Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 08:16 AM EST

PDB ID	:	4XA6
Title	:	Crystal Structure of the coiled-coil surrounding Skip 4 of MYH7
Authors	:	Taylor, K.C.; Buvoli, M.; Korkmaz, E.N.; Buvoli, A.; Zheng, Y.; Heinz, N.T.; Qiang, C.; Leinwand, L.A.; Rayment, I.
Deposited on	:	2014-12-12
Resolution	:	3.42 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

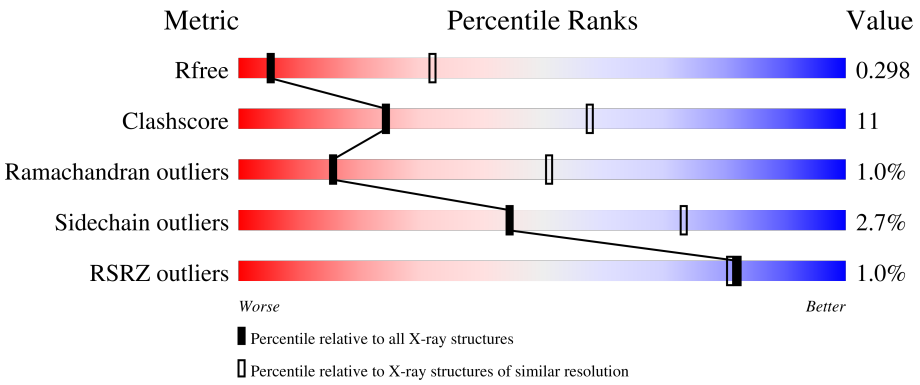
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 of 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	175	.% 69% 25% • •
1	B	175	2% 65% 27% • 6%
1	C	175	51% 15% 34%
1	D	175	45% 14% • 40%

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	1838	-	-	-	X
1	MLY	A	1842	-	-	-	X
1	MLY	C	1783	-	-	-	X
1	MLY	D	1791	-	-	-	X

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4726 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 Gp7-MYH7(1777-1855)-EB1 chimera protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	168	1427	894	252	277	1	3	0	0	0
1	B	165	1406	881	249	272	1	3	0	0	0
1	C	116	995	622	179	190	1	3	0	0	0
1	D	105	898	562	161	173	1	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

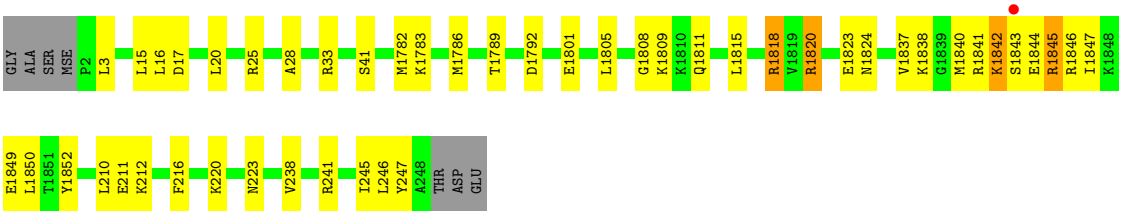
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P13848
A	-1	ALA	-	expression tag	UNP P13848
A	0	SER	-	expression tag	UNP P13848
A	1	MSE	-	expression tag	UNP P13848
B	-2	GLY	-	expression tag	UNP P13848
B	-1	ALA	-	expression tag	UNP P13848
B	0	SER	-	expression tag	UNP P13848
B	1	MSE	-	expression tag	UNP P13848
C	1724	GLY	-	expression tag	UNP P13848
C	1725	ALA	-	expression tag	UNP P13848
C	1726	SER	-	expression tag	UNP P13848
C	1727	MSE	-	expression tag	UNP P13848
D	1724	GLY	-	expression tag	UNP P13848
D	1725	ALA	-	expression tag	UNP P13848
D	1726	SER	-	expression tag	UNP P13848
D	1727	MSE	-	expression tag	UNP P13848

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

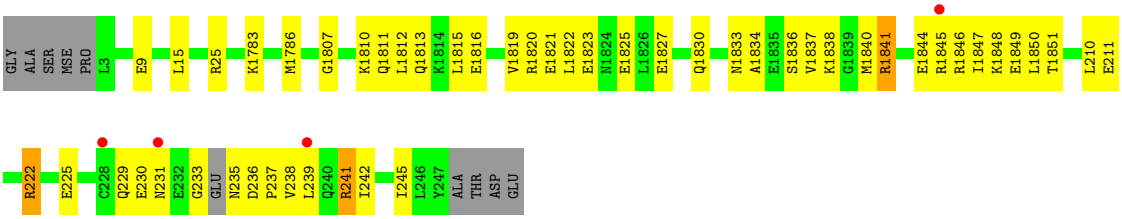
• Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein

Chain A:



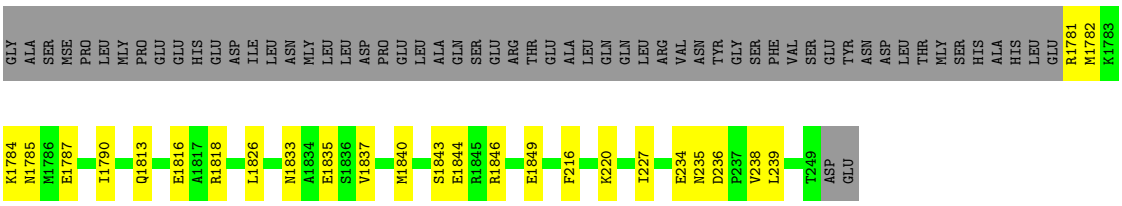
• Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein

Chain B:



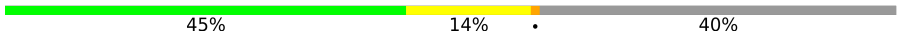
• Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein

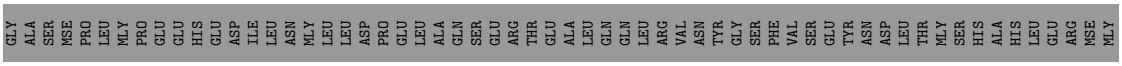
Chain C:

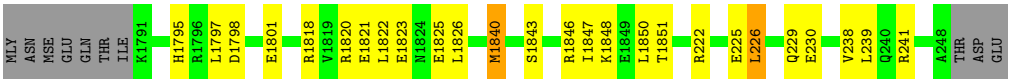


• Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein

Chain D:






MLY
ASN
MSE
GLU
GLN
THR
ILE
K1791
H1795
R1796
L1797
D1798
E1801
R1818
V1819
R1820
E1821
L1822
E1823
N1824
E1825
L1826
M1840
S1843
R1846
I1847
K1848
E1849
L1850
T1851
R222
E225
L226
Q229
E230
V238
L239
Q240
R241
A248
THR
ASP
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.55Å 46.89Å 169.06Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	43.89 – 3.42 44.88 – 3.42	Depositor EDS
% Data completeness (in resolution range)	88.8 (43.89-3.42) 83.8 (44.88-3.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.239 , 0.297 0.245 , 0.298	Depositor DCC
R_{free} test set	677 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.32	0/1263	0.51	0/1700
1	B	0.33	0/1240	0.50	0/1667
1	C	0.27	0/855	0.43	0/1144
1	D	0.30	0/783	0.58	1/1053 (0.1%)
All	All	0.31	0/4141	0.50	1/5564 (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	D	226	LEU	CA-CB-CG	7.24	131.95	115.30

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	1427	0	1443	43	0
1	B	1406	0	1421	49	0
1	C	995	0	1022	17	0
1	D	898	0	918	18	0
All	All	4726	0	4804	105	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 11.

