



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2016 – 03:46 PM EDT

PDB ID : 4CAV
Title : Crystal structure of *Aspergillus fumigatus* N-myristoyl transferase in complex with myristoyl CoA and a benzofuran ligand R0-09-4879
Authors : Robinson, D.A.; Fang, W.; Raimi, O.G.; Blair, D.E.; Harrison, J.; Ruda, G.F.; Lockhart, D.E.A.; Torrie, L.S.; Wyatt, P.G.; Gilbert, I.H.; Van Aalten, D.M.F.
Deposited on : 2013-10-09
Resolution : 1.89 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
<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

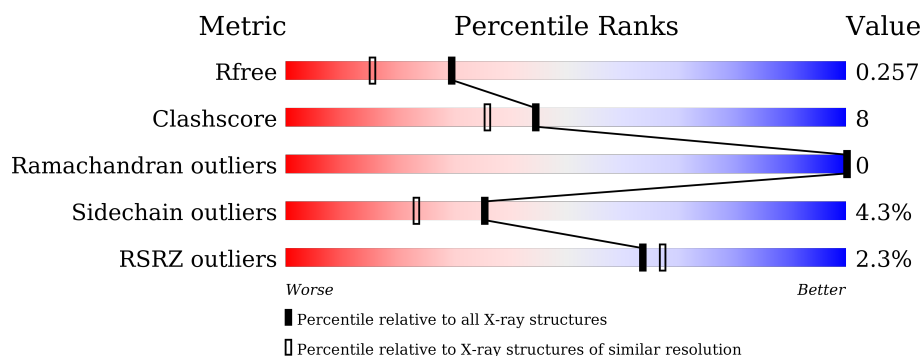
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	411	<div> <div>2%</div> <div>82%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3704 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 GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	1	0
			3195	2066	545	572	12			

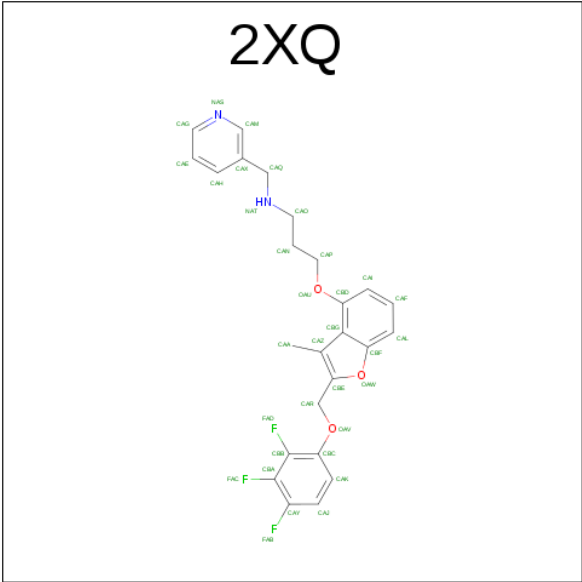
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLY	-	EXPRESSION TAG	UNP Q9UVX3
A	83	PRO	-	EXPRESSION TAG	UNP Q9UVX3
A	84	ARG	-	EXPRESSION TAG	UNP Q9UVX3
A	85	SER	-	EXPRESSION TAG	UNP Q9UVX3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

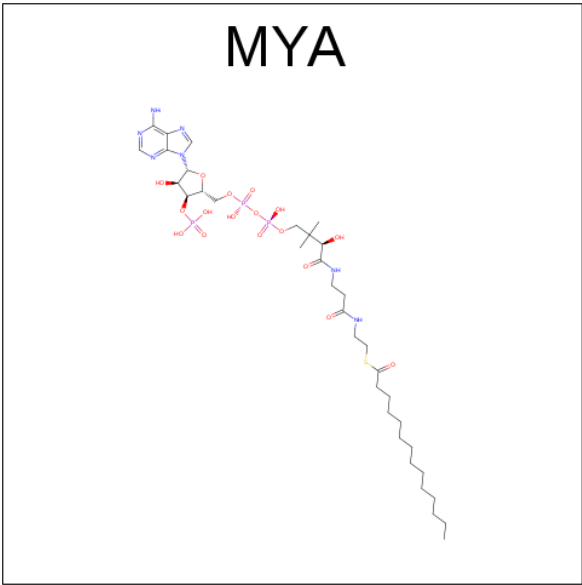
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 3-[[3-METHYL-2-[[2,3,4-TRIS(FLUORANYL)PHENOXY]METHYL]-1-BENZOFURAN-4-YL]OXY]-N-(PYRIDIN-3-YLMETHYL)PROPAN-1-AMINE (three-letter code: 2XQ) (formula: C₂₅H₂₃F₃N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	33	25	3	2	3	0	0

