Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID	:	1XKP
Title	:	Crystal structure of the virulence factor YopN in complex with its heterodimeric chaperone SycN-YscB
Authors	:	Schubot, F.D.; Jackson, M.W.; Penrose, K.J.; Cherry, S.; Tropea, J.E.; Plano, G.V.; Waugh, D.S.
Deposited on	:	2004-09-29
Resolution	:	1.70 Å(reported)

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

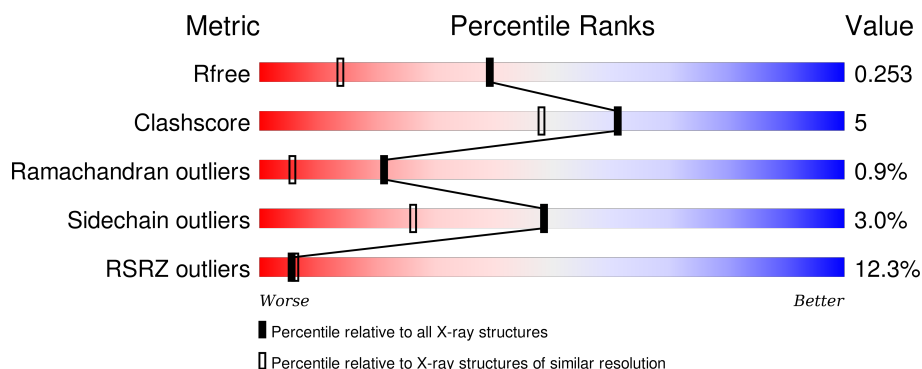|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.70 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		0.253
Clashscore		5
Ramachandran outliers		0.9%
Sidechain outliers		3.0%
RSRZ outliers		12.3%

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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	246	14% 80% 13% · 6%
2	B	124	5% 89% 8% · ·
3	C	143	10% 78% 9% · 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3952 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 putative membrane-bound Yop targeting protein YopN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1823	1146	309	363	5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	DMG	GLY	MODIFIED RESIDUE	GB 3822072
A	64	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	70	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	72	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	93	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	100	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	122	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	128	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	137	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	147	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	221	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	237	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	254	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	264	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	266	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	276	MLY	LYS	MODIFIED RESIDUE	GB 3822072

- Molecule 2 is a protein called Chaperone protein sycN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	945	608	161	172	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	MLY	LYS	MODIFIED RESIDUE	UNP P61380
B	74	MLY	LYS	MODIFIED RESIDUE	UNP P61380
B	123	PRO	SER	ENGINEERED	UNP P61380

• Molecule 3 is a protein called Chaperone protein yscB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	126	1005	643	181	177	4	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MLY	LYS	MODIFIED RESIDUE	UNP Q56973
C	15	MLY	LYS	MODIFIED RESIDUE	UNP Q56973
C	21	MLY	LYS	MODIFIED RESIDUE	UNP Q56973
C	31	MLY	LYS	MODIFIED RESIDUE	UNP Q56973
C	113	MLY	LYS	MODIFIED RESIDUE	UNP Q56973
C	138	HIS	-	EXPRESSION TAG	UNP Q56973
C	139	HIS	-	EXPRESSION TAG	UNP Q56973
C	140	HIS	-	EXPRESSION TAG	UNP Q56973
C	141	HIS	-	EXPRESSION TAG	UNP Q56973
C	142	HIS	-	EXPRESSION TAG	UNP Q56973
C	143	HIS	-	EXPRESSION TAG	UNP Q56973

• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	104	104	104	0	0
4	B	35	35	35	0	0
4	C	40	40	40	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.
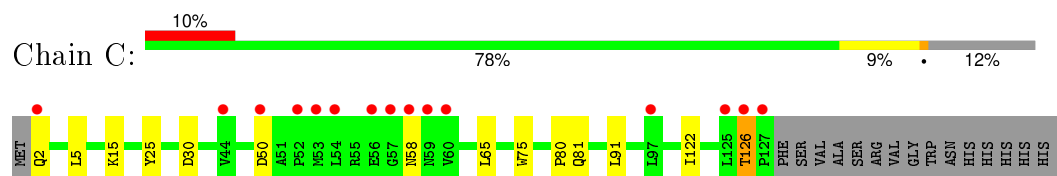
• Molecule 1: putative membrane-bound Yop targeting protein YopN
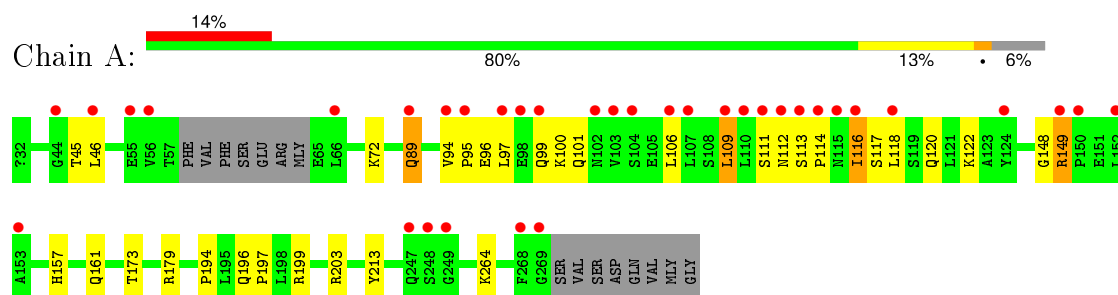
• Molecule 2: Chaperone protein sycN
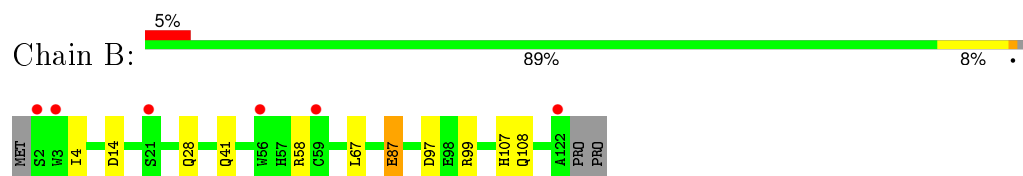
• Molecule 3: Chaperone protein yscB

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	60.72Å 60.72Å 140.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.86 – 1.70 42.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (60.86-1.70) 89.9 (42.93-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.82 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.242 0.213 , 0.253	Depositor DCC
R_{free} test set	2571 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.0	EDS
Estimated twinning fraction	0.063 for h,-k,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 50097 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3952	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

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	0.64	0/1695	0.75	2/2297 (0.1%)
2	B	0.57	0/943	0.68	0/1288
3	C	0.60	0/965	0.73	0/1316
All	All	0.61	0/3603	0.73	2/4901 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	213	TYR	CB-CG-CD1	5.10	124.06	121.00

There are no chirality outliers.

There are no planarity outliers.

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	1823	0	1844	29	0
2	B	945	0	965	9	0
3	C	1005	0	1064	9	0
4	A	104	0	0	6	0
4	B	35	0	0	1	0
4	C	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3952	0	3873	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 5.