All (105) 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:B:1844:GLU:HA	1:B:1847:ILE:HG22	1.58	0.84
1:C:238:VAL:HG11	1:D:239:LEU:HD21	1.66	0.78
1:A:1818:ARG:NH2	1:B:1823:GLU:OE2	2.20	0.74
1:B:1846:ARG:HA	1:B:1849:GLU:HB3	1.74	0.70
1:A:1820:ARG:O	1:A:1824:ASN:ND2	2.19	0.69
1:A:1846:ARG:HG2	1:B:1847:ILE:HD11	1.75	0.68
1:D:226:LEU:HA	1:D:229:GLN:OE1	1.95	0.66
1:D:222:ARG:HA	1:D:225:GLU:HB3	1.78	0.65
1:A:1850:LEU:HD21	1:B:1851:THR:HG23	1.79	0.64
1:A:1837:VAL:O	1:A:1841:ARG:NH1	2.32	0.63
1:A:1842:MLY:HG2	1:A:1845:ARG:HH21	1.64	0.63
1:B:222:ARG:HA	1:B:225:GLU:HB3	1.80	0.62
1:A:33:ARG:NH1	1:B:9:GLU:OE2	2.30	0.62
1:B:233:GLY:O	1:B:235:ASN:N	2.34	0.60
1:B:236:ASP:HB3	1:B:239:LEU:HB2	1.83	0.60
1:C:1787:GLU:HA	1:C:1790:ILE:HB	1.82	0.59
1:B:1840:MSE:HG3	1:B:1841:ARG:HD3	1.83	0.59
1:A:1823:GLU:HG3	1:B:1822:LEU:HD21	1.85	0.58
1:B:1841:ARG:NH2	1:B:1844:GLU:HB2	2.19	0.58
1:A:1840:MSE:C	1:A:1843:SER:H	2.08	0.57
1:B:1844:GLU:OE2	1:B:1848:MLY:HB2	2.04	0.56
1:A:1842:MLY:O	1:A:1845:ARG:NE	2.39	0.56
1:B:229:GLN:O	1:B:231:ASN:N	2.38	0.56
1:A:1838:MLY:O	1:A:1842:MLY:HB3	2.05	0.56
1:B:1837:VAL:HA	1:B:1840:MSE:HB3	1.87	0.55
1:A:16:LEU:HA	1:B:25:ARG:HD3	1.88	0.55
1:A:1847:ILE:HD11	1:B:1847:ILE:HB	1.88	0.55
1:A:238:VAL:HG11	1:B:239:LEU:HD11	1.89	0.54
1:C:216:PHE:HE2	1:C:220:MLY:HH13	1.73	0.54
1:B:1837:VAL:CA	1:B:1840:MSE:HB3	2.38	0.54
1:B:1837:VAL:O	1:B:1840:MSE:HB3	2.08	0.53
1:A:223:ASN:HB3	1:B:245:ILE:HD13	1.91	0.53
1:B:1816:GLU:HA	1:B:1819:VAL:HG22	1.90	0.53
1:B:1844:GLU:HA	1:B:1847:ILE:CG2	2.32	0.53
1:A:210:LEU:HD13	1:B:211:GLU:HB2	1.91	0.52
1:C:227:ILE:HD13	1:D:241:ARG:HB3	1.91	0.52
1:B:1841:ARG:O	1:B:1845:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1848:MLY:HA	1:D:1851:THR:HG22	1.92	0.51
1:C:234:GLU:O	1:C:236:ASP:N	2.44	0.51
1:A:1783:MLY:HG2	1:B:1786:MSE:HE1	1.92	0.50
1:B:1841:ARG:HD2	1:B:1844:GLU:CB	2.42	0.50
1:A:1842:MLY:HH22	1:A:1845:ARG:CZ	2.40	0.50
1:D:1843:SER:O	1:D:1847:ILE:N	2.43	0.49
1:C:1781:ARG:HD2	1:C:1784:MLY:HG2	1.94	0.49
1:D:1818:ARG:NH1	1:D:1821:GLU:OE2	2.46	0.49
1:B:1820:ARG:HG2	1:B:1823:GLU:HB2	1.95	0.49
1:C:216:PHE:CE2	1:C:220:MLY:HH13	2.48	0.48
1:A:1843:SER:HB3	1:A:1844:GLU:OE2	2.14	0.47
1:D:1840:MSE:HE3	1:D:1840:MSE:HB2	1.56	0.47
1:C:1781:ARG:HD3	1:C:1781:ARG:HA	1.53	0.47
1:A:1786:MSE:HE1	1:B:1783:MLY:HA	1.96	0.47
1:B:1834:ALA:O	1:B:1838:MLY:HG3	2.15	0.47
1:C:1782:MSE:HA	1:C:1785:ASN:HB3	1.97	0.47
1:C:1833:ASN:O	1:C:1837:VAL:HG23	2.15	0.46
1:A:211:GLU:HB2	1:B:210:LEU:HD21	1.96	0.46
1:B:1841:ARG:HD2	1:B:1844:GLU:HB2	1.97	0.46
1:A:1801:GLU:O	1:A:1805:LEU:HB2	2.16	0.46
1:C:1818:ARG:NH2	1:D:1823:GLU:OE2	2.42	0.46
1:B:241:ARG:H	1:B:241:ARG:HG2	1.53	0.46
