



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2019 – 05:16 PM EDT

PDB ID : 6H4X
Title : Crystal structure of human KDM4A in complex with compound 17b
Authors : Le Bihan, Y.V.; van Montfort, R.L.M.
Deposited on : 2018-07-23
Resolution : 2.34 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

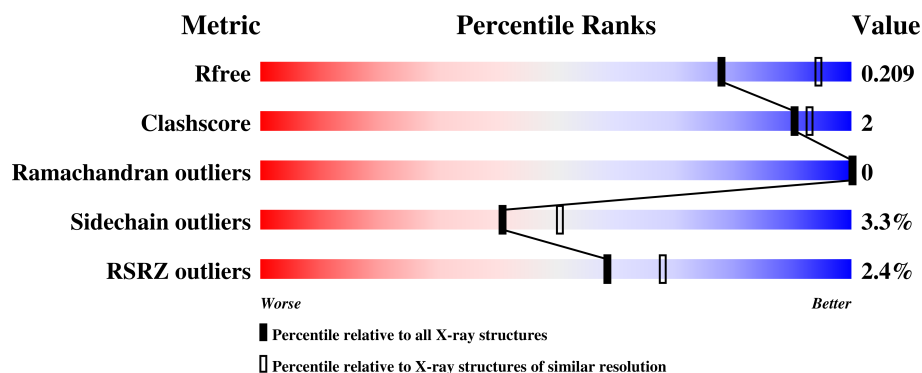
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	111664	1763 (2.36-2.32)
Clashscore	122126	1858 (2.36-2.32)
Ramachandran outliers	120053	1834 (2.36-2.32)
Sidechain outliers	120020	1835 (2.36-2.32)
RSRZ outliers	108989	1737 (2.36-2.32)

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 $\leq 5\%$. 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	360	<div> <div>3%</div> <div>87% 7% 6%</div> </div>
1	B	360	<div> <div>%</div> <div>89% 5% 6%</div> </div>
1	C	360	<div> <div>4%</div> <div>89% 6% 5%</div> </div>
1	D	360	<div> <div>%</div> <div>88% 5% 6%</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	GOL	A	405	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11342 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2674	1748	434	478	14			
1	B	340	Total	C	N	O	S	0	2	0
			2728	1774	449	490	15			
1	C	341	Total	C	N	O	S	0	1	0
			2652	1725	434	479	14			
1	D	337	Total	C	N	O	S	0	1	0
			2663	1738	437	473	15			

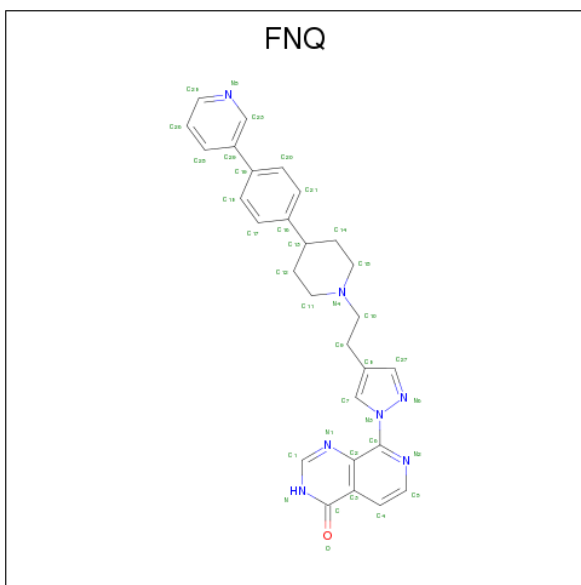
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164
C	0	SER	-	expression tag	UNP O75164
D	0	SER	-	expression tag	UNP O75164