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:100:MLY:HH21	4:A:342:HOH:O	1.63	0.96
1:A:100:MLY:CH2	4:A:342:HOH:O	2.22	0.81
1:A:100:MLY:NZ	4:A:342:HOH:O	2.20	0.74
1:A:100:MLY:HH11	4:A:342:HOH:O	1.90	0.70
1:A:100:MLY:CH1	4:A:342:HOH:O	2.42	0.67
1:A:157:HIS:CD2	1:A:161:GLN:HE21	2.15	0.65
1:A:264:MLY:HH11	4:A:331:HOH:O	1.97	0.65
1:A:148:GLY:O	1:A:149:ARG:HG3	1.99	0.62
1:A:196:GLN:NE2	1:A:199:ARG:HH21	1.98	0.62
2:B:14:ASP:OD2	2:B:107:HIS:HE1	1.85	0.60
1:A:173:THR:HG23	1:A:203:ARG:HD2	1.85	0.58
3:C:122:ILE:O	3:C:126:THR:OG1	2.21	0.57
1:A:116:ILE:N	1:A:116:ILE:HD12	2.18	0.57
2:B:4:ILE:HD11	2:B:41:GLN:HG2	1.88	0.55
1:A:117:SER:H	1:A:120:GLN:HE21	1.55	0.54
2:B:67:LEU:CD1	3:C:65:LEU:HD11	2.38	0.54
1:A:94:VAL:HG13	1:A:94:VAL:O	2.09	0.53
1:A:97:LEU:HD13	1:A:99:GLN:NE2	2.24	0.52
1:A:118:LEU:HG	1:A:122:MLY:HE2	1.93	0.51
3:C:2:GLN:HG2	3:C:5:LEU:H	1.75	0.51
2:B:97:ASP:OD2	2:B:99:ARG:NE	2.44	0.50
1:A:89:GLN:C	1:A:89:GLN:NE2	2.64	0.50
1:A:46:LEU:HD22	2:B:28:GLN:OE1	2.13	0.49
1:A:94:VAL:O	1:A:96:GLU:N	2.46	0.49
1:A:111:SER:O	1:A:113:SER:N	2.46	0.48
1:A:196:GLN:HE22	1:A:199:ARG:HH21	1.60	0.48
1:A:72:MLY:HH22	3:C:30:ASP:OD1	2.14	0.47
3:C:5:LEU:HD13	3:C:25:TYR:CD2	2.50	0.47
1:A:114:PRO:HG3	3:C:58:ASN:HD21	1.79	0.46
1:A:89:GLN:C	1:A:89:GLN:HE21	2.19	0.46
2:B:87:GLU:H	2:B:87:GLU:CD	2.21	0.45
1:A:113:SER:HB2	1:A:116:ILE:HG13	1.99	0.45
1:A:194:PRO:HG2	1:A:197:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:HD2	3:C:81:GLN:OE1	2.17	0.44
3:C:15:MLY:HH23	3:C:15:MLY:HD3	1.90	0.44
2:B:108:GLN:HG2	4:B:142:HOH:O	2.17	0.43
1:A:148:GLY:O	1:A:149:ARG:CB	2.66	0.43
1:A:116:ILE:N	1:A:116:ILE:CD1	2.82	0.43
1:A:101:GLN:HA	1:A:101:GLN:OE1	2.19	0.43
1:A:148:GLY:O	1:A:149:ARG:CG	2.65	0.42
2:B:4:ILE:HD11	2:B:41:GLN:CG	2.50	0.42
2:B:67:LEU:HD11	3:C:65:LEU:HD11	2.02	0.41

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	214/246 (87%)	206 (96%)	4 (2%)	4 (2%)	10	1
2	B	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
3	C	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
All	All	450/513 (88%)	440 (98%)	6 (1%)	4 (1%)	21	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	149	ARG
1	A	109	LEU
1	A	95	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	188/200 (94%)	182 (97%)	6 (3%)	46	24
2	B	101/104 (97%)	99 (98%)	2 (2%)	63	44
3	C	105/120 (88%)	101 (96%)	4 (4%)	40	17
All	All	394/424 (93%)	382 (97%)	12 (3%)	48	26

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	89	GLN
1	A	106	LEU
1	A	109	LEU
1	A	116	ILE
1	A	179	ARG
2	B	58	ARG
2	B	87	GLU
3	C	50	ASP
3	C	75	TRP
3	C	91	LEU
3	C	126	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	120	GLN
1	A	154	HIS
1	A	157	HIS
1	A	161	GLN
1	A	196	GLN
2	B	73	GLN
2	B	107	HIS
2	B	112	GLN

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Mol	Chain	Res	Type
3	C	32	HIS
3	C	58	ASN
3	C	105	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)

