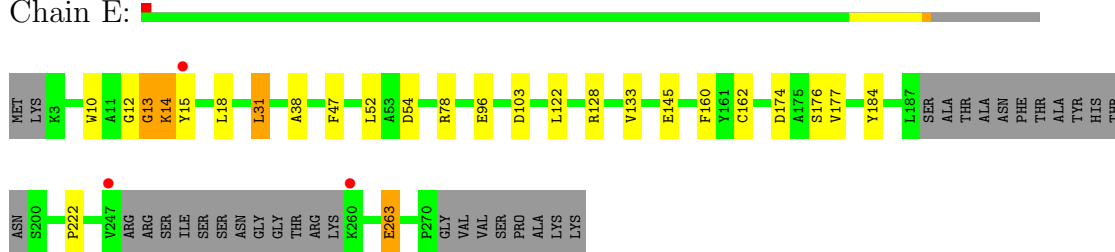
- Molecule 1: DNA adenine methylase

Chain D:



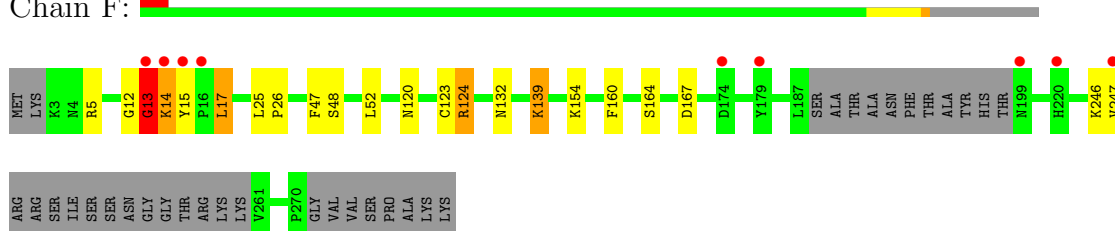
- Molecule 1: DNA adenine methylase

Chain E:



- Molecule 1: DNA adenine methylase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.04Å 161.04Å 95.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.55 – 2.45 29.55 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.55-2.45) 99.4 (29.55-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.209 , 0.248 0.203 , 0.240	Depositor DCC
R_{free} test set	2645 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.0	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 52435 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6065	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: 0Y0

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	D	1.19	5/2008 (0.2%)	0.94	4/2731 (0.1%)
1	E	1.07	0/1996	0.91	1/2719 (0.0%)
1	F	1.09	2/2016 (0.1%)	0.92	2/2742 (0.1%)
All	All	1.12	7/6020 (0.1%)	0.92	7/8192 (0.1%)

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	D	0	1
1	E	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	123	CYS	CB-SG	5.78	1.92	1.82
1	D	156	GLN	CG-CD	5.56	1.63	1.51
1	F	47	PHE	CE2-CZ	5.43	1.47	1.37
1	D	125	TYR	CD1-CE1	5.16	1.47	1.39
1	D	111	PHE	CE2-CZ	5.10	1.47	1.37
1	D	146	ALA	CA-CB	5.06	1.63	1.52
1	D	207	ALA	CA-CB	5.01	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	GLY	N-CA-C	-6.31	97.32	113.10
1	F	167	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	103	ASP	CB-CG-OD1	5.60	123.34	118.30
1	D	219	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	219	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	128	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	13	GLY	Peptide
1	E	13	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1954	0	1836	16	0
1	E	1941	0	1786	14	0
1	F	1961	0	1837	16	0
2	D	26	0	0	0	0
2	E	26	0	0	0	0
2	F	26	0	0	0	0
3	D	66	0	0	0	0
3	E	33	0	0	2	0
3	F	32	0	0	1	0
All	All	6065	0	5459	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:12:GLY:O	1:F:14:LYS:N	1.80	1.14