- Molecule 4 is TETRADECANOYL-COA (three-letter code: MYA) (formula: C₃₅H₆₂N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	63	35	7	17	3	1	0	0

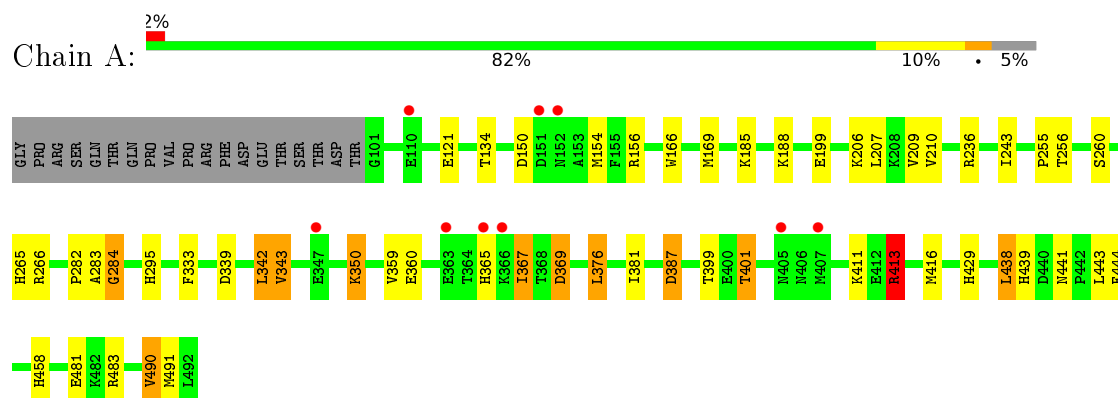
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	412	Total 412	O 412	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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.43Å 57.01Å 143.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 1.89 19.93 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.93-1.89) 94.1 (19.93-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.248 0.195 , 0.257	Depositor DCC
R_{free} test set	1766 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.9	EDS
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35154 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3704	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, 2XQ, 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	1.08	3/3282 (0.1%)	1.03	8/4461 (0.2%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	VAL	CB-CG1	5.39	1.64	1.52
1	A	166	TRP	CE3-CZ3	5.17	1.47	1.38
1	A	121	GLU	CD-OE2	-5.07	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ASP	CB-CG-OD1	-8.63	110.53	118.30
1	A	413	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	376	LEU	CB-CG-CD2	6.34	121.77	111.00
1	A	413	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	342	LEU	CB-CG-CD1	5.71	120.71	111.00
1	A	284	GLY	N-CA-C	-5.34	99.75	113.10
1	A	236	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	483	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	PRO	Peptide

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	3195	0	3185	52	0
2	A	1	0	0	0	0
3	A	33	0	23	2	0
4	A	63	0	58	0	1
5	A	412	0	0	23	1
All	All	3704	0	3266	52	1

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 8.

