wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 12:33 am BST

PDB ID	:	3HFH
Title	:	Crystal structure of tandem FF domains
Authors	:	Lu, M.; Yang, J.; Ren, Z.; Subir, S.; Bedford, M.T.; Jacobson, R.H.; McMurray, J.S.; Chen, X.
Deposited on	:	2009-05-11
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

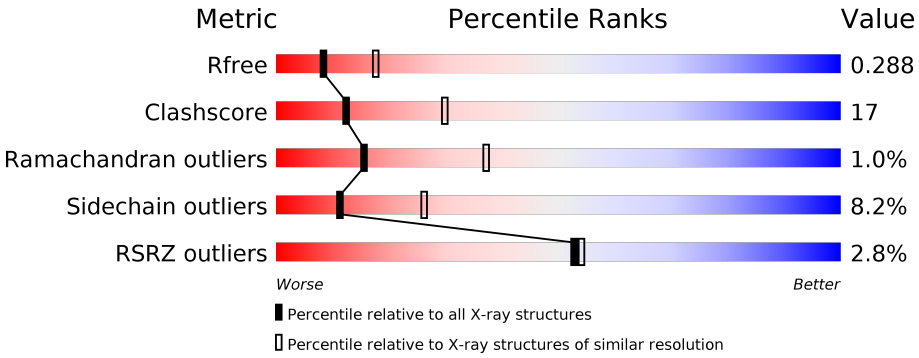
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. 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	190	3% 56% 29% . 12%
1	B	190	% 67% 28% .

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
1	MLY	A	734	-	-	-	X
1	MLY	A	765	-	-	-	X
1	MLY	A	785	-	-	-	X
1	MLY	A	789	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3178 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 Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	Se	0	0	0
			1475	951	255	262	7			
1	B	190	Total	C	N	O	Se	0	0	0
			1648	1061	285	295	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	-	EXPRESSION TAG	UNP O14776
A	657	PRO	-	EXPRESSION TAG	UNP O14776
A	658	LEU	-	EXPRESSION TAG	UNP O14776
A	659	GLY	-	EXPRESSION TAG	UNP O14776
A	660	SER	-	EXPRESSION TAG	UNP O14776
B	656	GLY	-	EXPRESSION TAG	UNP O14776
B	657	PRO	-	EXPRESSION TAG	UNP O14776
B	658	LEU	-	EXPRESSION TAG	UNP O14776
B	659	GLY	-	EXPRESSION TAG	UNP O14776
B	660	SER	-	EXPRESSION TAG	UNP O14776

- Molecule 2 is water.

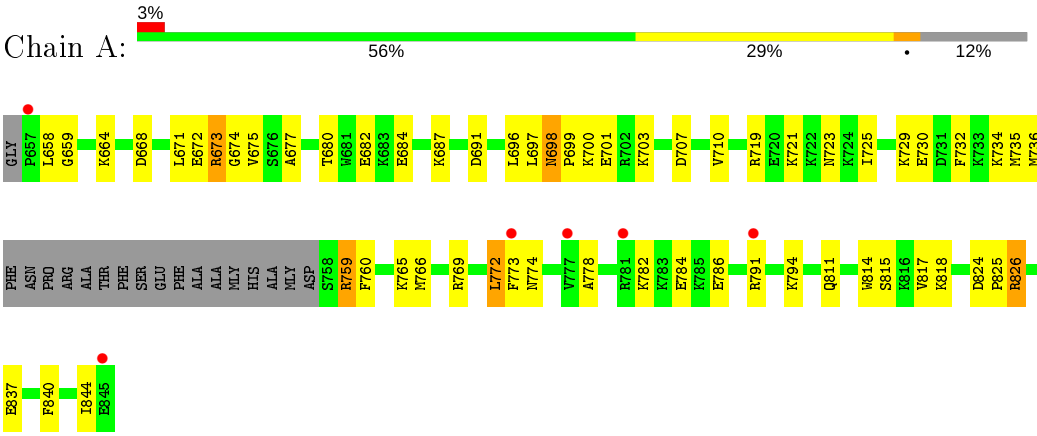
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	40	Total	O	0	0
			40	40		

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.

