World Wide PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:29 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
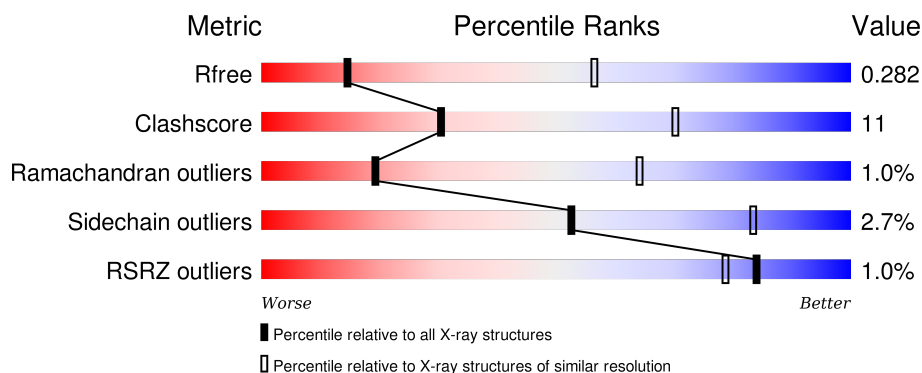
1   Overall quality at a glance (i)

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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	175	69% 26%
1	B	175	65% 27% 6%
1	C	175	51% 15% 34%
1	D	175	45% 14% 40%

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
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 ⓘ

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: Gp7-MYH7(1777-1855)-EB1 chimera protein
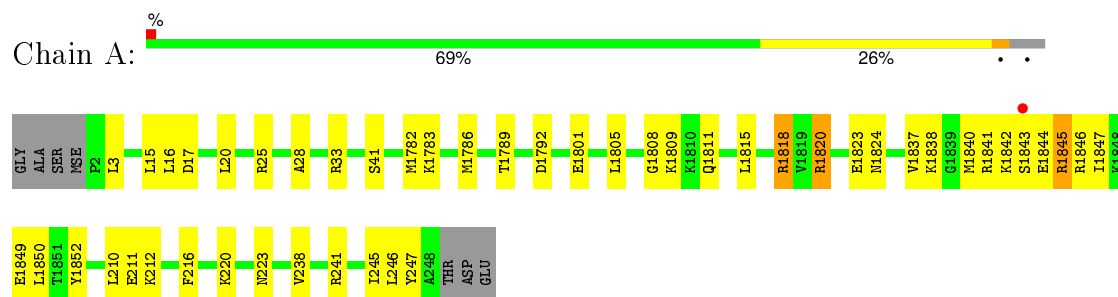
Chain A:

• 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:
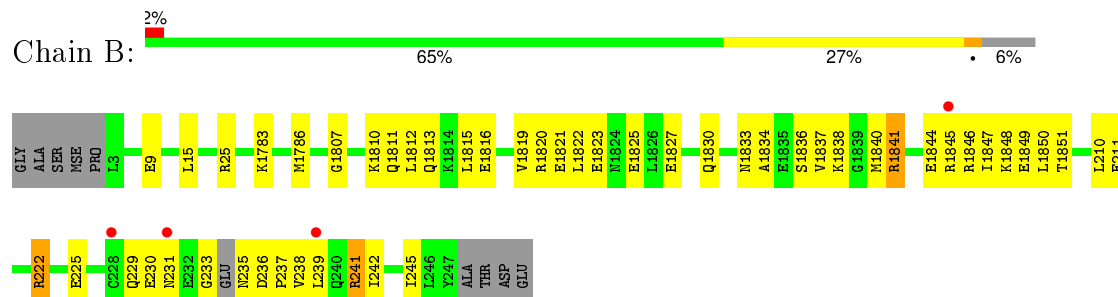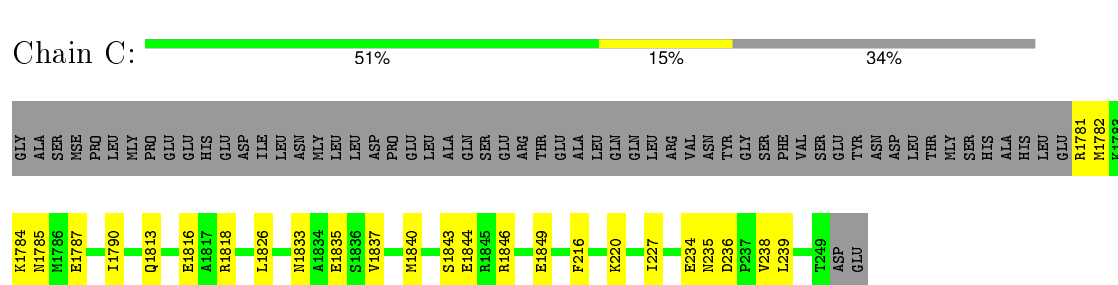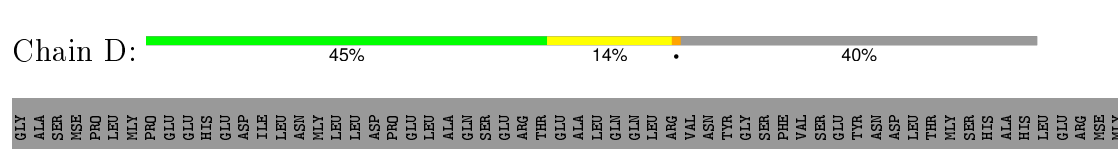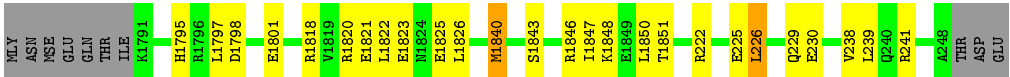
4 Data and refinement statistics (i)