All (52) 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:411:LYS:HE3	5:A:2354:HOH:O	1.53	1.08
1:A:199:GLU:OE2	1:A:206:LYS:HD2	1.53	1.07
1:A:199:GLU:CD	1:A:206:LYS:HD2	1.85	0.96
1:A:387:ASP:HB2	5:A:2335:HOH:O	1.66	0.95
1:A:387:ASP:HB3	5:A:2343:HOH:O	1.80	0.81
1:A:169:MET:HE2	5:A:2079:HOH:O	1.81	0.79
1:A:369:ASP:OD2	1:A:413:ARG:HD3	1.85	0.76
1:A:429:HIS:HE1	5:A:2365:HOH:O	1.71	0.73
1:A:438:LEU:HD21	1:A:490[A]:VAL:HG13	1.75	0.69
1:A:156:ARG:HG3	1:A:381:ILE:HD11	1.73	0.69
1:A:199:GLU:OE2	1:A:206:LYS:CD	2.37	0.69
1:A:491:MET:HE3	5:A:2174:HOH:O	1.93	0.68
1:A:367:ILE:HD12	1:A:367:ILE:C	2.14	0.67
1:A:169:MET:CE	5:A:2079:HOH:O	2.39	0.66
1:A:491:MET:CE	5:A:2174:HOH:O	2.44	0.64
1:A:150:ASP:HB3	5:A:2065:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:SER:OG	1:A:458:HIS:HD2	1.82	0.62
1:A:439:HIS:NE2	1:A:490[A]:VAL:CG2	2.64	0.61
1:A:411:LYS:CE	5:A:2354:HOH:O	2.24	0.60
1:A:134:THR:HG23	5:A:2039:HOH:O	2.03	0.58
1:A:199:GLU:CG	1:A:206:LYS:HD2	2.33	0.58
1:A:339:ASP:HA	1:A:343:VAL:HG13	1.86	0.58
1:A:188:LYS:CE	5:A:2128:HOH:O	2.53	0.56
1:A:443:LEU:HD23	1:A:481:GLU:HG2	1.90	0.54
1:A:413:ARG:HH21	1:A:416:MET:HE1	1.73	0.53
1:A:359:VAL:O	1:A:367:ILE:HA	2.09	0.53
1:A:265:HIS:HE1	3:A:1494:2XQ:OAW	1.92	0.52
1:A:458:HIS:HE1	5:A:2380:HOH:O	1.94	0.50
1:A:439:HIS:NE2	1:A:490[A]:VAL:HG22	2.26	0.50
1:A:401:THR:HG22	5:A:2330:HOH:O	2.11	0.48
1:A:413:ARG:NH2	1:A:416:MET:HE1	2.29	0.47
1:A:210:VAL:HG13	1:A:243:ILE:HG21	1.97	0.46
1:A:265:HIS:CE1	3:A:1494:2XQ:OAW	2.68	0.45
1:A:283:ALA:CB	5:A:2254:HOH:O	2.65	0.45
1:A:369:ASP:OD2	1:A:413:ARG:CD	2.59	0.45
1:A:188:LYS:HE2	5:A:2128:HOH:O	2.15	0.44
1:A:295:HIS:HD2	5:A:2131:HOH:O	2.00	0.44
1:A:185:LYS:HD3	1:A:185:LYS:C	2.38	0.44
1:A:188:LYS:HE3	5:A:2128:HOH:O	2.18	0.43
1:A:343:VAL:HA	5:A:2316:HOH:O	2.19	0.43
1:A:441:ASN:HA	1:A:444:PHE:CE2	2.54	0.43
1:A:439:HIS:HD2	5:A:2346:HOH:O	2.01	0.42
1:A:206:LYS:HB2	1:A:206:LYS:HE2	1.72	0.42
1:A:401:THR:CG2	1:A:413:ARG:HD2	2.50	0.41
1:A:255:PRO:C	1:A:256:THR:HG22	2.40	0.41
1:A:491:MET:HE2	5:A:2174:HOH:O	2.17	0.41
1:A:283:ALA:HB1	1:A:284:GLY:H	1.36	0.41
1:A:439:HIS:CD2	5:A:2346:HOH:O	2.72	0.41
1:A:429:HIS:CE1	5:A:2365:HOH:O	2.57	0.41
1:A:360:GLU:OE2	1:A:365:HIS:HD2	2.04	0.41
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.41
1:A:350:LYS:HA	1:A:350:LYS:HD3	1.77	0.40

All (1) 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)
4:A:1495:MYA:O9A	5:A:2265:HOH:O[3_554]	2.12	0.08

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	391/411 (95%)	381 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	347/367 (95%)	331 (95%)	16 (5%)	33	21