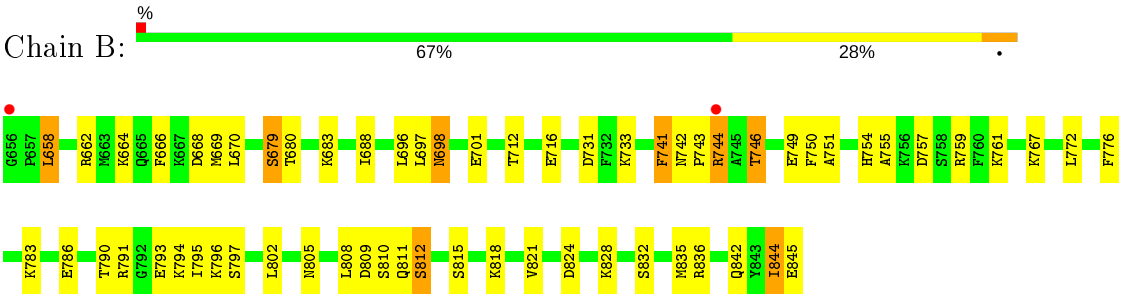
- Molecule 1: Transcription elongation regulator 1

Chain A:



- Molecule 1: Transcription elongation regulator 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α, β, γ	141.30Å 141.30Å 155.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.02 – 2.70 20.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.02-2.70) 96.2 (20.02-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.71Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.283 0.239 , 0.288	Depositor DCC
R_{free} test set	4631 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3178	wwPDB-VP
Average B, all atoms (Å^2)	91.0	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 68.92 % 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 4.0327e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.38	0/1195	0.55	0/1595
1	B	0.47	0/1347	0.61	1/1804 (0.1%)
All	All	0.43	0/2542	0.58	1/3399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	679	SER	CB-CA-C	-7.45	95.94	110.10

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	1475	0	1519	59	0
1	B	1648	0	1673	48	0
2	A	15	0	0	0	0
2	B	40	0	0	2	0
All	All	3178	0	3192	107	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 17.

The worst 5 of 107 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:826:ARG:HG3	1:A:826:ARG:HH11	1.13	1.12
1:B:679:SER:O	2:B:9:HOH:O	1.77	1.02
1:A:765:MLY:HG2	1:A:766:MSE:H	1.38	0.87
1:A:826:ARG:HH11	1:A:826:ARG:CG	1.88	0.86
1:A:826:ARG:HG3	1:A:826:ARG:NH1	1.92	0.84

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	137/190 (72%)	127 (93%)	9 (7%)	1 (1%)	22	46
1	B	158/190 (83%)	147 (93%)	9 (6%)	2 (1%)	12	30
All	All	295/380 (78%)	274 (93%)	18 (6%)	3 (1%)	15	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	741	PHE
1	B	812	SER
1	A	659	GLY

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	128/134 (96%)	119 (93%)	9 (7%)	15 35
1	B	141/134 (105%)	128 (91%)	13 (9%)	9 21
All	All	269/268 (100%)	247 (92%)	22 (8%)	11 26

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	658	LEU
1	B	744	ARG
1	B	835	MSE
1	B	680	THR
1	B	698	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	805	ASN
1	B	698	ASN
1	B	708	GLN
1	A	727	GLN
1	B	704	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