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:139:LYS:CD	1:D:139:LYS:H	1.68	1.01
1:F:12:GLY:C	1:F:14:LYS:N	2.17	0.96
1:F:12:GLY:C	1:F:14:LYS:H	1.69	0.95
1:D:139:LYS:HD2	1:D:139:LYS:H	1.28	0.95
1:F:139:LYS:HD3	1:F:139:LYS:H	1.41	0.85
1:F:124:ARG:HH11	1:F:124:ARG:CG	1.90	0.84
1:F:124:ARG:HH11	1:F:124:ARG:HG3	1.53	0.73
1:D:17:LEU:HD11	1:D:263:GLU:HG2	1.73	0.69
1:D:139:LYS:N	1:D:139:LYS:CD	2.50	0.68
1:D:10:TRP:HB3	1:D:38:ALA:HB2	1.74	0.67
1:E:10:TRP:HB3	1:E:38:ALA:HB2	1.76	0.66
1:E:78:ARG:NH1	1:E:145:GLU:OE2	2.26	0.66
1:D:15:TYR:O	1:D:17:LEU:N	2.32	0.63
1:F:14:LYS:HB3	1:F:17:LEU:HD21	1.84	0.59
1:F:124:ARG:HH11	1:F:124:ARG:HG2	1.67	0.57
1:E:78:ARG:HH12	1:E:145:GLU:CD	2.10	0.55
1:E:96:GLU:HG3	3:E:433:HOH:O	2.06	0.55
1:D:80:LEU:HD22	1:D:109:VAL:HG12	1.91	0.53
1:F:124:ARG:NH1	1:F:124:ARG:HG3	2.23	0.53
1:E:78:ARG:NH1	1:E:145:GLU:CD	2.62	0.53
1:E:128:ARG:NH1	3:E:429:HOH:O	2.24	0.52
1:F:164:SER:OG	3:F:411:HOH:O	2.19	0.51
1:D:177:VAL:HG12	1:D:178:VAL:N	2.27	0.50
1:F:12:GLY:O	1:F:14:LYS:HG2	2.12	0.50
1:E:52:LEU:O	1:E:160:PHE:HA	2.14	0.48
1:F:124:ARG:NH1	1:F:124:ARG:CG	2.61	0.48
1:F:246:LYS:O	1:F:247:VAL:HG13	2.15	0.47
1:D:78:ARG:HH21	1:D:145:GLU:CD	2.19	0.45
1:F:52:LEU:O	1:F:160:PHE:HA	2.16	0.45
1:D:15:TYR:N	1:D:16:PRO:CD	2.80	0.45
1:E:184:TYR:OH	1:E:263:GLU:OE2	2.26	0.45
1:D:82:VAL:HB	1:D:83:PRO:HD2	2.00	0.44
1:D:14:LYS:C	1:D:16:PRO:HD2	2.38	0.44
1:E:122:LEU:O	1:E:133:VAL:HG21	2.17	0.44
1:E:177:VAL:HG22	1:E:222:PRO:HG2	2.00	0.43
1:F:13:GLY:O	1:F:14:LYS:C	2.56	0.43
1:D:29:GLU:HB2	1:D:175:ALA:HB1	2.01	0.43
1:E:31:LEU:HG	1:E:47:PHE:CE1	2.54	0.43
1:E:78:ARG:NH1	1:E:145:GLU:OE1	2.53	0.42
1:D:240:ALA:HB2	1:D:268:TYR:CE2	2.54	0.42
1:F:25:LEU:HA	1:F:26:PRO:HD3	1.85	0.42
1:E:12:GLY:O	1:E:14:LYS:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:240:ALA:HB2	1:D:268:TYR:CZ	2.55	0.41
1:E:54:ASP:O	1:E:162:CYS:HA	2.21	0.41
1:D:177:VAL:CG1	1:D:178:VAL:N	2.83	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	D	237/278 (85%)	223 (94%)	10 (4%)	4 (2%)	14	20
1	E	238/278 (86%)	224 (94%)	12 (5%)	2 (1%)	27	43
1	F	238/278 (86%)	223 (94%)	13 (6%)	2 (1%)	27	43
All	All	713/834 (86%)	670 (94%)	35 (5%)	8 (1%)	21	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	13	GLY
1	F	14	LYS
1	D	14	LYS
1	D	17	LEU
1	E	13	GLY
1	D	200	SER
1	E	14	LYS
1	D	13	GLY