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

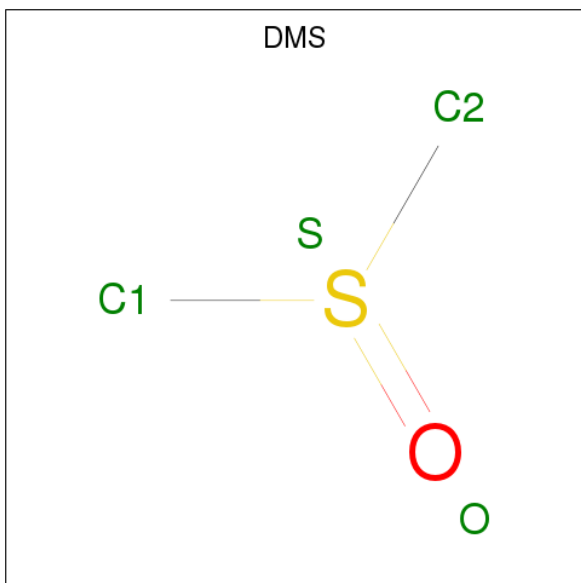
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 8-[4-[2-[4-(4-pyridin-3-ylphenyl)piperidin-1-yl]ethyl]pyrazol-1-yl]-3 {H}-pyrido [3,4-d]pyrimidin-4-one (three-letter code: FNQ) (formula: C₂₈H₂₇N₇O).



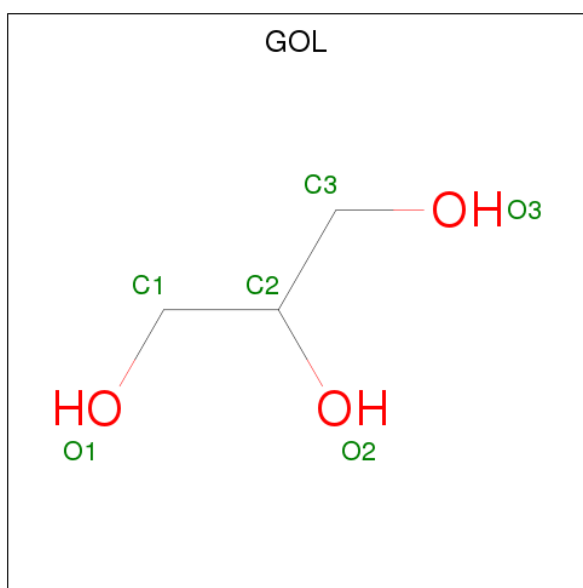
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	12	6	1		
3	B	1	Total	C	N	O	0	0
			31	24	6	1		
3	C	1	Total	C	N	O	0	0
			30	23	6	1		
3	D	1	Total	C	N	O	0	0
			25	18	6	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 124	O 124	0	1
7	B	151	Total 152	O 152	0	1
7	C	85	Total 85	O 85	0	0
7	D	121	Total 121	O 121	0	0

L346	L354	LYS
		GLU
		SER
		GLU
		LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.83Å 101.40Å 142.54Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	48.37 – 2.34 48.37 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.37-2.34) 99.8 (48.37-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.166 , 0.207 0.173 , 0.209	Depositor DCC
R_{free} test set	3380 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11342	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 25.11 % 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 3.3725e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, DMS, FNQ, CL

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	0/2759	0.66	0/3756
1	B	0.55	0/2815	0.67	0/3827
1	C	0.50	0/2737	0.66	0/3733
1	D	0.51	0/2750	0.65	0/3746
All	All	0.52	0/11061	0.66	0/15062

There are no bond length outliers.

There are no bond angle outliers.

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	2674	0	2452	13	0
1	B	2728	0	2515	8	0
1	C	2652	0	2371	10	0
1	D	2663	0	2435	6	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	0	1	0
3	C	30	0	0	1	0
3	D	25	0	0	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	6	0	8	5	0
5	B	6	0	8	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	124	0	0	0	0
7	B	152	0	0	0	0
7	C	85	0	0	0	0
7	D	121	0	0	0	0
All	All	11342	0	9813	40	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 2.