57 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	B	687	1	9,10,11	0.59	0	6,11,13	2.57	4 (66%)
1	MLY	A	664	1	9,10,11	0.40	0	6,11,13	2.43	4 (66%)
1	MLY	A	820	1	9,10,11	0.39	0	6,11,13	2.57	3 (50%)
1	MLY	B	721	1	9,10,11	0.49	0	6,11,13	2.42	4 (66%)
1	MLY	A	721	1	9,10,11	0.46	0	6,11,13	2.48	4 (66%)
1	MLY	A	683	1	9,10,11	0.49	0	6,11,13	2.66	3 (50%)
1	MLY	A	667	1	9,10,11	0.52	0	6,11,13	2.40	4 (66%)
1	MLY	A	687	1	9,10,11	0.49	0	6,11,13	2.54	4 (66%)
1	MLY	A	722	1	9,10,11	0.45	0	6,11,13	2.34	4 (66%)
1	MLY	B	828	1	9,10,11	0.37	0	6,11,13	2.43	4 (66%)
1	MLY	A	761	1	9,10,11	0.42	0	6,11,13	2.43	4 (66%)
1	MLY	B	818	1	9,10,11	0.42	0	6,11,13	2.43	4 (66%)
1	MLY	A	767	1	9,10,11	0.40	0	6,11,13	2.43	4 (66%)
1	MLY	B	783	1	9,10,11	0.37	0	6,11,13	2.34	4 (66%)
1	MLY	A	711	1	9,10,11	0.40	0	6,11,13	2.49	4 (66%)
1	MLY	A	794	1	9,10,11	0.45	0	6,11,13	2.13	3 (50%)
1	MLY	A	828	1	9,10,11	0.41	0	6,11,13	2.34	4 (66%)
1	MLY	A	796	1	9,10,11	0.44	0	6,11,13	2.18	3 (50%)
1	MLY	A	733	1	9,10,11	0.37	0	6,11,13	2.25	4 (66%)
1	MLY	B	782	1	9,10,11	0.45	0	6,11,13	2.42	4 (66%)
1	MLY	B	733	1	9,10,11	0.43	0	6,11,13	2.45	4 (66%)
1	MLY	B	785	1	9,10,11	0.42	0	6,11,13	2.38	4 (66%)
1	MLY	B	683	1	9,10,11	0.39	0	6,11,13	2.82	3 (50%)
1	MLY	B	711	1	9,10,11	0.48	0	6,11,13	2.42	4 (66%)
1	MLY	B	756	1	9,10,11	0.53	0	6,11,13	2.14	3 (50%)
1	MLY	B	740	1	3,4,11	0.77	0	2,4,13	1.12	0
1	MLY	A	789	1	9,10,11	0.43	0	6,11,13	2.32	4 (66%)
1	MLY	A	783	1	9,10,11	0.41	0	6,11,13	2.53	4 (66%)
1	MLY	B	722	1	9,10,11	0.46	0	6,11,13	2.35	4 (66%)
1	MLY	B	789	1	9,10,11	0.37	0	6,11,13	2.30	4 (66%)
1	MLY	A	785	1	9,10,11	0.43	0	6,11,13	2.22	4 (66%)
1	MLY	A	729	1	9,10,11	0.38	0	6,11,13	2.25	4 (66%)
1	MLY	A	700	1	9,10,11	0.46	0	6,11,13	2.34	4 (66%)
1	MLY	B	700	1	9,10,11	0.45	0	6,11,13	2.41	4 (66%)
1	MLY	A	816	1	9,10,11	0.57	0	6,11,13	2.23	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	B	703	1	9,10,11	0.44	0	6,11,13	2.37	4 (66%)
1	MLY	A	782	1	9,10,11	0.45	0	6,11,13	2.39	4 (66%)
1	MLY	B	765	1	9,10,11	0.56	0	6,11,13	2.24	4 (66%)
1	MLY	B	734	1	9,10,11	0.41	0	6,11,13	2.48	4 (66%)
1	MLY	A	818	1	9,10,11	0.39	0	6,11,13	2.46	4 (66%)
1	MLY	B	794	1	9,10,11	0.45	0	6,11,13	2.57	3 (50%)
1	MLY	A	734	1	9,10,11	0.43	0	6,11,13	2.33	4 (66%)
1	MLY	B	729	1	9,10,11	0.38	0	6,11,13	2.24	3 (50%)
1	MLY	B	841	1	9,10,11	0.34	0	6,11,13	2.27	3 (50%)
1	MLY	B	767	1	9,10,11	0.41	0	6,11,13	2.47	4 (66%)
1	MLY	A	841	1	9,10,11	0.34	0	6,11,13	2.41	4 (66%)
1	MLY	A	724	1	9,10,11	0.40	0	6,11,13	2.44	4 (66%)
1	MLY	B	724	1	9,10,11	0.41	0	6,11,13	2.53	4 (66%)
1	MLY	B	667	1	9,10,11	0.69	0	6,11,13	2.75	5 (83%)
1	MLY	B	796	1	9,10,11	0.40	0	6,11,13	2.35	4 (66%)
1	MLY	B	816	1	9,10,11	0.38	0	6,11,13	2.49	4 (66%)
1	MLY	B	664	1	9,10,11	0.61	0	6,11,13	2.45	3 (50%)
1	MLY	B	820	1	9,10,11	0.36	0	6,11,13	2.38	4 (66%)
1	MLY	B	761	1	9,10,11	0.34	0	6,11,13	2.38	4 (66%)
1	MLY	B	753	1	9,10,11	0.40	0	6,11,13	2.30	4 (66%)
1	MLY	A	765	1	9,10,11	0.41	0	6,11,13	2.52	4 (66%)
1	MLY	A	703	1	9,10,11	0.39	0	6,11,13	2.30	4 (66%)