1:A:1845:ARG:H	1:A:1845:ARG:HG3	1.58	0.45
1:C:1826:LEU:HA	1:D:1826:LEU:HD13	1.96	0.45
1:B:237:PRO:O	1:B:241:ARG:HG2	2.16	0.45
1:D:1795:HIS:HA	1:D:1798:ASP:HB2	1.99	0.44
1:A:17:ASP:HB3	1:A:20:LEU:HB2	1.98	0.44
1:B:1837:VAL:HA	1:B:1840:MSE:CB	2.46	0.44
1:A:1846:ARG:O	1:A:1850:LEU:N	2.34	0.44
1:A:241:ARG:O	1:A:245:ILE:HG13	2.18	0.44
1:B:1827:GLU:HA	1:B:1830:GLN:HG2	2.00	0.44
1:B:1841:ARG:HD2	1:B:1841:ARG:HA	1.68	0.44
1:A:1840:MSE:HA	1:A:1843:SER:H	1.82	0.44
1:C:239:LEU:HD11	1:D:238:VAL:HG11	2.00	0.44
1:D:1848:MLY:O	1:D:1851:THR:HG22	2.17	0.44
1:B:225:GLU:O	1:B:229:GLN:HG3	2.18	0.44
1:C:1840:MSE:HA	1:D:1840:MSE:CE	2.48	0.44
1:D:1822:LEU:HD12	1:D:1822:LEU:HA	1.84	0.43
1:D:1848:MLY:HH13	1:D:1848:MLY:HD2	1.85	0.43
1:A:1840:MSE:HA	1:A:1843:SER:N	2.34	0.43
1:D:1797:LEU:O	1:D:1801:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD21	1:A:28:ALA:HB3	2.00	0.43
1:B:1813:GLN:OE1	1:B:1816:GLU:HB2	2.18	0.43
1:A:25:ARG:HD3	1:B:15:LEU:O	2.20	0.42
1:A:1850:LEU:HD23	1:B:1850:LEU:HB3	2.01	0.42
1:B:1815:LEU:O	1:B:1819:VAL:HG13	2.20	0.42
1:B:1833:ASN:O	1:B:1836:SER:N	2.52	0.42
1:C:1813:GLN:HA	1:C:1816:GLU:HB2	2.01	0.42
1:A:1789:THR:O	1:A:1792:ASP:HB3	2.20	0.42
1:A:1809:MLY:HH23	1:A:1809:MLY:HD2	1.77	0.42
1:A:212:MLY:O	1:A:216:PHE:N	2.50	0.41
1:B:1846:ARG:O	1:B:1850:LEU:N	2.49	0.41
1:A:1844:GLU:HB3	1:A:1847:ILE:HD13	2.03	0.41
1:B:238:VAL:O	1:B:242:ILE:HG13	2.20	0.41
1:D:1846:ARG:HH12	1:D:1850:LEU:HD21	1.86	0.41
1:A:216:PHE:CZ	1:A:220:MLY:HH12	2.56	0.41
1:A:1842:MLY:HG2	1:A:1845:ARG:NH2	2.34	0.41
1:A:1782:MSE:O	1:A:1786:MSE:HG3	2.21	0.41
1:A:245:ILE:O	1:A:247:TYR:N	2.43	0.41
1:B:1807:GLY:HA3	1:B:1811:GLN:HB3	2.01	0.41
1:B:1810:MLY:HE3	1:B:1810:MLY:HB3	1.88	0.40
1:C:1846:ARG:HA	1:C:1849:GLU:HB3	2.02	0.40
1:A:1849:GLU:O	1:A:1852:TYR:HB3	2.21	0.40
1:C:1843:SER:OG	1:C:1844:GLU:N	2.54	0.40
1:A:1811:GLN:OE1	1:B:1812:LEU:HD21	2.22	0.40
1:B:1821:GLU:O	1:B:1825:GLU:HG2	2.22	0.40
1:A:1840:MSE:CA	1:A:1843:SER:H	2.34	0.40
1:A:1811:GLN:O	1:A:1815:LEU:HG	2.22	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	150/175 (86%)	141 (94%)	7 (5%)	2 (1%)	12	45
1	B	145/175 (83%)	133 (92%)	11 (8%)	1 (1%)	22	58
1	C	101/175 (58%)	92 (91%)	8 (8%)	1 (1%)	15	51
1	D	93/175 (53%)	85 (91%)	7 (8%)	1 (1%)	14	49
All	All	489/700 (70%)	451 (92%)	33 (7%)	5 (1%)	15	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ASN
1	D	230	GLU
1	B	230	GLU
1	A	246	LEU
1	A	1808	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	137/138 (99%)	132 (96%)	5 (4%)	35	66
1	B	135/138 (98%)	132 (98%)	3 (2%)	52	78
1	C	92/138 (67%)	91 (99%)	1 (1%)	73	87
1	D	83/138 (60%)	80 (96%)	3 (4%)	35	66
All	All	447/552 (81%)	435 (97%)	12 (3%)	44	73

