



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 PM UTC

PDB ID : 4XA6 / pdb_00004xa6
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

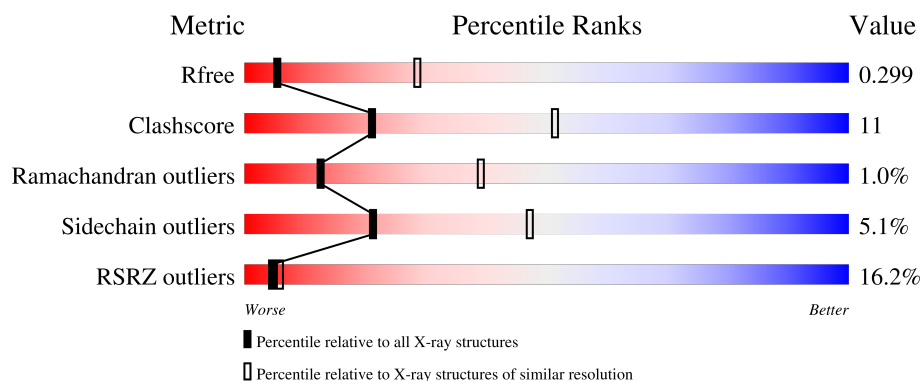
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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 $\leq 5\%$. 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	175	
1	B	175	
1	C	175	
1	D	175	

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	C	1783	-	-	-	X

2 Entry composition

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

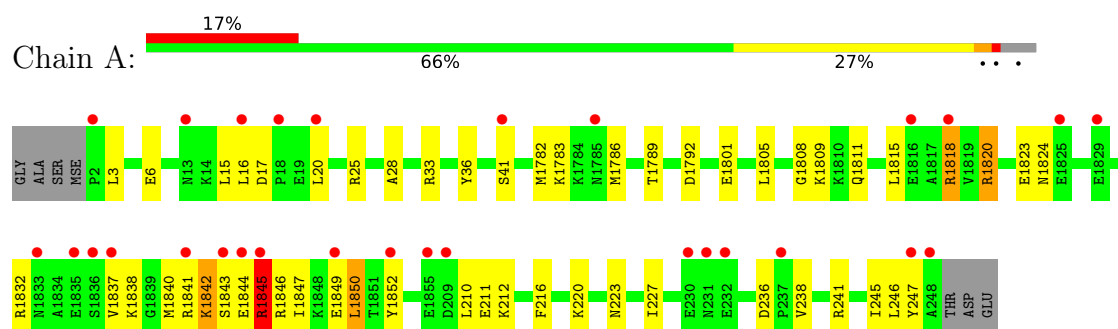
There are 16 discrepancies between the modelled and reference sequences:

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

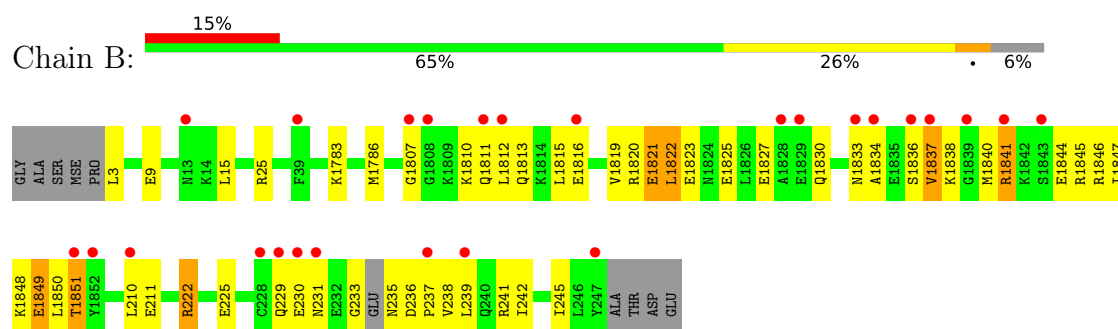
3 Residue-property plots [i](#)

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.