20 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	100	1	9,10,11	1.06	1 (11%)	9,11,13	1.47	2 (22%)
1	MLY	A	122	1	9,10,11	0.59	0	9,11,13	0.86	1 (11%)
1	MLY	A	128	1	9,10,11	0.54	0	9,11,13	0.89	0
1	MLY	A	137	1	9,10,11	0.63	0	9,11,13	1.13	0
1	MLY	A	147	1	9,10,11	0.59	0	9,11,13	0.77	0
1	MLY	A	221	1	9,10,11	0.72	0	9,11,13	1.02	1 (11%)
1	MLY	A	237	1	9,10,11	0.55	0	9,11,13	1.25	1 (11%)
1	MLY	A	254	1	9,10,11	0.62	0	9,11,13	0.76	0
1	MLY	A	264	1	9,10,11	0.69	0	9,11,13	1.06	1 (11%)
1	MLY	A	266	1	9,10,11	0.55	0	9,11,13	1.03	0
1	MLY	A	70	1	9,10,11	0.72	0	9,11,13	1.01	1 (11%)
1	MLY	A	72	1	9,10,11	0.74	0	9,11,13	1.23	1 (11%)
1	MLY	A	93	1	9,10,11	0.61	0	9,11,13	0.95	0
2	MLY	B	65	2	9,10,11	0.47	0	9,11,13	1.21	1 (11%)
2	MLY	B	74	2	9,10,11	0.69	0	9,11,13	0.70	0
3	MLY	C	113	3	9,10,11	0.71	0	9,11,13	0.81	1 (11%)
3	MLY	C	15	3	9,10,11	0.65	0	9,11,13	0.97	1 (11%)
3	MLY	C	21	3	9,10,11	0.62	0	9,11,13	0.95	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	MLY	C	31	3	9,10,11	0.61	0	9,11,13	1.08	1 (11%)
3	MLY	C	6	3	9,10,11	0.61	0	9,11,13	0.95	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
1	MLY	A	100	1	-	0/7/9/11	0/0/0/0
1	MLY	A	122	1	-	0/7/9/11	0/0/0/0
1	MLY	A	128	1	-	0/7/9/11	0/0/0/0
1	MLY	A	137	1	-	0/7/9/11	0/0/0/0
1	MLY	A	147	1	-	0/7/9/11	0/0/0/0
1	MLY	A	221	1	-	0/7/9/11	0/0/0/0
1	MLY	A	237	1	-	0/7/9/11	0/0/0/0
1	MLY	A	254	1	-	0/7/9/11	0/0/0/0
1	MLY	A	264	1	-	0/7/9/11	0/0/0/0
1	MLY	A	266	1	-	0/7/9/11	0/0/0/0
1	MLY	A	70	1	-	0/7/9/11	0/0/0/0
1	MLY	A	72	1	-	0/7/9/11	0/0/0/0
1	MLY	A	93	1	-	0/7/9/11	0/0/0/0
2	MLY	B	65	2	-	0/7/9/11	0/0/0/0
2	MLY	B	74	2	-	0/7/9/11	0/0/0/0
3	MLY	C	113	3	-	0/7/9/11	0/0/0/0
3	MLY	C	15	3	-	0/7/9/11	0/0/0/0
3	MLY	C	21	3	-	0/7/9/11	0/0/0/0
3	MLY	C	31	3	-	0/7/9/11	0/0/0/0
3	MLY	C	6	3	-	0/7/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	MLY	CB-CA	-2.39	1.51	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	31	MLY	O-C-CA	-2.58	118.77	125.49
1	A	221	MLY	O-C-CA	-2.30	119.50	125.49
1	A	72	MLY	O-C-CA	-2.27	119.59	125.49
1	A	264	MLY	O-C-CA	-2.24	119.67	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	MLY	O-C-CA	-2.24	119.67	125.49
3	C	113	MLY	O-C-CA	-2.17	119.83	125.49
2	B	65	MLY	CD-CE-NZ	-2.16	108.37	113.92
3	C	15	MLY	O-C-CA	-2.11	119.98	125.49
1	A	237	MLY	O-C-CA	-2.07	120.09	125.49
1	A	100	MLY	CD-CG-CB	-2.06	106.34	113.66
1	A	122	MLY	O-C-CA	-2.01	120.26	125.49
3	C	21	MLY	O-C-CA	-2.00	120.27	125.49
1	A	100	MLY	CH2-NZ-CH1	2.63	116.76	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	100	MLY	5	0
1	A	122	MLY	1	0
1	A	264	MLY	1	0
1	A	72	MLY	1	0
3	C	15	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	217/246 (88%)	1.19	35 (16%)	3	3	23, 31, 66, 70	0
2	B	119/124 (95%)	0.75	6 (5%)	32	35	28, 32, 42, 53	0
3	C	121/143 (84%)	1.10	15 (12%)	5	6	26, 34, 50, 51	0
All	All	457/513 (89%)	1.05	56 (12%)	5	6	23, 32, 52, 70	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	25.4
3	C	127	PRO	11.9
1	A	112	ASN	11.6
1	A	107	LEU	8.6
1	A	109	LEU	8.3
1	A	113	SER	7.6
1	A	97	LEU	7.5
1	A	114	PRO	7.0
2	B	56	TRP	7.0
1	A	247	GLN	6.9
3	C	126	THR	6.8
1	A	104	SER	6.6
3	C	58	ASN	5.3
1	A	111	SER	5.3
3	C	56	GLU	5.3
3	C	60	VAL	5.3
1	A	124	TYR	5.1
3	C	59	ASN	4.8
3	C	57	GLY	4.7
1	A	248	SER	4.6
3	C	125	LEU	4.1
2	B	122	ALA	4.1
1	A	102	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	269	GLY	3.8
1	A	99	GLN	3.7
1	A	66	LEU	3.7
1	A	153	ALA	3.5
1	A	152	LEU	3.5
3	C	54	LEU	3.4
3	C	52	PRO	3.4
1	A	98	GLU	3.3
1	A	94	VAL	3.2
2	B	21	SER	3.1
1	A	249	GLY	3.0
1	A	89	GLN	2.9
1	A	56	VAL	2.9
1	A	103	VAL	2.9
2	B	2	SER	2.9
1	A	106	LEU	2.7
3	C	2	GLN	2.6
3	C	53	MET	2.5
1	A	150	PRO	2.5
1	A	118	LEU	2.5
1	A	55	GLU	2.5
1	A	149	ARG	2.5
3	C	50	ASP	2.4
1	A	268	PHE	2.3
1	A	44	GLY	2.3
2	B	59	CYS	2.3
1	A	95	PRO	2.2
1	A	46	LEU	2.2
2	B	3	TRP	2.2
1	A	115	ASN	2.2
1	A	116	ILE	2.1
3	C	97	LEU	2.1
3	C	44	VAL	2.0