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	B	687	1	-	2/8/9/11	-
1	MLY	A	664	1	-	5/8/9/11	-
1	MLY	A	820	1	-	4/8/9/11	-
1	MLY	B	721	1	-	1/8/9/11	-
1	MLY	A	721	1	-	5/8/9/11	-
1	MLY	A	683	1	-	2/8/9/11	-
1	MLY	A	667	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	687	1	-	1/8/9/11	-
1	MLY	A	722	1	-	3/8/9/11	-
1	MLY	B	828	1	-	1/8/9/11	-
1	MLY	A	761	1	-	2/8/9/11	-
1	MLY	B	818	1	-	3/8/9/11	-
1	MLY	A	767	1	-	2/8/9/11	-
1	MLY	B	783	1	-	5/8/9/11	-
1	MLY	A	711	1	-	5/8/9/11	-
1	MLY	A	794	1	-	2/8/9/11	-
1	MLY	A	828	1	-	1/8/9/11	-
1	MLY	A	796	1	-	3/8/9/11	-
1	MLY	A	733	1	-	5/8/9/11	-
1	MLY	B	782	1	-	2/8/9/11	-
1	MLY	B	733	1	-	4/8/9/11	-
1	MLY	B	785	1	-	3/8/9/11	-
1	MLY	B	683	1	-	4/8/9/11	-
1	MLY	B	711	1	-	1/8/9/11	-
1	MLY	B	756	1	-	1/8/9/11	-
1	MLY	B	740	1	-	0/0/2/11	-
1	MLY	A	789	1	-	1/8/9/11	-
1	MLY	A	783	1	-	3/8/9/11	-
1	MLY	B	722	1	-	1/8/9/11	-
1	MLY	B	789	1	-	3/8/9/11	-
1	MLY	A	785	1	-	3/8/9/11	-
1	MLY	A	729	1	-	3/8/9/11	-
1	MLY	A	700	1	-	3/8/9/11	-
1	MLY	B	700	1	-	4/8/9/11	-
1	MLY	A	816	1	-	4/8/9/11	-
1	MLY	B	703	1	-	4/8/9/11	-
1	MLY	A	782	1	-	2/8/9/11	-
1	MLY	B	765	1	-	3/8/9/11	-
1	MLY	B	734	1	-	5/8/9/11	-
1	MLY	A	818	1	-	2/8/9/11	-
1	MLY	B	794	1	-	5/8/9/11	-
1	MLY	A	734	1	-	5/8/9/11	-
1	MLY	B	729	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	841	1	-	2/8/9/11	-
1	MLY	B	767	1	-	3/8/9/11	-
1	MLY	A	841	1	-	2/8/9/11	-
1	MLY	A	724	1	-	2/8/9/11	-
1	MLY	B	724	1	-	1/8/9/11	-
1	MLY	B	667	1	-	4/8/9/11	-
1	MLY	B	796	1	-	3/8/9/11	-
1	MLY	B	816	1	-	5/8/9/11	-
1	MLY	B	664	1	-	4/8/9/11	-
1	MLY	B	820	1	-	2/8/9/11	-
1	MLY	B	761	1	-	4/8/9/11	-
1	MLY	B	753	1	-	2/8/9/11	-
1	MLY	A	765	1	-	4/8/9/11	-
1	MLY	A	703	1	-	3/8/9/11	-

There are no bond length outliers.

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	683	MLY	CH2-NZ-CH1	4.78	122.08	109.73
1	B	683	MLY	CD-CE-NZ	-4.44	101.76	113.79
1	B	794	MLY	CH2-NZ-CH1	4.24	120.70	109.73
1	B	687	MLY	CH2-NZ-CH1	4.24	120.68	109.73
1	A	820	MLY	CH2-NZ-CH1	4.19	120.56	109.73

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	820	MLY	C-CA-CB-CG
1	A	721	MLY	N-CA-CB-CG
1	A	721	MLY	C-CA-CB-CG
1	A	722	MLY	N-CA-CB-CG
1	A	722	MLY	C-CA-CB-CG

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	664	MLY	1	0
1	A	721	MLY	1	0
1	A	687	MLY	1	0
1	B	828	MLY	1	0
1	B	818	MLY	1	0
1	B	783	MLY	2	0
1	A	794	MLY	2	0
1	B	733	MLY	1	0
1	B	683	MLY	1	0
1	A	729	MLY	1	0
1	A	700	MLY	1	0
1	A	782	MLY	1	0
1	A	818	MLY	2	0
1	B	794	MLY	1	0
1	A	734	MLY	3	0
1	B	767	MLY	1	0
1	B	796	MLY	2	0
1	B	664	MLY	1	0
1	B	761	MLY	1	0
1	A	765	MLY	5	0
1	A	703	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

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, 95^{th} 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	134/190 (70%)	0.19	6 (4%)	33 31	51, 94, 161, 172	0
1	B	153/190 (80%)	-0.15	2 (1%)	77 78	44, 71, 123, 144	0
All	All	287/380 (75%)	0.01	8 (2%)	53 54	44, 79, 145, 172	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	656	GLY	5.4
1	A	773	PHE	4.0
1	A	791	ARG	3.8
1	A	657	PRO	3.7
1	A	777	VAL	2.9