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

Mol	Chain	Res	Type
1	A	3	LEU
1	A	41	SER
1	A	1818	ARG
1	A	1820	ARG
1	A	1845	ARG
1	B	1841	ARG

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Mol	Chain	Res	Type
1	B	222	ARG
1	B	241	ARG
1	C	1835	GLU
1	D	1820	ARG
1	D	1825	GLU
1	D	1840	MSE

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

Mol	Chain	Res	Type
1	D	1824	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)

56 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	220	1	9,10,11	0.58	0	6,11,13	0.89	0
1	MLY	D	1848	1	9,10,11	0.58	0	6,11,13	0.85	0
1	MLY	C	1831	1	9,10,11	0.58	0	6,11,13	0.71	0
1	MLY	B	1842	1	9,10,11	0.58	0	6,11,13	0.72	0
1	MLY	A	212	1	9,10,11	0.59	0	6,11,13	0.80	0
1	MLY	B	1848	1	9,10,11	0.51	0	6,11,13	0.93	0
1	MLY	B	212	1	9,10,11	0.56	0	6,11,13	0.84	0
1	MLY	D	220	1	9,10,11	0.58	0	6,11,13	0.79	0
1	MLY	A	220	1	9,10,11	0.60	0	6,11,13	0.59	0
1	MLY	B	1784	1	9,10,11	0.54	0	6,11,13	0.83	0
1	MLY	A	1784	1	9,10,11	0.57	0	6,11,13	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	B	1806	1	9,10,11	0.51	0	6,11,13	0.84	0
1	MLY	A	1838	1	9,10,11	0.68	0	6,11,13	0.60	0
1	MLY	D	212	1	9,10,11	0.67	0	6,11,13	0.73	0
1	MLY	B	48	1	9,10,11	0.58	0	6,11,13	0.83	0
1	MLY	B	4	1	9,10,11	0.51	0	6,11,13	0.89	0
1	MLY	A	1842	1	9,10,11	0.65	0	6,11,13	1.12	1 (16%)
1	MLY	C	212	1	9,10,11	0.58	0	6,11,13	0.79	0
1	MLY	D	1806	1	9,10,11	0.55	0	6,11,13	0.83	0
1	MLY	B	1791	1	9,10,11	0.49	0	6,11,13	0.81	0
1	MLY	D	1838	1	9,10,11	0.58	0	6,11,13	0.82	0
1	MLY	B	14	1	9,10,11	0.54	0	6,11,13	0.74	0
1	MLY	A	1810	1	9,10,11	0.56	0	6,11,13	0.87	0
1	MLY	B	1814	1	9,10,11	0.58	0	6,11,13	0.79	0
1	MLY	C	1806	1	9,10,11	0.53	0	6,11,13	0.83	0
1	MLY	C	1838	1	9,10,11	0.68	0	6,11,13	0.73	0
1	MLY	D	1809	1	9,10,11	0.54	0	6,11,13	0.81	0
1	MLY	C	1809	1	9,10,11	0.56	0	6,11,13	0.78	0
1	MLY	D	1810	1	9,10,11	0.59	0	6,11,13	0.78	0
1	MLY	C	1784	1	9,10,11	0.46	0	6,11,13	0.80	0
1	MLY	A	1848	1	9,10,11	0.54	0	6,11,13	0.81	0
1	MLY	B	1809	1	9,10,11	0.54	0	6,11,13	0.77	0
1	MLY	C	1783	1	9,10,11	0.70	0	6,11,13	0.63	0
1	MLY	D	1791	1	9,10,11	0.61	0	6,11,13	0.67	0
1	MLY	A	1809	1	9,10,11	0.56	0	6,11,13	0.72	0
1	MLY	D	1831	1	9,10,11	0.53	0	6,11,13	0.79	0
1	MLY	C	220	1	9,10,11	0.62	0	6,11,13	1.01	0
1	MLY	A	4	1	9,10,11	0.59	0	6,11,13	0.76	0
1	MLY	A	1806	1	9,10,11	0.54	0	6,11,13	0.80	0
1	MLY	D	1814	1	9,10,11	0.61	0	6,11,13	0.46	0
1	MLY	D	1842	1	9,10,11	0.61	0	6,11,13	0.61	0
