



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:27 pm GMT

PDB ID : 3QWZ
Title : Crystal structure of FAF1 UBX-p97N-domain complex
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Deposited on : 2011-02-28
Resolution : 2.00 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
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) : trunk31020

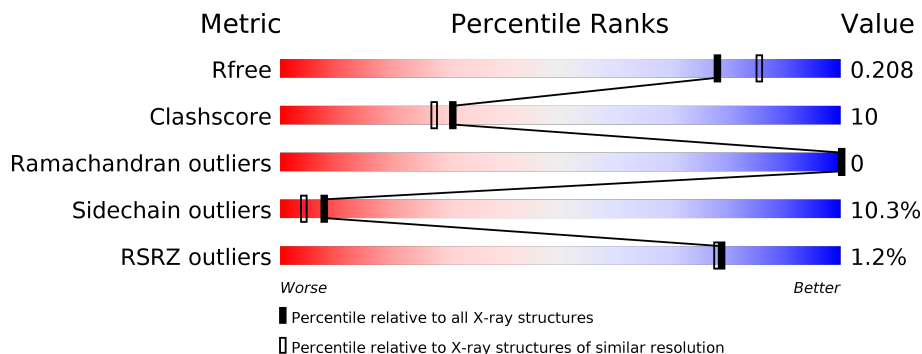
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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	211	<div> <div></div> <div>58%18%7%16%</div> </div>
2	B	84	<div> <div></div> <div>69%23%5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2258 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1416	891	248	269	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P55072
A	-1	SER	-	EXPRESSION TAG	UNP P55072
A	0	HIS	-	EXPRESSION TAG	UNP P55072

- Molecule 2 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			679	444	112	122	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	567	GLY	-	EXPRESSION TAG	UNP Q9UNN5
B	568	SER	-	EXPRESSION TAG	UNP Q9UNN5
B	569	HIS	-	EXPRESSION TAG	UNP Q9UNN5
B	570	MET	-	EXPRESSION TAG	UNP Q9UNN5

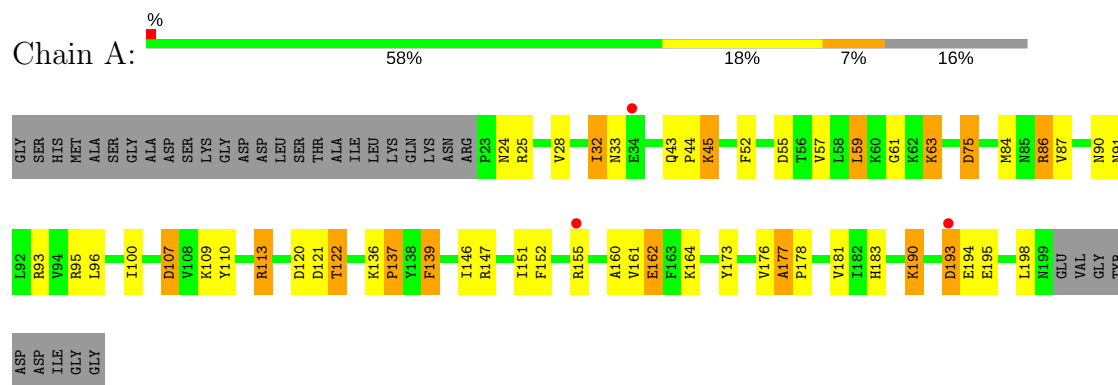
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	49	Total	O	0	0
			49	49		

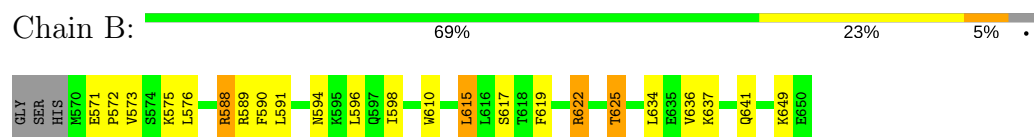
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Transitional endoplasmic reticulum ATPase



- Molecule 2: FAS-associated factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.49Å 59.94Å 75.54Å 90.00° 114.83° 90.00°	Depositor
Resolution (Å)	19.33 – 2.00 42.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.33-2.00) 96.1 (42.84-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.249 0.214 , 0.208	Depositor DCC
R_{free} test set	932 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2258	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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, 0.333 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: MLY