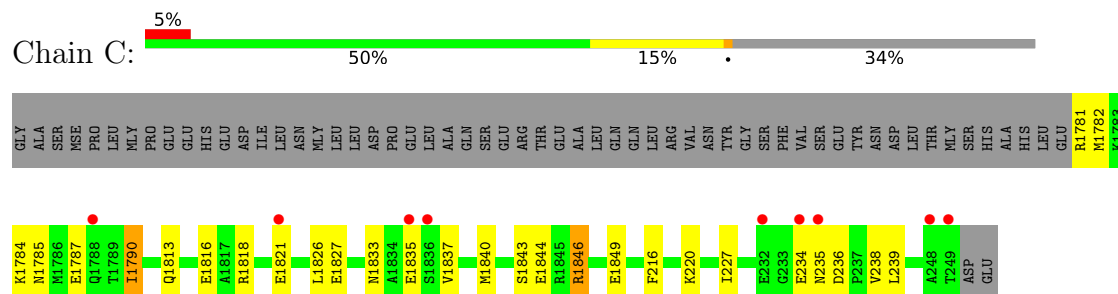
- Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein



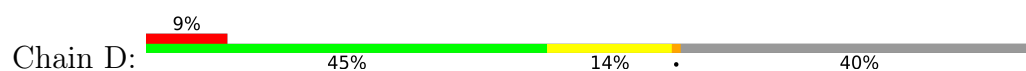
- Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein

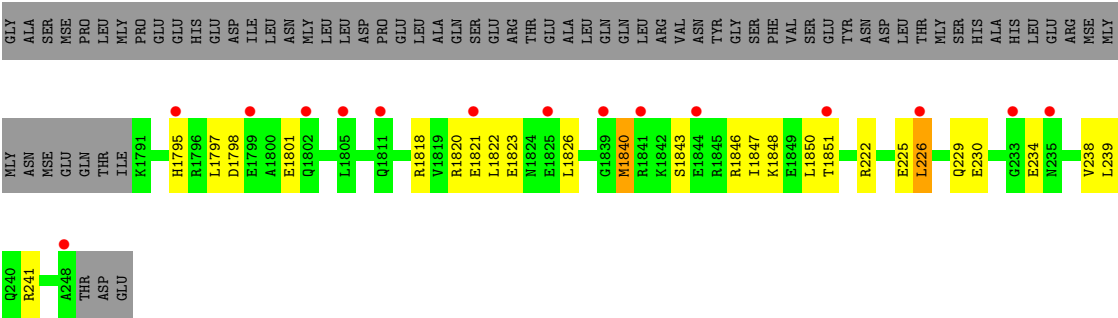


- Molecule 1: Gp7-MYH7(1777-1855)-EB1 chimera protein



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





4 Data and refinement statistics

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 43.89 – 3.42	Depositor EDS
% Data completeness (in resolution range)	88.8 (43.89-3.42) 83.7 (43.89-3.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.239 , 0.297 0.246 , 0.299	Depositor DCC
R_{free} test set	677 reflections (2.13%)	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)	0.31 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	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.*

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 [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	0.35	0/1263	0.79	3/1700 (0.2%)
1	B	0.36	0/1240	0.74	1/1667 (0.1%)
1	C	0.30	0/855	0.72	1/1144 (0.1%)
1	D	0.32	0/783	0.82	0/1053
All	All	0.34	0/4141	0.77	5/5564 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1821	GLU	N-CA-C	-7.51	104.12	113.28
1	A	1845	ARG	N-CA-C	-6.72	105.05	113.18
1	A	236	ASP	CA-C-N	5.46	126.67	119.84
1	A	236	ASP	C-N-CA	5.46	126.67	119.84
1	C	1846	ARG	N-CA-C	-5.38	108.49	114.62

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	1444	43	0
1	B	1406	0	1422	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	995	0	1022	17	0
1	D	898	0	918	18	0
All	All	4726	0	4806	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:A:1840:MSE:C	1:A:1843:SER:H	2.08	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:36:TYR:OH	1:B:3:LEU:O	2.36	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: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%)	9	33
1	B	145/175 (83%)	133 (92%)	11 (8%)	1 (1%)	18	47
1	C	101/175 (58%)	92 (91%)	8 (8%)	1 (1%)	12	39
1	D	93/175 (53%)	85 (91%)	7 (8%)	1 (1%)	11	37
All	All	489/700 (70%)	451 (92%)	33 (7%)	5 (1%)	12	39

