Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2016 – 04:46 PM EST

PDB ID	:	5U4X
Title	:	Coactivator-associated arginine methyltransferase 1
Authors	:	DONG, A.; ZENG, H.; Saikatendu, K.S.; STONE, H.; WALKER, J.R.; Boun-tra, C.; Arrowsmith, C.H.; Edwards, A.M.; BROWN, P.J.; WU, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2016-12-06
Resolution	:	1.88 Å(reported)

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

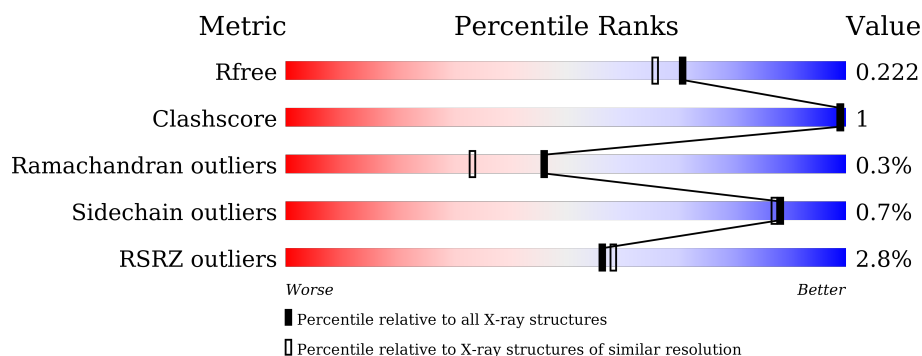|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.88 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		1
Ramachandran outliers		0.3%
Sidechain outliers		0.7%
RSRZ outliers		2.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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. 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 <=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	341	2% ... 94%
1	B	341	4% ... 96%
1	C	341	% ... 94%
1	D	341	4% ... 95%

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 crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	D	504	-	-	-	X
4	UNX	D	509	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11750 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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	13	1
			2725	1763	450	495	17			
1	B	331	Total	C	N	O	S	0	9	1
			2674	1734	434	489	17			
1	C	331	Total	C	N	O	S	0	11	1
			2703	1749	444	493	17			
1	D	332	Total	C	N	O	S	0	9	1
			2690	1744	439	491	16			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
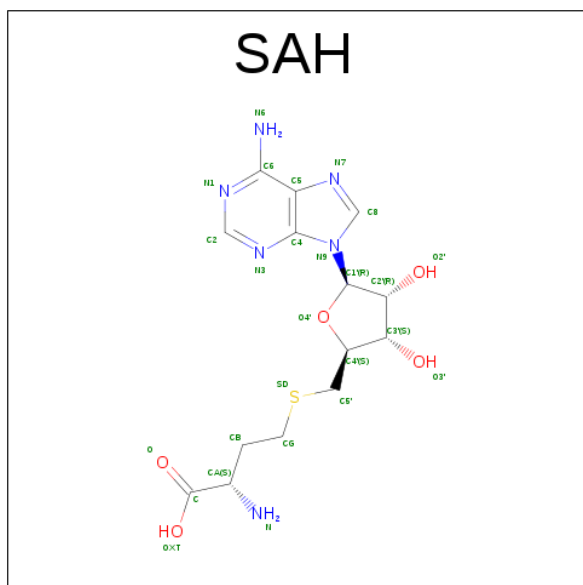
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is N-methyl-N-[(2-{1-[2-(methylamino)ethyl]piperidin-4-yl}pyridin-4-yl)methyl]-3-phenoxybenzamide (three-letter code: 7VM) (formula: $C_{28}H_{34}N_4O_2$).
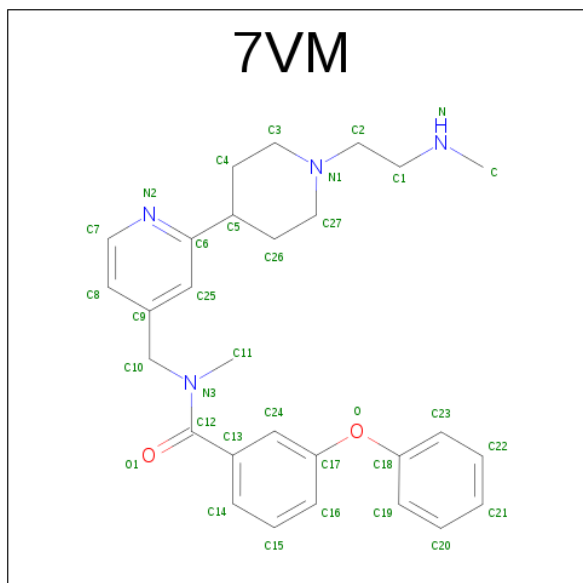
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	28	4	2		
3	B	1	Total	C	N	O	0	0
			34	28	4	2		
3	C	1	Total	C	N	O	0	0
			34	28	4	2		
3	D	1	Total	C	N	O	0	0
			34	28	4	2		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	X	0	0
			5	5		
4	A	2	Total	X	0	0
			2	2		
4	D	7	Total	X	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total 4	X 4	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total 131	O 131	0	1
5	B	169	Total 174	O 174	0	5
5	C	198	Total 201	O 201	0	3
5	D	190	Total 194	O 194	0	4