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	D	198/239 (83%)	192 (97%)	6 (3%)	53	78
1	E	191/239 (80%)	185 (97%)	6 (3%)	52	77
1	F	197/239 (82%)	188 (95%)	9 (5%)	37	60
All	All	586/717 (82%)	565 (96%)	21 (4%)	47	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	LEU
1	D	48	SER
1	D	139	LYS
1	D	174	ASP
1	D	187	LEU
1	D	226	SER
1	E	15	TYR
1	E	18	LEU
1	E	31	LEU
1	E	174	ASP
1	E	176	SER
1	E	263	GLU
1	F	5	ARG
1	F	15	TYR
1	F	17	LEU
1	F	48	SER
1	F	120	ASN
1	F	124	ARG
1	F	132	ASN
1	F	139	LYS
1	F	154	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	102	GLN
1	D	120	ASN
1	D	157	ASN
1	F	132	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands 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	0Y0	D	301	-	28,28,28	2.54	13 (46%)	40,40,40	2.61	12 (30%)
2	0Y0	E	301	-	28,28,28	1.55	4 (14%)	40,40,40	2.78	12 (30%)
2	0Y0	F	301	-	28,28,28	1.69	7 (25%)	40,40,40	2.60	16 (40%)

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	0Y0	D	301	-	-	0/15/31/31	0/3/3/3
2	0Y0	E	301	-	-	0/15/31/31	0/3/3/3
2	0Y0	F	301	-	-	0/15/31/31	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	0Y0	CAC-CAD	-5.04	1.46	1.53
2	E	301	0Y0	C6-N6	4.89	1.50	1.34
2	F	301	0Y0	C6-N6	4.36	1.48	1.34
2	D	301	0Y0	OAH-CAB	-4.28	1.32	1.43
2	D	301	0Y0	C6-N6	4.04	1.47	1.34
2	D	301	0Y0	C4-N9	-4.03	1.31	1.37
2	D	301	0Y0	CAC-CAB	-3.71	1.43	1.53
2	D	301	0Y0	OAE-CAD	-3.53	1.36	1.41
2	D	301	0Y0	C8-N9	-3.44	1.31	1.36
2	D	301	0Y0	CAF-CAA	-3.29	1.43	1.51
2	E	301	0Y0	OAH-CAB	-2.96	1.35	1.43
2	D	301	0Y0	OAI-CAC	-2.91	1.35	1.43
2	F	301	0Y0	OAE-CAD	2.91	1.44	1.41
2	F	301	0Y0	CAF-CAA	-2.88	1.44	1.51
2	D	301	0Y0	CAB-CAA	-2.77	1.45	1.53
2	F	301	0Y0	CAC-CAD	-2.71	1.49	1.53
2	E	301	0Y0	OXT-C	2.68	1.31	1.22
2	F	301	0Y0	OAH-CAB	-2.65	1.36	1.43
2	F	301	0Y0	OXT-C	2.63	1.31	1.22
2	D	301	0Y0	C4-N3	-2.46	1.31	1.35
2	D	301	0Y0	C5-N7	-2.29	1.31	1.39
2	D	301	0Y0	OXT-C	2.21	1.29	1.22
2	F	301	0Y0	C2-N3	2.18	1.35	1.32
2	E	301	0Y0	C2-N3	2.06	1.35	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	0Y0	N3-C2-N1	-9.82	120.25	128.89
2	F	301	0Y0	N3-C2-N1	-8.85	121.11	128.89
2	D	301	0Y0	N3-C2-N1	-8.29	121.60	128.89
2	E	301	0Y0	C5-C4-N3	-8.06	118.12	125.98
2	D	301	0Y0	C5-C4-N3	-7.23	118.93	125.98
2	F	301	0Y0	C5-C4-N3	-6.89	119.26	125.98
2	E	301	0Y0	N3-C4-N9	5.89	135.50	125.39