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%)	128 (93%)	9 (7%)	15	40
1	B	135/138 (98%)	129 (96%)	6 (4%)	25	50
1	C	92/138 (67%)	88 (96%)	4 (4%)	26	50
1	D	83/138 (60%)	79 (95%)	4 (5%)	23	48
All	All	447/552 (81%)	424 (95%)	23 (5%)	21	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	GLU
1	A	41	SER
1	A	1818	ARG
1	A	1820	ARG
1	A	1832	ARG
1	A	1845	ARG
1	A	1850	LEU
1	A	227	ILE
1	B	1822	LEU
1	B	1837	VAL
1	B	1841	ARG
1	B	1849	GLU
1	B	1851	THR
1	B	222	ARG
1	C	1790	ILE
1	C	1821	GLU
1	C	1827	GLU
1	C	1835	GLU
1	D	1820	ARG
1	D	1840	MSE
1	D	226	LEU
1	D	234	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1802	GLN
1	A	1813	GLN
1	B	1788	GLN
1	B	1830	GLN
1	B	1853	GLN
1	C	1802	GLN
1	D	1824	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	C	1831	1	9,10,11	0.58	0	6,11,13	0.72	0
1	MLY	B	1838	1	9,10,11	0.47	0	6,11,13	0.88	0
1	MLY	C	220	1	9,10,11	0.62	0	6,11,13	1.00	0
1	MLY	A	1810	1	9,10,11	0.56	0	6,11,13	0.86	0
1	MLY	A	1784	1	9,10,11	0.58	0	6,11,13	0.84	0
1	MLY	B	1842	1	9,10,11	0.58	0	6,11,13	0.72	0
1	MLY	C	1838	1	9,10,11	0.69	0	6,11,13	0.73	0
1	MLY	A	1842	1	9,10,11	0.67	0	6,11,13	1.12	1 (16%)
1	MLY	A	1848	1	9,10,11	0.54	0	6,11,13	0.81	0
1	MLY	A	1809	1	9,10,11	0.56	0	6,11,13	0.72	0
1	MLY	A	1831	1	9,10,11	0.61	0	6,11,13	0.83	0
1	MLY	B	220	1	9,10,11	0.59	0	6,11,13	0.88	0
1	MLY	C	1783	1	9,10,11	0.71	0	6,11,13	0.62	0
1	MLY	D	212	1	9,10,11	0.68	0	6,11,13	0.74	0
1	MLY	A	1838	1	9,10,11	0.68	0	6,11,13	0.60	0
1	MLY	D	1814	1	9,10,11	0.62	0	6,11,13	0.46	0
1	MLY	B	1784	1	9,10,11	0.54	0	6,11,13	0.82	0
1	MLY	B	1791	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	C	1848	1	9,10,11	0.57	0	6,11,13	0.83	0
1	MLY	C	1791	1	9,10,11	0.55	0	6,11,13	0.79	0
1	MLY	C	1810	1	9,10,11	0.61	0	6,11,13	0.73	0
1	MLY	C	1784	1	9,10,11	0.46	0	6,11,13	0.80	0
1	MLY	D	1848	1	9,10,11	0.58	0	6,11,13	0.84	0
1	MLY	D	1791	1	9,10,11	0.61	0	6,11,13	0.67	0
1	MLY	C	1809	1	9,10,11	0.56	0	6,11,13	0.78	0
1	MLY	C	1842	1	9,10,11	0.59	0	6,11,13	0.73	0
1	MLY	B	1814	1	9,10,11	0.59	0	6,11,13	0.80	0
1	MLY	A	14	1	9,10,11	0.59	0	6,11,13	0.71	0
1	MLY	A	1791	1	9,10,11	0.49	0	6,11,13	0.86	0
1	MLY	B	4	1	9,10,11	0.51	0	6,11,13	0.89	0
1	MLY	A	1806	1	9,10,11	0.55	0	6,11,13	0.80	0
1	MLY	B	212	1	9,10,11	0.57	0	6,11,13	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	1810	1	9,10,11	0.59	0	6,11,13	0.78	0
1	MLY	B	14	1	9,10,11	0.54	0	6,11,13	0.74	0
1	MLY	B	1831	1	9,10,11	0.57	0	6,11,13	0.85	0
1	MLY	C	1806	1	9,10,11	0.52	0	6,11,13	0.83	0
1	MLY	B	1783	1	9,10,11	0.55	0	6,11,13	0.77	0
1	MLY	D	1809	1	9,10,11	0.55	0	6,11,13	0.81	0