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.
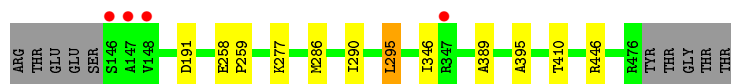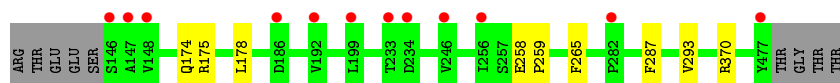
- Molecule 1: Histone-arginine methyltransferase CARM1
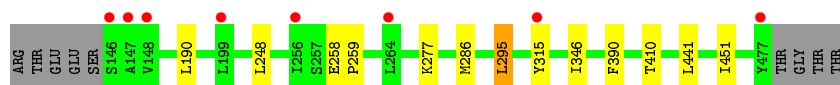
- Molecule 1: Histone-arginine methyltransferase CARM1
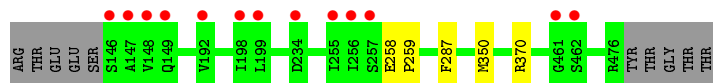
- Molecule 1: Histone-arginine methyltransferase CARM1

- Molecule 1: Histone-arginine methyltransferase CARM1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.09Å　　98.92Å　　207.55Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　1.88 27.67　–　1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.88) 99.7 (27.67-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.43 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188　,　0.215 0.198　,　0.222	Depositor DCC
R_{free} test set	2521 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11750	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2378e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, SAH, 7VM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.45	0/2808	0.65	1/3807 (0.0%)
1	B	0.47	0/2757	0.67	2/3741 (0.1%)
1	C	0.48	0/2787	0.68	2/3779 (0.1%)
1	D	0.50	0/2765	0.70	2/3751 (0.1%)
All	All	0.48	0/11117	0.68	7/15078 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	370	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	D	370	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	191	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	295	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	175	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	446	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2725	0	2647	6	0
1	B	2674	0	2608	1	0
1	C	2703	0	2631	6	0
1	D	2690	0	2621	2	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	34	0	0	0	0
3	B	34	0	0	0	0
3	C	34	0	0	0	0
3	D	34	0	0	0	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
5	A	131	0	0	0	0
5	B	174	0	0	0	0
5	C	201	0	0	0	0
5	D	194	0	0	0	0
All	All	11750	0	10583	15	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 1.

All (15) 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:441:LEU:HD22	1:A:451:ILE:HG12	1.83	0.60
1:C:277:LYS:HD3	1:C:286[A]:MET:SD	2.45	0.57
1:C:346:ILE:HG21	1:C:410:THR:HG23	1.90	0.53
1:D:265:PHE:CE2	1:D:293[A]:VAL:HG21	2.47	0.50
1:C:346:ILE:HD13	1:C:410:THR:HG22	1.94	0.49
1:A:190:LEU:HD13	1:A:248:LEU:HD21	1.96	0.48
1:A:277:LYS:HD3	1:A:286[A]:MET:SD	2.54	0.47
1:B:350[B]:MET:HE2	1:B:350[B]:MET:HA	1.98	0.46
1:A:346:ILE:HG21	1:A:410:THR:CG2	2.47	0.44
1:D:174:GLN:HG2	1:D:178[A]:LEU:HD12	2.00	0.44
1:C:346:ILE:HG21	1:C:410:THR:CG2	2.47	0.44
1:A:346:ILE:HG21	1:A:410:THR:HG22	2.00	0.43
1:C:295:LEU:HA	1:C:389:ALA:O	2.19	0.42
1:A:295:LEU:HG	1:A:390:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HG12	1:C:395:ALA:HB3	2.02	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	343/341 (101%)	331 (96%)	11 (3%)	1 (0%)	46	33
1	B	338/341 (99%)	326 (96%)	11 (3%)	1 (0%)	46	33
1	C	340/341 (100%)	329 (97%)	10 (3%)	1 (0%)	46	33
1	D	339/341 (99%)	330 (97%)	8 (2%)	1 (0%)	46	33
All	All	1360/1364 (100%)	1316 (97%)	40 (3%)	4 (0%)	46	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	PRO
1	C	259	PRO
1	A	259	PRO
1	D	259	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	291/296 (98%)	289 (99%)	2 (1%)	88	87
1	B	286/296 (97%)	284 (99%)	2 (1%)	88	87
1	C	290/296 (98%)	288 (99%)	2 (1%)	88	87
1	D	288/296 (97%)	286 (99%)	2 (1%)	88	87
All	All	1155/1184 (98%)	1147 (99%)	8 (1%)	88	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	A	315	TYR
1	B	258	GLU
1	B	287	PHE
1	C	258	GLU
1	C	295	LEU
1	D	258	GLU
1	D	287	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	381	HIS