All (40) 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:126:THR:HB	5:A:405:GOL:H2	1.48	0.93
1:A:76:THR:HA	5:A:405:GOL:H12	1.61	0.82
5:A:405:GOL:H11	1:C:126:THR:HB	1.72	0.72
1:D:10:PRO:HD2	1:D:12:ALA:H	1.65	0.61
1:C:236:ALA:HB1	1:C:239:ARG:HG3	1.88	0.56
1:B:126:THR:O	5:B:405:GOL:H11	2.06	0.56
1:A:294:ARG:HG2	1:A:294:ARG:HH21	1.69	0.56
1:A:153:LEU:HD11	1:A:197:ILE:HG21	1.89	0.55
1:D:153:LEU:HD11	1:D:197:ILE:HG21	1.89	0.55
1:B:153:LEU:HD11	1:B:197:ILE:HG21	1.89	0.54
1:C:153:LEU:HD11	1:C:197:ILE:HG21	1.88	0.54
1:B:126:THR:HB	5:B:405:GOL:H11	1.90	0.53
1:B:82:PHE:HB2	1:B:244:LEU:HB2	1.90	0.53
1:A:136:VAL:HB	1:A:176:LEU:HB2	1.90	0.53
1:A:154:ARG:HA	1:A:158:ASP:OD2	2.08	0.53
3:A:403:FNQ:N1	3:A:403:FNQ:C7	2.73	0.52
3:B:403:FNQ:N1	3:B:403:FNQ:C7	2.73	0.52
3:C:403:FNQ:C7	3:C:403:FNQ:N1	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:403:FNQ:N1	3:D:403:FNQ:C7	2.73	0.51
5:A:405:GOL:H11	1:C:126:THR:CB	2.40	0.51
1:B:186:ALA:HA	1:B:244:LEU:HD23	1.92	0.50
1:A:150:ILE:HG22	1:A:174:PRO:HB3	1.94	0.50
1:C:150:ILE:HG22	1:C:174:PRO:HB3	1.94	0.49
1:A:141:TYR:CE2	1:A:149:ASN:HA	2.47	0.48
1:A:82:PHE:HB2	1:A:244:LEU:HB2	1.95	0.48
1:A:186:ALA:HA	1:A:244:LEU:CD2	2.43	0.47
1:A:186:ALA:HB1	1:A:243:THR:O	2.15	0.47
1:B:126:THR:HB	5:B:405:GOL:H32	1.97	0.46
1:B:186:ALA:HA	1:B:244:LEU:CD2	2.45	0.46
1:A:342:ASP:HB3	1:A:345:LEU:HD12	1.98	0.44
1:C:342:ASP:HB3	1:C:345:LEU:HD12	1.99	0.44
1:B:342:ASP:HB3	1:B:345:LEU:HD12	1.99	0.44
1:D:342:ASP:HB3	1:D:345:LEU:HD12	2.00	0.43
1:D:215:HIS:CD2	1:D:256:PRO:HG2	2.53	0.43
1:A:74:LEU:HB3	1:C:74:LEU:HD22	2.01	0.42
1:C:155:THR:HG21	1:C:291:PHE:HB2	2.01	0.42
5:A:405:GOL:H32	1:C:126:THR:HB	2.03	0.41
1:D:186:ALA:HA	1:D:244:LEU:HD23	2.03	0.41
1:C:215:HIS:CD2	1:C:256:PRO:HG2	2.56	0.40
1:D:82:PHE:HB2	1:D:244:LEU:HB2	2.03	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	334/360 (93%)	325 (97%)	9 (3%)	0	100	100
1	B	338/360 (94%)	333 (98%)	5 (2%)	0	100	100
1	C	336/360 (93%)	331 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	334/360 (93%)	330 (99%)	4 (1%)	0	100	100
All	All	1342/1440 (93%)	1319 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/316 (81%)	249 (97%)	8 (3%)	43	53
1	B	267/316 (84%)	257 (96%)	10 (4%)	37	47
1	C	247/316 (78%)	239 (97%)	8 (3%)	42	51
1	D	255/316 (81%)	247 (97%)	8 (3%)	43	53
All	All	1026/1264 (81%)	992 (97%)	34 (3%)	41	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	71	ILE
1	A	74	LEU
1	A	132	TYR
1	A	182	LYS
1	A	184	SER
1	A	288	SER
1	A	289	THR
1	B	58	SER
1	B	63	ASP
1	B	74	LEU
1	B	132	TYR
1	B	137	ASN
1	B	182	LYS
1	B	184	SER
1	B	235	GLU