1	MLY	D	1842	1	9,10,11	0.61	0	6,11,13	0.61	0
1	MLY	A	212	1	9,10,11	0.60	0	6,11,13	0.80	0
1	MLY	A	220	1	9,10,11	0.60	0	6,11,13	0.58	0
1	MLY	A	1814	1	9,10,11	0.55	0	6,11,13	0.83	0
1	MLY	B	48	1	9,10,11	0.59	0	6,11,13	0.82	0
1	MLY	D	1806	1	9,10,11	0.56	0	6,11,13	0.83	0
1	MLY	D	1831	1	9,10,11	0.54	0	6,11,13	0.78	0
1	MLY	D	220	1	9,10,11	0.58	0	6,11,13	0.79	0
1	MLY	B	1809	1	9,10,11	0.55	0	6,11,13	0.77	0
1	MLY	D	1838	1	9,10,11	0.58	0	6,11,13	0.81	0
1	MLY	A	1783	1	9,10,11	0.51	0	6,11,13	0.86	0
1	MLY	B	1806	1	9,10,11	0.52	0	6,11,13	0.84	0
1	MLY	B	1810	1	9,10,11	0.52	0	6,11,13	0.80	0
1	MLY	A	4	1	9,10,11	0.59	0	6,11,13	0.76	0
1	MLY	C	1814	1	9,10,11	0.59	0	6,11,13	0.77	0
1	MLY	B	1848	1	9,10,11	0.52	0	6,11,13	0.92	0
1	MLY	C	212	1	9,10,11	0.59	0	6,11,13	0.79	0
1	MLY	A	48	1	9,10,11	0.65	0	6,11,13	0.81	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	C	1831	1	-	0/8/9/11	-
1	MLY	B	1838	1	-	2/8/9/11	-
1	MLY	C	220	1	-	1/8/9/11	-
1	MLY	A	1810	1	-	3/8/9/11	-
1	MLY	A	1784	1	-	6/8/9/11	-
1	MLY	B	1842	1	-	2/8/9/11	-
1	MLY	C	1838	1	-	4/8/9/11	-
1	MLY	A	1842	1	-	5/8/9/11	-
1	MLY	A	1848	1	-	0/8/9/11	-
1	MLY	A	1809	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	1831	1	-	1/8/9/11	-
1	MLY	B	220	1	-	2/8/9/11	-
1	MLY	C	1783	1	-	1/8/9/11	-
1	MLY	D	212	1	-	2/8/9/11	-
1	MLY	A	1838	1	-	2/8/9/11	-
1	MLY	D	1814	1	-	5/8/9/11	-
1	MLY	B	1784	1	-	0/8/9/11	-
1	MLY	B	1791	1	-	1/8/9/11	-
1	MLY	C	1848	1	-	2/8/9/11	-
1	MLY	C	1791	1	-	3/8/9/11	-
1	MLY	C	1810	1	-	2/8/9/11	-
1	MLY	C	1784	1	-	2/8/9/11	-
1	MLY	D	1848	1	-	3/8/9/11	-
1	MLY	D	1791	1	-	0/8/9/11	-
1	MLY	C	1809	1	-	4/8/9/11	-
1	MLY	C	1842	1	-	2/8/9/11	-
1	MLY	B	1814	1	-	1/8/9/11	-
1	MLY	A	14	1	-	1/8/9/11	-
1	MLY	A	1791	1	-	0/8/9/11	-
1	MLY	B	4	1	-	0/8/9/11	-
1	MLY	A	1806	1	-	0/8/9/11	-
1	MLY	B	212	1	-	0/8/9/11	-
1	MLY	D	1810	1	-	1/8/9/11	-
1	MLY	B	14	1	-	2/8/9/11	-
1	MLY	B	1831	1	-	2/8/9/11	-
1	MLY	C	1806	1	-	2/8/9/11	-
1	MLY	B	1783	1	-	2/8/9/11	-
1	MLY	D	1809	1	-	4/8/9/11	-
1	MLY	D	1842	1	-	2/8/9/11	-
1	MLY	A	212	1	-	1/8/9/11	-
1	MLY	A	220	1	-	1/8/9/11	-
1	MLY	A	1814	1	-	2/8/9/11	-
1	MLY	B	48	1	-	0/8/9/11	-
1	MLY	D	1806	1	-	3/8/9/11	-
1	MLY	D	1831	1	-	0/8/9/11	-
1	MLY	D	220	1	-	2/8/9/11	-
1	MLY	B	1809	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	1838	1	-	0/8/9/11	-
1	MLY	A	1783	1	-	0/8/9/11	-
1	MLY	B	1806	1	-	3/8/9/11	-
1	MLY	B	1810	1	-	1/8/9/11	-
1	MLY	A	4	1	-	3/8/9/11	-
1	MLY	C	1814	1	-	3/8/9/11	-
1	MLY	B	1848	1	-	0/8/9/11	-
1	MLY	C	212	1	-	0/8/9/11	-
1	MLY	A	48	1	-	3/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1842	MLY	CH2-NZ-CE	-2.06	102.56	110.75