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	1.79	16/1416 (1.1%)	1.11	7/1916 (0.4%)
2	B	1.77	2/673 (0.3%)	1.07	2/908 (0.2%)
All	All	1.79	18/2089 (0.9%)	1.10	9/2824 (0.3%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	VAL	CB-CG2	-5.96	1.40	1.52
1	A	95	ARG	CB-CG	-5.88	1.36	1.52
1	A	146	ILE	CB-CG2	-5.85	1.34	1.52
1	A	28	VAL	CB-CG1	-5.82	1.40	1.52
1	A	162	GLU	CD-OE1	-5.79	1.19	1.25
1	A	45	LYS	CD-CE	-5.77	1.36	1.51
1	A	28	VAL	CB-CG2	-5.75	1.40	1.52
2	B	625	THR	CB-CG2	-5.66	1.33	1.52
1	A	137	PRO	CB-CG	-5.51	1.22	1.50
2	B	636	VAL	CB-CG2	-5.43	1.41	1.52
1	A	177	ALA	CA-CB	-5.37	1.41	1.52
1	A	160	ALA	CA-CB	-5.30	1.41	1.52
1	A	61	GLY	C-O	-5.27	1.15	1.23
1	A	139	PHE	CD1-CE1	-5.26	1.28	1.39
1	A	110	TYR	CD1-CE1	-5.22	1.31	1.39
1	A	57	VAL	CB-CG1	-5.13	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	PHE	CD2-CE2	-5.08	1.29	1.39
1	A	63	LYS	CB-CG	-5.04	1.39	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	75	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	107	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	155	ARG	CB-CA-C	-6.35	97.69	110.40
1	A	93	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	B	615	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	93	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	59	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	576	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	MET	Mainchain

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	1416	0	1439	33	0
2	B	679	0	694	10	0
3	A	114	0	0	2	0
3	B	49	0	0	1	0
All	All	2258	0	2133	42	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 10.

All (42) 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:122:THR:HG21	1:A:162:GLU:N	1.69	1.05
1:A:122:THR:HG21	1:A:162:GLU:H	0.88	1.04
1:A:122:THR:HG23	1:A:161:VAL:HA	1.45	0.98
1:A:122:THR:CG2	1:A:161:VAL:HA	1.94	0.96
1:A:113:ARG:HE	1:A:183:HIS:HE1	1.21	0.87
2:B:571:GLU:HG2	2:B:572:PRO:HD2	1.68	0.74
1:A:113:ARG:HE	1:A:183:HIS:CE1	2.07	0.72
1:A:122:THR:HG23	1:A:122:THR:O	1.91	0.69
2:B:575:LYS:HG3	3:B:72:HOH:O	1.91	0.69
1:A:113:ARG:NE	1:A:183:HIS:HE1	1.89	0.68
1:A:122:THR:CG2	1:A:122:THR:O	2.41	0.68
1:A:91:ASN:HD21	1:A:151:ILE:H	1.46	0.63
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.81	0.62
1:A:193:ASP:HB2	3:A:302:HOH:O	1.98	0.61
1:A:190:LYS:HB3	1:A:190:LYS:NZ	2.16	0.60
1:A:32:ILE:HD12	1:A:32:ILE:H	1.66	0.60
1:A:90:ASN:HD21	1:A:198:LEU:H	1.50	0.60
1:A:43:GLN:N	1:A:44:PRO:HD2	2.16	0.60
1:A:90:ASN:ND2	1:A:198:LEU:H	2.01	0.58
2:B:571:GLU:CG	2:B:572:PRO:HD2	2.35	0.56
1:A:164:MLY:HH23	3:A:246:HOH:O	2.07	0.54
1:A:107:ASP:O	1:A:109:LYS:HE2	2.06	0.54
1:A:100:ILE:C	1:A:100:ILE:HD12	2.28	0.53
1:A:136:LYS:N	1:A:137:PRO:CD	2.72	0.53
1:A:122:THR:HG21	1:A:161:VAL:HA	1.82	0.53
1:A:86:ARG:H	1:A:86:ARG:CZ	2.22	0.52
1:A:190:LYS:HB3	1:A:190:LYS:HZ1	1.76	0.51
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.94	0.50
2:B:617:SER:OG	2:B:622:ARG:HG2	2.14	0.47
2:B:573:VAL:HG23	2:B:590:PHE:O	2.15	0.47
1:A:120:ASP:OD1	1:A:121:ASP:N	2.47	0.47
2:B:594:ASN:HB3	2:B:598:ILE:HD12	1.96	0.46
2:B:610:TRP:CH2	2:B:649:MLY:HH11	2.51	0.46
1:A:164:MLY:HH12	1:A:195:GLU:OE2	2.17	0.45
2:B:588:ARG:HG2	2:B:590:PHE:CZ	2.51	0.45
1:A:113:ARG:HG3	1:A:181:VAL:HB	1.98	0.45
2:B:588:ARG:HG3	2:B:589:ARG:N	2.32	0.44
1:A:177:ALA:HB1	1:A:178:PRO:CD	2.47	0.43
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.54	0.42
1:A:33:ASN:HD21	2:B:619:PHE:HE2	1.66	0.42
1:A:91:ASN:ND2	1:A:151:ILE:H	2.16	0.41
1:A:52:PHE:HB2	1:A:55:ASP:OD2	2.20	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	173/211 (82%)	162 (94%)	11 (6%)	0	100	100
2	B	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
All	All	250/295 (85%)	234 (94%)	16 (6%)	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	160/185 (86%)	145 (91%)	15 (9%)	9	5
2	B	74/76 (97%)	65 (88%)	9 (12%)	5	3
All	All	234/261 (90%)	210 (90%)	24 (10%)	8	4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	ARG
1	A	32	ILE
1	A	45	LYS
1	A	59	LEU