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	MET
1	A	207	LEU
1	A	266	ARG
1	A	333	PHE
1	A	342	LEU
1	A	343	VAL
1	A	350	LYS
1	A	367	ILE

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Mol	Chain	Res	Type
1	A	369	ASP
1	A	376	LEU
1	A	399	THR
1	A	401	THR
1	A	413	ARG
1	A	438	LEU
1	A	490[A]	VAL
1	A	490[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	290	GLN
1	A	295	HIS
1	A	321	GLN
1	A	365	HIS
1	A	419	ASN
1	A	447	GLN
1	A	456	GLN
1	A	458	HIS
1	A	477	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	2XQ	A	1494	-	32,36,36	1.64	6 (18%)	35,49,49	1.39	5 (14%)
4	MYA	A	1495	-	53,65,65	0.96	3 (5%)	64,91,91	1.94	14 (21%)

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	2XQ	A	1494	-	-	0/12/14/14	0/3/4/4
4	MYA	A	1495	-	-	0/59/80/80	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1494	2XQ	CAR-CBE	-5.60	1.38	1.50
3	A	1494	2XQ	CBD-CBG	-2.24	1.37	1.42
4	A	1495	MYA	C6-C5	2.04	1.55	1.51
3	A	1494	2XQ	OAV-CAR	2.04	1.49	1.43
4	A	1495	MYA	O10-C10	2.29	1.46	1.42
3	A	1494	2XQ	CAF-CAL	2.30	1.41	1.36
3	A	1494	2XQ	CAJ-CAY	2.50	1.43	1.37
3	A	1494	2XQ	CAA-CAZ	2.57	1.57	1.51
4	A	1495	MYA	P3X-O9A	2.76	1.59	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1495	MYA	N3A-C2A-N1A	-7.73	122.80	128.87
4	A	1495	MYA	C4M-C3M-C2M	-3.67	103.41	113.97
3	A	1494	2XQ	CAE-CAH-CAX	-3.29	115.66	120.65
4	A	1495	MYA	C2X-C3X-C4X	-2.93	97.63	103.25
4	A	1495	MYA	C3-C2-S1	-2.48	106.23	113.84
4	A	1495	MYA	O3X-C3X-C2X	-2.44	102.66	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1495	MYA	C13-C11-C12	-2.29	105.53	108.50
3	A	1494	2XQ	OAV-CAR-CBE	-2.04	103.78	108.03
4	A	1495	MYA	C2A-N1A-C6A	2.25	122.79	118.77
3	A	1494	2XQ	FAD-CBB-CBC	2.28	122.26	119.49
4	A	1495	MYA	C13-C11-C10	2.32	113.40	109.17
4	A	1495	MYA	N6A-C6A-N1A	2.47	122.65	118.52
3	A	1494	2XQ	FAB-CAY-CAJ	2.53	124.20	118.46
4	A	1495	MYA	O5A-P2A-O4A	2.63	126.23	112.56
4	A	1495	MYA	C14-C11-C10	2.73	114.15	109.17
3	A	1494	2XQ	CAH-CAX-CAM	3.25	121.70	117.07
4	A	1495	MYA	O4X-C1X-N9A	3.42	114.56	108.11
4	A	1495	MYA	C2-S1-C2M	5.22	107.72	100.70
4	A	1495	MYA	O2M-C2M-C3M	5.86	119.88	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1494	2XQ	2	0
4	A	1495	MYA	0	1

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 [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	392/411 (95%)	0.15	9 (2%) 64 67	13, 23, 39, 56	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	3.3
1	A	110	GLU	3.0
1	A	347	GLU	2.8
1	A	363	GLU	2.5
1	A	407	MET	2.4
1	A	405	ASN	2.4
1	A	152	ASN	2.3
1	A	366	LYS	2.2
1	A	365	HIS	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(\AA^2)	Q<0.9
4	MYA	A	1495	63/63	0.95	0.10	-0.36	11,19,29,39	0
3	2XQ	A	1494	33/33	0.96	0.08	-1.13	14,21,35,41	0
2	CL	A	1493	1/1	0.83	0.07	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.