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Mol	Chain	Res	Type
1	B	289	THR
1	B	338	ASN
1	C	58	SER
1	C	74	LEU
1	C	132	TYR
1	C	163	GLU
1	C	182	LYS
1	C	184	SER
1	C	289	THR
1	C	318	ASP
1	D	11	SER
1	D	58	SER
1	D	74	LEU
1	D	132	TYR
1	D	171	VAL
1	D	182	LYS
1	D	289	THR
1	D	318	ASP

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

Mol	Chain	Res	Type
1	A	215	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z > 2$
3	FNQ	A	403	2	16,21,41	0.69	0	17,29,57	1.99	6 (35%)
4	DMS	A	404	-	3,3,3	0.31	0	3,3,3	0.21	0
5	GOL	A	405	-	5,5,5	0.19	0	5,5,5	0.52	0
3	FNQ	B	403	2	31,35,41	0.49	0	38,49,57	1.35	7 (18%)
4	DMS	B	404	-	3,3,3	0.32	0	3,3,3	0.23	0
5	GOL	B	405	-	5,5,5	0.17	0	5,5,5	0.72	0
3	FNQ	C	403	2	30,34,41	0.53	0	36,47,57	1.41	7 (19%)
4	DMS	C	404	-	3,3,3	0.30	0	3,3,3	0.25	0
3	FNQ	D	403	2	24,28,41	0.56	0	28,39,57	1.60	6 (21%)
4	DMS	D	404	-	3,3,3	0.22	0	3,3,3	0.23	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
3	FNQ	A	403	2	-	0/3/7/27	0/3/3/6
4	DMS	A	404	-	-	0/0/0/0	0/0/0/0
5	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	FNQ	B	403	2	-	0/9/23/27	0/5/5/6
4	DMS	B	404	-	-	0/0/0/0	0/0/0/0
5	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	FNQ	C	403	2	-	0/9/23/27	0/5/5/6
4	DMS	C	404	-	-	0/0/0/0	0/0/0/0
3	FNQ	D	403	2	-	0/5/19/27	0/4/4/6
4	DMS	D	404	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	FNQ	C6-C2-C3	-4.36	115.01	119.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	FNQ	C6-C2-C3	-4.19	115.19	119.63
3	A	403	FNQ	C6-C2-C3	-4.17	115.21	119.63
3	D	403	FNQ	C6-C2-C3	-4.07	115.32	119.63
3	D	403	FNQ	C5-C4-C3	-2.54	117.38	119.72
3	B	403	FNQ	C5-C4-C3	-2.35	117.56	119.72
3	A	403	FNQ	C5-C4-C3	-2.21	117.69	119.72
3	B	403	FNQ	N1-C1-N	-2.16	125.19	128.68
3	C	403	FNQ	N1-C1-N	-2.16	125.20	128.68
3	A	403	FNQ	N1-C1-N	-2.14	125.23	128.68
3	D	403	FNQ	N1-C1-N	-2.13	125.25	128.68
3	C	403	FNQ	C-C3-C2	-2.05	118.40	119.92
3	B	403	FNQ	C-C3-C2	-2.04	118.41	119.92
3	C	403	FNQ	C5-C4-C3	-2.00	117.88	119.72
3	D	403	FNQ	C1-N1-C2	2.13	116.11	114.64
3	B	403	FNQ	C1-N1-C2	2.13	116.11	114.64
3	A	403	FNQ	C1-N1-C2	2.17	116.14	114.64
3	C	403	FNQ	C1-N1-C2	2.32	116.24	114.64
3	C	403	FNQ	C4-C3-C2	3.23	121.00	118.15
3	B	403	FNQ	C4-C3-C2	3.30	121.06	118.15
3	A	403	FNQ	C4-C3-C2	3.33	121.09	118.15
3	D	403	FNQ	C4-C3-C2	3.47	121.21	118.15