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 26 ligands modelled in this entry, 18 are unknown - leaving 8 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	#$|Z| > 2$
2	SAH	A	501	-	22,28,28	1.06	2 (9%)	18,40,40	2.41	4 (22%)
3	7VM	A	502	-	37,37,37	0.25	0	47,49,49	0.73	1 (2%)
2	SAH	B	501	-	22,28,28	0.96	1 (4%)	18,40,40	2.20	3 (16%)
3	7VM	B	502	-	37,37,37	0.20	0	47,49,49	0.92	1 (2%)
2	SAH	C	501	-	22,28,28	1.28	3 (13%)	18,40,40	2.57	4 (22%)
3	7VM	C	502	-	37,37,37	0.27	0	47,49,49	0.76	1 (2%)
2	SAH	D	501	-	22,28,28	1.08	2 (9%)	18,40,40	2.15	4 (22%)
3	7VM	D	502	-	37,37,37	0.25	0	47,49,49	0.84	1 (2%)

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	SAH	A	501	-	-	0/7/31/31	0/3/3/3
3	7VM	A	502	-	-	0/24/34/34	0/4/4/4
2	SAH	B	501	-	-	0/7/31/31	0/3/3/3
3	7VM	B	502	-	-	0/24/34/34	0/4/4/4
2	SAH	C	501	-	-	0/7/31/31	0/3/3/3
3	7VM	C	502	-	-	0/24/34/34	0/4/4/4
2	SAH	D	501	-	-	0/7/31/31	0/3/3/3
3	7VM	D	502	-	-	0/24/34/34	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	C2-N3	2.11	1.35	1.32
2	D	501	SAH	C2-N3	2.28	1.36	1.32
2	C	501	SAH	C2-N3	2.58	1.36	1.32
2	D	501	SAH	C5-C4	2.61	1.46	1.40
2	B	501	SAH	C5-C4	2.90	1.47	1.40
2	C	501	SAH	C5-C4	3.08	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	SAH	O4'-C1'	3.13	1.45	1.41
2	A	501	SAH	C5-C4	3.17	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	SAH	N3-C2-N1	-8.81	121.95	128.87
2	A	501	SAH	N3-C2-N1	-8.54	122.16	128.87
2	B	501	SAH	N3-C2-N1	-7.94	122.64	128.87
2	D	501	SAH	N3-C2-N1	-7.34	123.11	128.87
2	D	501	SAH	C1'-N9-C4	-2.57	123.94	126.81
2	A	501	SAH	C1'-N9-C4	-2.31	124.23	126.81
2	C	501	SAH	C1'-N9-C4	-2.27	124.27	126.81
2	B	501	SAH	O4'-C1'-N9	-2.20	103.94	108.11
2	D	501	SAH	O4'-C1'-N9	-2.16	104.02	108.11
3	C	502	7VM	C-N-C1	2.20	116.15	111.78
3	A	502	7VM	C-N-C1	2.26	116.27	111.78
2	A	501	SAH	C2-N1-C6	2.33	122.92	118.77
2	B	501	SAH	N6-C6-N1	2.35	122.45	118.52
2	C	501	SAH	C2-N1-C6	2.57	123.36	118.77
2	D	501	SAH	N6-C6-N1	3.01	123.56	118.52
3	D	502	7VM	C-N-C1	3.19	118.10	111.78
2	A	501	SAH	N6-C6-N1	3.27	124.00	118.52
2	C	501	SAH	N6-C6-N1	4.43	125.95	118.52
3	B	502	7VM	C-N-C1	4.77	121.23	111.78