There are no chirality outliers.

All (97) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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	C	1809	MLY	CD-CE-NZ-CH1
1	C	1809	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	220	MLY	CG-CD-CE-NZ
1	B	1838	MLY	CG-CD-CE-NZ
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	A	220	MLY	CD-CE-NZ-CH2
1	C	1810	MLY	CD-CE-NZ-CH1
1	C	1810	MLY	CD-CE-NZ-CH2
1	D	1806	MLY	CD-CE-NZ-CH1
1	D	1809	MLY	CD-CE-NZ-CH2
1	D	1814	MLY	CD-CE-NZ-CH1
1	C	1784	MLY	CG-CD-CE-NZ
1	B	1783	MLY	CD-CE-NZ-CH2
1	B	1809	MLY	CD-CE-NZ-CH2
1	C	1838	MLY	CG-CD-CE-NZ
1	B	1809	MLY	CA-CB-CG-CD
1	B	1814	MLY	CA-CB-CG-CD
1	C	220	MLY	CD-CE-NZ-CH2
1	D	1809	MLY	CD-CE-NZ-CH1
1	D	1842	MLY	CD-CE-NZ-CH2
1	A	1838	MLY	CA-CB-CG-CD
1	C	1814	MLY	CA-CB-CG-CD
1	C	1809	MLY	CE-CD-CG-CB
1	D	1814	MLY	CG-CD-CE-NZ
1	D	1848	MLY	CG-CD-CE-NZ
1	A	1838	MLY	CE-CD-CG-CB
1	B	1810	MLY	CA-CB-CG-CD
1	B	1806	MLY	CA-CB-CG-CD
1	B	1842	MLY	CA-CB-CG-CD
1	A	1842	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	A	212	MLY	CD-CE-NZ-CH2
1	D	1809	MLY	CG-CD-CE-NZ
1	C	1838	MLY	CA-CB-CG-CD
1	B	14	MLY	CE-CD-CG-CB
1	A	1842	MLY	CG-CD-CE-NZ
1	B	1842	MLY	CE-CD-CG-CB
1	B	1838	MLY	CE-CD-CG-CB
1	D	1810	MLY	CA-CB-CG-CD
1	C	1814	MLY	CE-CD-CG-CB
1	C	1791	MLY	CA-CB-CG-CD
1	A	1831	MLY	C-CA-CB-CG
1	C	1842	MLY	C-CA-CB-CG
1	D	1806	MLY	C-CA-CB-CG
1	B	1806	MLY	CD-CE-NZ-CH2
1	C	1838	MLY	CD-CE-NZ-CH1
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	B	1783	MLY	CA-CB-CG-CD
1	D	220	MLY	CA-CB-CG-CD
1	D	212	MLY	CE-CD-CG-CB
1	D	1814	MLY	CD-CE-NZ-CH2
1	A	48	MLY	CE-CD-CG-CB
1	A	1784	MLY	CA-CB-CG-CD
1	B	14	MLY	CD-CE-NZ-CH2
1	C	1842	MLY	CG-CD-CE-NZ
1	C	1784	MLY	CA-CB-CG-CD
1	A	4	MLY	CE-CD-CG-CB
1	A	1842	MLY	CE-CD-CG-CB
1	B	1791	MLY	C-CA-CB-CG
1	B	1806	MLY	C-CA-CB-CG
1	A	1810	MLY	CA-CB-CG-CD
1	D	212	MLY	CG-CD-CE-NZ