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

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
1	MLY	A	137	11/12	0.86	0.18	-	28,31,45,45	0
1	MLY	A	72	11/12	0.78	0.23	-	30,32,44,46	0
1	MLY	A	221	11/12	0.92	0.17	-	27,29,48,51	0
1	MLY	A	100	11/12	0.50	0.52	-	64,65,70,70	0
1	MLY	A	266	11/12	0.68	0.19	-	39,44,48,51	0
1	MLY	A	147	11/12	0.74	0.27	-	45,47,54,54	0
3	MLY	C	21	11/12	0.84	0.29	-	34,36,46,46	0
3	MLY	C	113	11/12	0.95	0.12	-	28,30,41,43	0
3	MLY	C	6	11/12	0.87	0.23	-	33,36,49,49	0
1	MLY	A	254	11/12	0.88	0.17	-	31,36,52,54	0
1	MLY	A	70	11/12	0.84	0.25	-	33,34,48,48	0
3	MLY	C	31	11/12	0.78	0.21	-	30,31,47,48	0
1	MLY	A	122	11/12	0.87	0.18	-	34,35,49,49	0
1	MLY	A	237	11/12	0.94	0.11	-	21,23,30,32	0
1	MLY	A	264	11/12	0.86	0.14	-	32,37,44,45	0
3	MLY	C	15	11/12	0.93	0.16	-	38,39,48,49	0
2	MLY	B	74	11/12	0.91	0.18	-	32,34,45,45	0
1	MLY	A	93	11/12	0.81	0.34	-	48,52,60,61	0
2	MLY	B	65	11/12	0.86	0.18	-	29,30,40,42	0
1	MLY	A	128	11/12	0.87	0.15	-	33,33,37,39	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.