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Mol	Chain	Res	Type
1	A	63	LYS
1	A	75	ASP
1	A	86	ARG
1	A	96	LEU
1	A	113	ARG
1	A	122	THR
1	A	173	TYR
1	A	190	LYS
1	A	193	ASP
1	A	194	GLU
2	B	588	ARG
2	B	591	LEU
2	B	596	LEU
2	B	615	LEU
2	B	622	ARG
2	B	625	THR
2	B	634	LEU
2	B	637	LYS
2	B	641	GLN

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

Mol	Chain	Res	Type
1	A	36	ASN
1	A	90	ASN
1	A	91	ASN
1	A	183	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
1	MLY	A	164	1	10,10,11	3.41	3 (30%)	8,11,13	5.44	4 (50%)
1	MLY	A	62	1	10,10,11	1.70	2 (20%)	8,11,13	3.43	2 (25%)
2	MLY	B	614	2	10,10,11	2.12	1 (10%)	8,11,13	2.20	1 (12%)
2	MLY	B	649	2	10,10,11	3.15	2 (20%)	8,11,13	4.66	3 (37%)

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
1	MLY	A	164	1	-	0/7/9/11	0/0/0/0
1	MLY	A	62	1	-	0/7/9/11	0/0/0/0
2	MLY	B	614	2	-	0/7/9/11	0/0/0/0
2	MLY	B	649	2	-	0/7/9/11	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	MLY	CH2-NZ	-9.67	1.15	1.46
2	B	649	MLY	CH1-NZ	-8.70	1.18	1.46
1	A	62	MLY	CH1-NZ	-3.98	1.33	1.46
1	A	164	MLY	CB-CA	-2.31	1.50	1.53
1	A	62	MLY	CA-C	2.35	1.53	1.50
1	A	164	MLY	CA-C	2.93	1.54	1.50
2	B	649	MLY	CH2-NZ	3.36	1.56	1.46
2	B	614	MLY	CH2-NZ	6.31	1.65	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	MLY	CH1-NZ-CE	-6.45	84.81	110.75
2	B	649	MLY	CH2-NZ-CE	-6.14	86.04	110.75
1	A	62	MLY	CH1-NZ-CE	-3.41	97.05	110.75
1	A	164	MLY	O-C-CA	-2.00	119.46	124.96
2	B	614	MLY	CH1-NZ-CE	5.21	131.71	110.75
1	A	164	MLY	CH2-NZ-CE	5.35	132.27	110.75
2	B	649	MLY	CH1-NZ-CE	7.67	141.63	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	649	MLY	CH2-NZ-CH1	8.40	131.86	109.73
1	A	62	MLY	CH2-NZ-CH1	8.78	132.84	109.73
1	A	164	MLY	CH2-NZ-CH1	12.52	142.71	109.73

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
1	A	164	MLY	2	0
2	B	649	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	175/211 (82%)	-0.36	3 (1%) 70 68	11, 24, 45, 62	0
2	B	79/84 (94%)	-0.47	0 100 100	13, 25, 52, 69	0
All	All	254/295 (86%)	-0.39	3 (1%) 79 78	11, 24, 47, 69	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	5.4
1	A	34	GLU	2.2
1	A	193	ASP	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, 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
1	MLY	A	164	11/12	0.88	0.14	21,22,32,32	0
2	MLY	B	614	11/12	0.93	0.13	12,15,21,29	0
2	MLY	B	649	11/12	0.94	0.09	17,20,27,27	0
1	MLY	A	62	11/12	0.97	0.08	15,17,20,25	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.