3	A	403	FNQ	C1-N-C	4.12	122.84	115.89
3	D	403	FNQ	C1-N-C	4.13	122.85	115.89
3	B	403	FNQ	C1-N-C	4.18	122.94	115.89
3	C	403	FNQ	C1-N-C	4.19	122.96	115.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	FNQ	1	0
5	A	405	GOL	5	0
3	B	403	FNQ	1	0
5	B	405	GOL	3	0
3	C	403	FNQ	1	0
3	D	403	FNQ	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, 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	340/360 (94%)	0.16	9 (2%) 56 64	36, 58, 97, 115	0
1	B	340/360 (94%)	0.00	3 (0%) 84 89	35, 50, 80, 112	0
1	C	341/360 (94%)	0.22	16 (4%) 31 43	41, 66, 105, 130	0
1	D	337/360 (93%)	0.06	4 (1%) 79 85	35, 59, 102, 123	0
All	All	1358/1440 (94%)	0.11	32 (2%) 59 68	35, 58, 100, 130	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	LEU	4.7
1	B	353	PHE	3.5
1	A	336	LYS	3.1
1	D	312	MET	3.0
1	A	308	CYS	2.9
1	A	332	TRP	2.8
1	D	311	ASP	2.8
1	C	339	THR	2.7
1	C	338	ASN	2.6
1	A	335	GLY	2.6
1	C	337	ASP	2.6
1	C	20	THR	2.6
1	A	307	SER	2.5
1	C	335	GLY	2.5
1	C	332	TRP	2.5
1	C	348	PRO	2.4
1	C	170	GLY	2.4
1	C	326	PRO	2.4
1	C	329	TYR	2.4
1	B	114[A]	PHE	2.4
1	C	144	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	334	ALA	2.2
1	C	350	ALA	2.1
1	C	330	LYS	2.1
1	B	338	ASN	2.1
1	D	337	ASP	2.1
1	C	349	GLU	2.1
1	A	334	ALA	2.1
1	C	167	THR	2.1
1	A	326	PRO	2.1
1	A	324	PHE	2.0
1	D	334	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
6	CL	B	406	1/1	0.24	0.36	116,116,116,116	0
4	DMS	B	404	4/4	0.77	0.25	122,122,123,123	0
4	DMS	A	404	4/4	0.78	0.28	117,117,118,118	0
4	DMS	D	404	4/4	0.84	0.25	117,117,119,119	0
6	CL	A	406	1/1	0.86	0.23	109,109,109,109	0
5	GOL	A	405	6/6	0.88	0.41	37,45,47,48	6
4	DMS	C	404	4/4	0.88	0.18	97,97,97,98	4
3	FNQ	A	403	19/36	0.93	0.18	52,60,66,67	19
3	FNQ	D	403	25/36	0.94	0.14	50,60,74,74	25
5	GOL	B	405	6/6	0.95	0.30	24,34,37,37	6
3	FNQ	B	403	31/36	0.96	0.18	36,51,84,85	31
3	FNQ	C	403	30/36	0.96	0.15	47,62,93,95	30

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	C	401	1/1	0.98	0.13	61,61,61,61	0
2	ZN	A	401	1/1	0.98	0.11	63,63,63,63	0
2	ZN	B	401	1/1	0.98	0.17	46,46,46,46	1
2	ZN	A	402	1/1	0.99	0.11	70,70,70,70	1
2	ZN	D	402	1/1	0.99	0.10	60,60,60,60	1
2	ZN	C	402	1/1	0.99	0.15	64,64,64,64	1
2	ZN	D	401	1/1	0.99	0.15	43,43,43,43	1
2	ZN	B	402	1/1	1.00	0.14	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.