2	F	301	0Y0	N3-C4-N9	5.75	135.25	125.39
2	D	301	0Y0	N3-C4-N9	5.40	134.66	125.39
2	D	301	0Y0	CAS-CB-CA	4.93	123.70	112.26
2	E	301	0Y0	CAS-CB-CA	3.65	120.73	112.26
2	F	301	0Y0	C8-N9-C4	3.25	109.60	106.96
2	E	301	0Y0	CAA-CAF-NAR	3.24	120.84	113.64
2	E	301	0Y0	C2-N3-C4	3.17	122.39	113.27
2	D	301	0Y0	C8-N9-C4	3.11	109.48	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	0Y0	OAE-CAA-CAF	-3.09	103.88	108.78
2	D	301	0Y0	CAF-CAA-CAB	-3.04	109.92	116.74
2	E	301	0Y0	CB-CAS-NAR	3.00	119.64	111.96
2	F	301	0Y0	CAD-N9-C4	-2.93	121.57	126.64
2	D	301	0Y0	OAE-CAD-CAC	-2.89	102.47	106.69
2	E	301	0Y0	C-CA-N	2.88	114.07	109.31
2	F	301	0Y0	C-CA-N	2.75	113.85	109.31
2	E	301	0Y0	O-C-OXT	-2.74	117.91	124.05
2	D	301	0Y0	OAE-CAA-CAF	-2.74	104.44	108.78
2	D	301	0Y0	CB-CA-C	-2.74	104.72	110.22
2	E	301	0Y0	CAD-N9-C4	-2.62	122.11	126.64
2	D	301	0Y0	C2-N3-C4	2.61	120.79	113.27
2	F	301	0Y0	C2-N3-C4	2.55	120.60	113.27
2	F	301	0Y0	CAC-CAB-CAA	2.51	107.66	102.64
2	F	301	0Y0	O-C-OXT	-2.49	118.46	124.05
2	D	301	0Y0	C4-C5-N7	-2.49	107.01	109.41
2	F	301	0Y0	CB-CAS-NAR	2.47	118.29	111.96
2	E	301	0Y0	O-C-CA	2.42	122.42	116.90
2	F	301	0Y0	CAA-CAF-NAR	2.40	118.98	113.64
2	D	301	0Y0	O-C-OXT	-2.34	118.80	124.05
2	F	301	0Y0	O-C-CA	2.28	122.10	116.90
2	F	301	0Y0	CAC-CAD-N9	2.26	119.51	113.35
2	F	301	0Y0	CB-CA-C	-2.21	105.76	110.22
2	F	301	0Y0	CAS-CB-CA	2.18	117.33	112.26
2	E	301	0Y0	C8-N9-C4	2.16	108.71	106.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	D	243/278 (87%)	-0.44	6 (2%) 54 56	26, 39, 62, 86	0
1	E	244/278 (87%)	-0.28	3 (1%) 75 76	29, 44, 68, 99	0
1	F	244/278 (87%)	-0.17	9 (3%) 39 40	28, 43, 63, 94	1 (0%)
All	All	731/834 (87%)	-0.30	18 (2%) 54 56	26, 42, 66, 99	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	16	PRO	5.4
1	E	15	TYR	5.4
1	F	15	TYR	5.2
1	E	260	LYS	4.6
1	D	199	ASN	4.3
1	F	199	ASN	3.9
1	F	247	VAL	3.4
1	D	16	PRO	3.1
1	F	14	LYS	2.9
1	D	261	VAL	2.9
1	F	220	HIS	2.7
1	E	247	VAL	2.7
1	D	14	LYS	2.6
1	F	174	ASP	2.4
1	D	187	LEU	2.3
1	F	179	TYR	2.3
1	D	220	HIS	2.2
1	F	13	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	0Y0	E	301	26/26	0.12	0.07	43,50,58,59	0
2	0Y0	F	301	26/26	0.15	-0.11	41,45,54,56	0
2	0Y0	D	301	26/26	0.10	-0.43	45,52,62,62	0

6.5 Other polymers

There are no such residues in this entry.