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. The B-factors column lists the minimum, median, 95^{th} 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	765	11/12	0.72	0.44	123,133,139,139	0
1	MLY	A	816	11/12	0.73	0.26	100,113,131,132	0
1	MLY	A	785	11/12	0.75	0.45	153,163,167,167	0
1	MLY	A	782	11/12	0.76	0.33	164,175,190,191	0
1	MLY	A	789	11/12	0.79	0.40	147,154,170,171	0
1	MLY	A	734	11/12	0.79	0.42	144,157,170,170	0
1	MLY	B	756	11/12	0.82	0.21	70,86,102,107	0
1	MLY	A	783	11/12	0.83	0.36	158,166,170,170	0
1	MLY	A	828	11/12	0.83	0.41	103,119,136,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	700	11/12	0.84	0.40	53,66,98,101	0
1	MLY	B	765	11/12	0.84	0.28	64,74,107,107	0
1	MLY	A	818	11/12	0.84	0.29	98,115,159,162	0
1	MLY	A	733	11/12	0.85	0.34	146,157,169,171	0
1	MLY	B	796	11/12	0.85	0.30	77,82,110,111	0
1	MLY	B	828	11/12	0.85	0.36	91,102,126,128	0
1	MLY	A	761	11/12	0.86	0.24	133,143,155,158	0
1	MLY	A	820	11/12	0.86	0.16	113,120,127,129	0
1	MLY	B	789	11/12	0.86	0.36	113,134,169,169	0
1	MLY	B	740	5/12	0.86	0.27	120,134,137,138	0
1	MLY	A	767	11/12	0.87	0.42	114,125,148,148	0
1	MLY	A	794	11/12	0.87	0.29	105,111,116,116	0
1	MLY	B	816	11/12	0.88	0.20	103,117,148,149	0
1	MLY	A	796	11/12	0.89	0.35	100,105,120,121	0
1	MLY	A	711	11/12	0.89	0.33	67,83,120,120	0
1	MLY	A	729	11/12	0.89	0.26	119,126,148,150	0
1	MLY	B	794	11/12	0.90	0.28	86,96,115,115	0
1	MLY	B	734	11/12	0.90	0.32	84,96,136,138	0
1	MLY	B	721	11/12	0.91	0.22	74,86,124,128	0
1	MLY	B	722	11/12	0.91	0.34	63,82,122,126	0
1	MLY	A	722	11/12	0.91	0.34	113,149,155,157	0
1	MLY	B	818	11/12	0.91	0.23	91,98,133,133	0
1	MLY	B	785	11/12	0.91	0.30	103,109,132,133	0
1	MLY	B	767	11/12	0.92	0.24	60,75,102,109	0
1	MLY	A	664	11/12	0.92	0.20	54,58,78,81	0
1	MLY	A	683	11/12	0.92	0.17	65,73,85,90	0
1	MLY	B	783	11/12	0.92	0.36	103,106,131,134	0
1	MLY	A	667	11/12	0.92	0.23	53,63,100,100	0
1	MLY	A	721	11/12	0.93	0.21	109,116,121,122	0
1	MLY	B	761	11/12	0.93	0.18	64,69,95,100	0
1	MLY	B	711	11/12	0.93	0.26	55,71,115,116	0
1	MLY	A	703	11/12	0.93	0.28	54,75,122,122	0
1	MLY	B	667	11/12	0.94	0.22	52,64,84,89	0
1	MLY	B	782	11/12	0.94	0.32	93,113,142,143	0
1	MLY	B	729	11/12	0.94	0.30	70,86,125,128	0
1	MLY	B	820	11/12	0.94	0.17	95,106,121,123	0
1	MLY	B	841	11/12	0.94	0.27	64,84,111,111	0
1	MLY	B	753	11/12	0.94	0.22	69,72,108,109	0
1	MLY	B	733	11/12	0.94	0.20	72,86,114,117	0
1	MLY	A	700	11/12	0.94	0.42	56,68,111,111	0
1	MLY	A	841	11/12	0.95	0.23	69,82,120,121	0
1	MLY	B	664	11/12	0.95	0.20	52,60,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	724	11/12	0.96	0.29	60,79,105,107	0
1	MLY	B	683	11/12	0.96	0.16	51,54,65,68	0
1	MLY	A	724	11/12	0.96	0.16	110,118,122,122	0
1	MLY	B	703	11/12	0.97	0.15	55,61,100,103	0
1	MLY	A	687	11/12	0.98	0.19	51,58,80,84	0
1	MLY	B	687	11/12	0.98	0.16	47,52,71,73	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.