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 ⓘ

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	332/341 (97%)	0.06	8 (2%)	62	64	22, 31, 41, 64	0
1	B	331/341 (97%)	0.00	13 (3%)	43	45	21, 28, 40, 55	0
1	C	331/341 (97%)	-0.12	4 (1%)	81	83	17, 26, 38, 56	1 (0%)
1	D	332/341 (97%)	0.02	12 (3%)	46	48	18, 26, 44, 58	0
All	All	1326/1364 (97%)	-0.01	37 (2%)	56	58	17, 28, 41, 64	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	TYR	7.7
1	A	146	SER	7.5
1	D	477	TYR	7.2
1	C	148	VAL	5.7
1	A	148	VAL	5.0
1	D	148	VAL	5.0
1	B	148	VAL	4.5
1	D	147	ALA	4.3
1	C	146	SER	3.6
1	B	192	VAL	3.2
1	D	199	LEU	3.2
1	A	264	LEU	3.0
1	A	147	ALA	3.0
1	B	147	ALA	2.8
1	A	315	TYR	2.8
1	B	149	GLN	2.8
1	D	256	ILE	2.7
1	B	234	ASP	2.7
1	C	347	ARG	2.6
1	B	199	LEU	2.6
1	B	146	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	198	ILE	2.5
1	B	256	ILE	2.4
1	D	233	THR	2.4
1	B	461	GLY	2.4
1	D	234	ASP	2.4
1	B	462	SER	2.3
1	A	256	ILE	2.3
1	C	147	ALA	2.3
1	D	192	VAL	2.3
1	B	257	SER	2.3
1	B	255	ILE	2.2
1	A	199	LEU	2.2
1	D	282[A]	PRO	2.1
1	D	186	ASP	2.1
1	D	246	VAL	2.1
1	D	146	SER	2.1

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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	UNX	D	504	1/1	0.90	0.51	11.05	30,30,30,30	0
4	UNX	D	509	1/1	0.82	0.22	5.12	30,30,30,30	0
2	SAH	D	501	26/26	0.95	0.13	0.23	21,23,27,29	0
3	7VM	A	502	34/34	0.87	0.13	-0.09	24,29,32,32	0
2	SAH	A	501	26/26	0.97	0.11	-0.20	22,24,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	7VM	C	502	34/34	0.92	0.11	-0.25	20,23,27,27	0
2	SAH	B	501	26/26	0.95	0.12	-0.25	21,22,24,24	0
2	SAH	C	501	26/26	0.98	0.09	-0.48	16,18,20,21	0
3	7VM	D	502	34/34	0.94	0.09	-0.61	21,23,24,25	0
3	7VM	B	502	34/34	0.94	0.09	-0.65	23,26,28,28	0
4	UNX	B	504	1/1	0.75	0.25	-	30,30,30,30	0
4	UNX	B	503	1/1	0.74	0.19	-	30,30,30,30	0
4	UNX	C	505	1/1	0.80	0.19	-	30,30,30,30	0
4	UNX	B	506	1/1	0.73	0.16	-	30,30,30,30	1
4	UNX	C	506	1/1	0.77	0.18	-	30,30,30,30	0
4	UNX	D	503	1/1	0.62	0.46	-	30,30,30,30	0
4	UNX	C	503	1/1	0.80	0.12	-	30,30,30,30	0
4	UNX	A	503	1/1	0.86	0.20	-	30,30,30,30	0
4	UNX	A	504	1/1	0.75	0.15	-	30,30,30,30	0
4	UNX	D	506	1/1	0.73	0.21	-	30,30,30,30	0
4	UNX	C	504	1/1	0.52	0.15	-	30,30,30,30	0
4	UNX	D	505	1/1	0.84	0.23	-	30,30,30,30	0
4	UNX	D	507	1/1	0.81	0.16	-	30,30,30,30	0
4	UNX	D	508	1/1	0.73	0.21	-	30,30,30,30	0
4	UNX	B	507	1/1	0.69	0.19	-	30,30,30,30	0
4	UNX	B	505	1/1	0.86	0.18	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.