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1838	MLY	1	0
1	C	220	MLY	2	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	0.96	29 (19%) 3 4	16, 69, 131, 161	0
1	B	146/175 (83%)	1.02	26 (17%) 4 5	21, 73, 138, 174	0
1	C	100/175 (57%)	0.81	9 (9%) 15 14	21, 66, 96, 124	0
1	D	93/175 (53%)	1.11	15 (16%) 4 6	43, 74, 113, 126	0
All	All	488/700 (69%)	0.98	79 (16%) 4 6	16, 71, 126, 174	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ASN	5.0
1	B	1852	TYR	4.3
1	D	1821	GLU	3.8
1	B	39	PHE	3.7
1	D	1841	ARG	3.7
1	A	1855	GLU	3.6
1	A	1845	ARG	3.5
1	D	235	ASN	3.4
1	C	234	GLU	3.4
1	A	247	TYR	3.3
1	A	2	PRO	3.3
1	C	235	ASN	3.3
1	A	209	ASP	3.3
1	B	1837	VAL	3.2
1	D	1839	GLY	3.2
1	B	1843	SER	3.1
1	B	239	LEU	3.1
1	A	1829	GLU	3.1
1	A	1843	SER	3.1
1	B	1807	GLY	3.0
1	C	232	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1829	GLU	2.9
1	B	1841	ARG	2.9
1	D	248	ALA	2.9
1	A	1841	ARG	2.9
1	B	247	TYR	2.8
1	A	1836	SER	2.8
1	C	248	ALA	2.8
1	D	1802	GLN	2.8
1	B	1812	LEU	2.8
1	B	1833	ASN	2.8
1	C	1821	GLU	2.8
1	B	1836	SER	2.7
1	B	1839	GLY	2.7
1	C	249	THR	2.7
1	A	1785	ASN	2.6
1	B	228	CYS	2.6
1	D	226	LEU	2.6
1	A	232	GLU	2.6
1	A	1837	VAL	2.6
1	D	1795	HIS	2.5
1	A	13	ASN	2.5
1	A	1825	GLU	2.5
1	D	1844	GLU	2.5
1	B	1851	THR	2.5
1	A	1818	ARG	2.5
1	B	1811	GLN	2.5
1	A	1849	GLU	2.5
1	D	1805	LEU	2.5
1	B	1828	ALA	2.5
1	A	1835	GLU	2.5
1	D	1811	GLN	2.5
1	B	1816	GLU	2.4
1	A	18	PRO	2.4
1	C	1836	SER	2.4
1	D	233	GLY	2.4
1	A	20	LEU	2.3
1	C	1788	GLN	2.3
1	D	1825	GLU	2.3
1	B	237	PRO	2.3
1	A	1844	GLU	2.3
1	D	1851	THR	2.3
1	B	1834	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	GLU	2.2
1	A	231	ASN	2.2
1	B	13	ASN	2.2
1	B	230	GLU	2.2
1	A	41	SER	2.1
1	A	248	ALA	2.1
1	A	1816	GLU	2.1
1	A	1833	ASN	2.1
1	A	16	LEU	2.1
1	C	1835	GLU	2.1
1	D	1799	GLU	2.1
1	A	1852	TYR	2.1
1	B	229	GLN	2.1
1	B	1808	GLY	2.0
1	A	237	PRO	2.0
1	B	210	LEU	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. 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	1784	11/12	0.41	0.29	102,116,122,123	0
1	MLY	C	1783	11/12	0.55	0.43	75,93,110,115	0
1	MLY	A	1838	11/12	0.62	0.32	105,118,127,131	0
1	MLY	A	4	11/12	0.64	0.28	82,98,106,106	0
1	MLY	A	1842	11/12	0.64	0.40	167,172,176,176	0
1	MLY	B	1810	11/12	0.67	0.33	115,123,150,151	0
1	MLY	C	1809	11/12	0.69	0.31	81,106,126,126	0