1	MLY	C	1848	1	9,10,11	0.57	0	6,11,13	0.83	0
1	MLY	A	1814	1	9,10,11	0.54	0	6,11,13	0.84	0
1	MLY	C	1842	1	9,10,11	0.59	0	6,11,13	0.74	0
1	MLY	B	1810	1	9,10,11	0.52	0	6,11,13	0.80	0
1	MLY	B	1838	1	9,10,11	0.47	0	6,11,13	0.88	0
1	MLY	B	1831	1	9,10,11	0.56	0	6,11,13	0.86	0
1	MLY	C	1791	1	9,10,11	0.54	0	6,11,13	0.79	0
1	MLY	A	1791	1	9,10,11	0.49	0	6,11,13	0.87	0
1	MLY	C	1814	1	9,10,11	0.58	0	6,11,13	0.77	0
1	MLY	A	14	1	9,10,11	0.59	0	6,11,13	0.72	0
1	MLY	A	1783	1	9,10,11	0.51	0	6,11,13	0.87	0
1	MLY	A	48	1	9,10,11	0.65	0	6,11,13	0.81	0
1	MLY	B	1783	1	9,10,11	0.55	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	C	1810	1	9,10,11	0.61	0	6,11,13	0.73	0
1	MLY	A	1831	1	9,10,11	0.60	0	6,11,13	0.84	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	B	220	1	-	2/8/9/11	-
1	MLY	D	1848	1	-	3/8/9/11	-
1	MLY	C	1831	1	-	0/8/9/11	-
1	MLY	B	1842	1	-	2/8/9/11	-
1	MLY	A	212	1	-	1/8/9/11	-
1	MLY	B	1848	1	-	0/8/9/11	-
1	MLY	B	212	1	-	0/8/9/11	-
1	MLY	D	220	1	-	2/8/9/11	-
1	MLY	A	220	1	-	1/8/9/11	-
1	MLY	B	1784	1	-	0/8/9/11	-
1	MLY	A	1784	1	-	6/8/9/11	-
1	MLY	B	1806	1	-	2/8/9/11	-
1	MLY	A	1838	1	-	2/8/9/11	-
1	MLY	D	212	1	-	1/8/9/11	-
1	MLY	B	48	1	-	0/8/9/11	-
1	MLY	B	4	1	-	0/8/9/11	-
1	MLY	A	1842	1	-	5/8/9/11	-
1	MLY	C	212	1	-	0/8/9/11	-
1	MLY	D	1806	1	-	2/8/9/11	-
1	MLY	B	1791	1	-	0/8/9/11	-
1	MLY	D	1838	1	-	0/8/9/11	-
1	MLY	B	14	1	-	2/8/9/11	-
1	MLY	A	1810	1	-	3/8/9/11	-
1	MLY	B	1814	1	-	1/8/9/11	-
1	MLY	C	1806	1	-	2/8/9/11	-
1	MLY	C	1838	1	-	4/8/9/11	-
1	MLY	D	1809	1	-	4/8/9/11	-
1	MLY	C	1809	1	-	4/8/9/11	-
1	MLY	D	1810	1	-	1/8/9/11	-
1	MLY	C	1784	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	1848	1	-	0/8/9/11	-
1	MLY	B	1809	1	-	3/8/9/11	-
1	MLY	C	1783	1	-	1/8/9/11	-
1	MLY	D	1791	1	-	0/8/9/11	-
1	MLY	A	1809	1	-	0/8/9/11	-
1	MLY	D	1831	1	-	0/8/9/11	-
1	MLY	C	220	1	-	1/8/9/11	-
1	MLY	A	4	1	-	3/8/9/11	-
1	MLY	A	1806	1	-	0/8/9/11	-
1	MLY	D	1814	1	-	5/8/9/11	-
1	MLY	D	1842	1	-	2/8/9/11	-
1	MLY	C	1848	1	-	2/8/9/11	-
1	MLY	A	1814	1	-	2/8/9/11	-
1	MLY	C	1842	1	-	2/8/9/11	-
1	MLY	B	1810	1	-	1/8/9/11	-
1	MLY	B	1838	1	-	2/8/9/11	-
1	MLY	B	1831	1	-	2/8/9/11	-
1	MLY	C	1791	1	-	3/8/9/11	-
1	MLY	A	1791	1	-	0/8/9/11	-
1	MLY	C	1814	1	-	3/8/9/11	-
1	MLY	A	14	1	-	1/8/9/11	-
1	MLY	A	1783	1	-	0/8/9/11	-
1	MLY	A	48	1	-	3/8/9/11	-
1	MLY	B	1783	1	-	2/8/9/11	-
1	MLY	C	1810	1	-	2/8/9/11	-
1	MLY	A	1831	1	-	1/8/9/11	-