1	MLY	A	1831	11/12	0.70	0.28	126,130,133,134	0
1	MLY	D	212	11/12	0.73	0.28	62,72,103,106	0
1	MLY	D	1838	11/12	0.74	0.26	72,88,92,92	0
1	MLY	B	1831	11/12	0.74	0.25	111,118,129,130	0
1	MLY	D	1791	11/12	0.75	0.28	52,75,94,94	0
1	MLY	A	1848	11/12	0.76	0.25	96,106,112,112	0
1	MLY	B	1809	11/12	0.76	0.30	105,119,123,123	0
1	MLY	B	1806	11/12	0.77	0.28	76,80,107,108	0
1	MLY	D	1809	11/12	0.77	0.22	88,96,112,121	0
1	MLY	B	4	11/12	0.78	0.26	83,109,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	D	1810	11/12	0.79	0.34	101,109,117,118	0
1	MLY	B	1842	11/12	0.79	0.23	95,106,149,150	0
1	MLY	C	1810	11/12	0.79	0.32	73,90,110,110	0
1	MLY	C	1838	11/12	0.80	0.27	54,78,103,103	0
1	MLY	A	1810	11/12	0.80	0.27	84,97,112,112	0
1	MLY	B	1848	11/12	0.80	0.24	102,115,123,123	0
1	MLY	C	1848	11/12	0.82	0.27	78,93,110,110	0
1	MLY	B	14	11/12	0.82	0.25	63,84,108,108	0
1	MLY	C	1791	11/12	0.84	0.18	57,63,66,68	0
1	MLY	C	1814	11/12	0.84	0.22	54,61,78,88	0
1	MLY	A	14	11/12	0.84	0.23	71,80,93,93	0
1	MLY	D	1806	11/12	0.85	0.26	70,83,104,107	0
1	MLY	A	212	11/12	0.85	0.28	75,94,120,122	0
1	MLY	C	1842	11/12	0.85	0.21	48,69,91,92	0
1	MLY	A	1809	11/12	0.85	0.22	63,80,87,90	0
1	MLY	B	1814	11/12	0.85	0.20	70,82,89,100	0
1	MLY	D	1842	11/12	0.86	0.25	74,82,100,100	0
1	MLY	A	1806	11/12	0.87	0.18	37,47,68,74	0
1	MLY	C	212	11/12	0.87	0.21	51,72,104,105	0
1	MLY	D	1848	11/12	0.87	0.19	53,64,87,90	0
1	MLY	D	1831	11/12	0.87	0.18	50,64,70,77	0
1	MLY	B	1838	11/12	0.88	0.24	146,153,162,168	0
1	MLY	D	1814	11/12	0.89	0.17	71,88,95,97	0
1	MLY	A	1814	11/12	0.89	0.21	76,86,115,115	0
1	MLY	A	220	11/12	0.89	0.17	48,57,70,71	0
1	MLY	A	1784	11/12	0.90	0.18	42,60,97,97	0
1	MLY	C	1831	11/12	0.90	0.20	51,68,74,75	0
1	MLY	A	48	11/12	0.91	0.20	20,41,77,80	0
1	MLY	D	220	11/12	0.91	0.15	42,56,66,68	0
1	MLY	A	1791	11/12	0.92	0.15	29,47,61,63	0
1	MLY	B	48	11/12	0.92	0.15	22,29,57,62	0
1	MLY	B	1784	11/12	0.92	0.13	32,48,65,70	0
1	MLY	C	1806	11/12	0.93	0.15	75,85,95,95	0
1	MLY	B	1783	11/12	0.93	0.16	19,27,50,52	0
1	MLY	B	212	11/12	0.93	0.17	70,79,88,89	0
1	MLY	B	220	11/12	0.93	0.18	52,60,90,92	0
1	MLY	C	220	11/12	0.94	0.15	37,43,81,83	0
1	MLY	B	1791	11/12	0.95	0.10	19,29,51,53	0
1	MLY	A	1783	11/12	0.96	0.10	11,37,63,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.