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	A	1842	MLY	CH2-NZ-CE	-2.06	102.56	110.74

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	14	MLY	O-C-CA-CB
1	A	48	MLY	C-CA-CB-CG
1	A	1784	MLY	N-CA-CB-CG
1	A	1784	MLY	C-CA-CB-CG
1	A	1784	MLY	O-C-CA-CB
1	A	1810	MLY	N-CA-CB-CG
1	A	1810	MLY	C-CA-CB-CG
1	A	1842	MLY	N-CA-CB-CG
1	A	1842	MLY	C-CA-CB-CG
1	B	1831	MLY	N-CA-CB-CG
1	B	1831	MLY	C-CA-CB-CG
1	B	220	MLY	N-CA-CB-CG
1	B	220	MLY	C-CA-CB-CG
1	C	1791	MLY	N-CA-CB-CG
1	C	1791	MLY	C-CA-CB-CG
1	C	1806	MLY	C-CA-CB-CG
1	C	1806	MLY	O-C-CA-CB
1	C	1809	MLY	C-CA-CB-CG
1	C	1814	MLY	O-C-CA-CB
1	D	1814	MLY	N-CA-CB-CG
1	D	1814	MLY	C-CA-CB-CG
1	D	1842	MLY	C-CA-CB-CG
1	D	1848	MLY	N-CA-CB-CG
1	D	1848	MLY	C-CA-CB-CG
1	B	1809	MLY	CD-CE-NZ-CH1
1	A	1784	MLY	CD-CE-NZ-CH1
1	A	1784	MLY	CD-CE-NZ-CH2
1	A	1814	MLY	CD-CE-NZ-CH1
1	A	1814	MLY	CD-CE-NZ-CH2
1	C	1809	MLY	CD-CE-NZ-CH1
1	C	1809	MLY	CD-CE-NZ-CH2
1	C	1810	MLY	CD-CE-NZ-CH1
1	C	1810	MLY	CD-CE-NZ-CH2
1	C	1848	MLY	CD-CE-NZ-CH1
1	C	1848	MLY	CD-CE-NZ-CH2
1	D	1806	MLY	CD-CE-NZ-CH2
1	D	1809	MLY	CD-CE-NZ-CH2
1	B	1838	MLY	CG-CD-CE-NZ
1	D	220	MLY	CG-CD-CE-NZ
1	C	1784	MLY	CG-CD-CE-NZ
1	A	220	MLY	CD-CE-NZ-CH2
1	B	1809	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	D	1806	MLY	CD-CE-NZ-CH1
1	D	1814	MLY	CD-CE-NZ-CH1
1	B	1809	MLY	CA-CB-CG-CD
1	B	1814	MLY	CA-CB-CG-CD
1	B	1783	MLY	CD-CE-NZ-CH2
1	C	1838	MLY	CG-CD-CE-NZ
1	A	1838	MLY	CA-CB-CG-CD
1	D	1809	MLY	CD-CE-NZ-CH1
1	C	1814	MLY	CA-CB-CG-CD
1	C	220	MLY	CD-CE-NZ-CH2
1	D	1842	MLY	CD-CE-NZ-CH2
1	B	1806	MLY	CA-CB-CG-CD
1	B	1810	MLY	CA-CB-CG-CD
1	B	1842	MLY	CA-CB-CG-CD
1	C	1838	MLY	CA-CB-CG-CD
1	C	1809	MLY	CE-CD-CG-CB
1	A	1838	MLY	CE-CD-CG-CB
1	D	1814	MLY	CG-CD-CE-NZ
1	D	1848	MLY	CG-CD-CE-NZ
1	D	1810	MLY	CA-CB-CG-CD
1	A	1842	MLY	CD-CE-NZ-CH1
1	C	1791	MLY	CA-CB-CG-CD
1	A	212	MLY	CD-CE-NZ-CH2
1	D	1809	MLY	CG-CD-CE-NZ
1	B	1806	MLY	CD-CE-NZ-CH2
1	B	1842	MLY	CE-CD-CG-CB
1	C	1838	MLY	CD-CE-NZ-CH1
1	B	14	MLY	CE-CD-CG-CB
1	A	1842	MLY	CG-CD-CE-NZ
1	B	1838	MLY	CE-CD-CG-CB
1	C	1814	MLY	CE-CD-CG-CB
1	B	1783	MLY	CA-CB-CG-CD
1	D	220	MLY	CA-CB-CG-CD
1	D	1814	MLY	CD-CE-NZ-CH2
1	D	1809	MLY	CA-CB-CG-CD
1	A	4	MLY	N-CA-CB-CG
1	A	48	MLY	N-CA-CB-CG
1	C	1783	MLY	N-CA-CB-CG
1	C	1838	MLY	N-CA-CB-CG
1	A	1831	MLY	C-CA-CB-CG
1	C	1842	MLY	C-CA-CB-CG
1	D	212	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	C	1784	MLY	CA-CB-CG-CD
1	A	1784	MLY	CA-CB-CG-CD
1	B	14	MLY	CD-CE-NZ-CH2
1	A	48	MLY	CE-CD-CG-CB
1	C	1842	MLY	CG-CD-CE-NZ
1	A	4	MLY	CE-CD-CG-CB
1	A	1842	MLY	CE-CD-CG-CB
1	A	1810	MLY	CA-CB-CG-CD

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1848	MLY	3	0
1	A	212	MLY	1	0
1	B	1848	MLY	1	0
1	A	220	MLY	1	0
1	A	1838	MLY	1	0
1	A	1842	MLY	5	0
1	C	1784	MLY	1	0
1	A	1809	MLY	1	0
1	C	220	MLY	2	0
1	B	1810	MLY	1	0
1	B	1838	MLY	1	0
1	A	1783	MLY	1	0
1	B	1783	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	149/175 (85%)	0.04	1 (0%)	87	86	16, 69, 131, 161	0
1	B	146/175 (83%)	0.09	4 (2%)	54	53	21, 73, 138, 174	0
1	C	100/175 (57%)	0.03	0	100	100	21, 66, 96, 124	0
1	D	93/175 (53%)	0.09	0	100	100	43, 74, 113, 126	0
All	All	488/700 (69%)	0.06	5 (1%)	82	81	16, 71, 126, 174	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ASN	3.7
1	B	239	LEU	3.4
1	A	1843	SER	2.4
1	B	1845	ARG	2.2
1	B	228	CYS	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	C	1783	11/12	0.71	0.56	75,93,110,115	0
1	MLY	A	1838	11/12	0.74	0.43	105,118,127,131	0
1	MLY	D	1791	11/12	0.75	0.41	52,75,94,94	0
1	MLY	A	1842	11/12	0.76	0.59	167,172,176,176	0
1	MLY	C	1784	11/12	0.81	0.27	102,116,122,123	0
1	MLY	B	1831	11/12	0.82	0.30	111,118,129,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	C	1809	11/12	0.83	0.30	81,106,126,126	0
1	MLY	B	1810	11/12	0.83	0.39	115,123,150,151	0
1	MLY	B	1809	11/12	0.84	0.32	105,119,123,123	0
1	MLY	B	1838	11/12	0.84	0.42	146,153,162,168	0
1	MLY	A	4	11/12	0.85	0.34	82,98,106,106	0
1	MLY	A	1831	11/12	0.85	0.35	126,130,133,134	0
1	MLY	D	1806	11/12	0.85	0.42	70,83,104,107	0
1	MLY	B	1806	11/12	0.86	0.31	76,80,107,108	0
1	MLY	A	1810	11/12	0.86	0.35	84,97,112,112	0
1	MLY	B	1842	11/12	0.86	0.22	95,106,149,150	0
1	MLY	A	1848	11/12	0.86	0.46	96,106,112,112	0
1	MLY	D	1809	11/12	0.86	0.31	88,96,112,121	0
1	MLY	D	1810	11/12	0.86	0.41	101,109,117,118	0
1	MLY	D	1842	11/12	0.86	0.31	74,82,100,100	0
1	MLY	C	1810	11/12	0.87	0.40	73,90,110,110	0
1	MLY	B	1848	11/12	0.87	0.33	102,115,123,123	0
1	MLY	D	1838	11/12	0.88	0.25	72,88,92,92	0
1	MLY	B	1814	11/12	0.88	0.34	70,82,89,100	0
1	MLY	D	212	11/12	0.88	0.27	62,72,103,106	0
1	MLY	A	14	11/12	0.89	0.40	71,80,93,93	0
1	MLY	C	1831	11/12	0.89	0.38	51,68,74,75	0
1	MLY	D	1814	11/12	0.89	0.27	71,88,95,97	0
1	MLY	A	1814	11/12	0.90	0.33	76,86,115,115	0
1	MLY	C	1848	11/12	0.90	0.27	78,93,110,110	0
1	MLY	A	212	11/12	0.90	0.34	75,94,120,122	0
1	MLY	B	4	11/12	0.90	0.29	83,109,136,136	0
1	MLY	C	1814	11/12	0.90	0.39	54,61,78,88	0
1	MLY	B	14	11/12	0.91	0.26	63,84,108,108	0
1	MLY	B	212	11/12	0.91	0.33	70,79,88,89	0
1	MLY	C	1842	11/12	0.91	0.26	48,69,91,92	0
1	MLY	D	1848	11/12	0.91	0.24	53,64,87,90	0
1	MLY	A	1809	11/12	0.91	0.25	63,80,87,90	0
1	MLY	C	212	11/12	0.92	0.45	51,72,104,105	0
1	MLY	A	48	11/12	0.93	0.28	20,41,77,80	0
1	MLY	C	1791	11/12	0.93	0.24	57,63,66,68	0
1	MLY	C	1838	11/12	0.93	0.39	54,78,103,103	0
1	MLY	A	1806	11/12	0.93	0.27	37,47,68,74	0
1	MLY	A	220	11/12	0.93	0.27	48,57,70,71	0
1	MLY	C	220	11/12	0.94	0.27	37,43,81,83	0
1	MLY	D	1831	11/12	0.94	0.18	50,64,70,77	0
1	MLY	A	1784	11/12	0.94	0.29	42,60,97,97	0
1	MLY	A	1791	11/12	0.94	0.22	29,47,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	48	11/12	0.94	0.23	22,29,57,62	0
1	MLY	C	1806	11/12	0.94	0.35	75,85,95,95	0
1	MLY	B	220	11/12	0.95	0.32	52,60,90,92	0
1	MLY	B	1784	11/12	0.95	0.22	32,48,65,70	0
1	MLY	B	1783	11/12	0.95	0.25	19,27,50,52	0
1	MLY	D	220	11/12	0.95	0.17	42,56,66,68	0
1	MLY	B	1791	11/12	0.96	0.21	19,29,51,53	0
1	MLY	A	1783	11/12	0.97	0.20	11,37,63,65	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.