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]	12.95 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.239 , 0.297 0.237 , 0.282	Depositor DCC
R_{free} test set	632 reflections (4.46%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 59.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	1 of 15109 reflections (0.007%)	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 8.20% 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 (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:B:1816:GLU:HA	1:B:1819:VAL:HG22	1.90	0.53
1:A:223:ASN:HB3	1:B:245:ILE:HD13	1.91	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:B:1841:ARG:HD2	1:B:1844:GLU:CB	2.42	0.50
1:A:1783:MLY:HG2	1:B:1786:MSE:HE1	1.92	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:HA	1:C:1781:ARG:HD3	1.53	0.47
1:A:1786:MSE:HE1	1:B:1783:MLY:HA	1.96	0.47
1:C:1782:MSE:HA	1:C:1785:ASN:HB3	1.97	0.47
1:B:1834:ALA:O	1:B:1838:MLY:HG3	2.15	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:C:1818:ARG:NH2	1:D:1823:GLU:OE2	2.42	0.46
1:A:1801:GLU:O	1:A:1805:LEU:HB2	2.16	0.46
1:B:241:ARG:HG2	1:B:241:ARG:H	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:B:1837:VAL:HA	1:B:1840:MSE:CB	2.46	0.44
1:A:17:ASP:HB3	1:A:20:LEU:HB2	1.98	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:HA	1:B:1841:ARG:HD2	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:HA	1:D:1822:LEU:HD12	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:B:1813:GLN:OE1	1:B:1816:GLU:HB2	2.18	0.43
1:A:15:LEU:HD21	1:A:28:ALA:HB3	2.00	0.43
1:A:1850:LEU:HD23	1:B:1850:LEU:HB3	2.01	0.42
1:A:25:ARG:HD3	1:B:15:LEU:O	2.20	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:HD2	1:A:1809:MLY:HH23	1.77	0.42
1:B:1846:ARG:O	1:B:1850:LEU:N	2.49	0.41
1:A:212:MLY:O	1:A:216:PHE:N	2.50	0.41
1:A:1844:GLU:HB3	1:A:1847:ILE:HD13	2.03	0.41
1:D:1846:ARG:HH12	1:D:1850:LEU:HD21	1.86	0.41
1:B:238:VAL:O	1:B:242:ILE:HG13	2.20	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:C:1846:ARG:HA	1:C:1849:GLU:HB3	2.02	0.40
1:B:1810:MLY:HE3	1:B:1810:MLY:HB3	1.88	0.40
1:C:1843:SER:OG	1:C:1844:GLU:N	2.54	0.40
1:A:1849:GLU:O	1:A:1852:TYR:HB3	2.21	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%)	15	58
1	B	145/175 (83%)	133 (92%)	11 (8%)	1 (1%)	26	70
1	C	101/175 (58%)	92 (91%)	8 (8%)	1 (1%)	19	64
1	D	93/175 (53%)	85 (91%)	7 (8%)	1 (1%)	17	62
All	All	489/700 (70%)	451 (92%)	33 (7%)	5 (1%)	19	64

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%)	42	78
1	B	135/138 (98%)	132 (98%)	3 (2%)	60	86
1	C	92/138 (67%)	91 (99%)	1 (1%)	80	92
1	D	83/138 (60%)	80 (96%)	3 (4%)	42	78
All	All	447/552 (81%)	435 (97%)	12 (3%)	52	83

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

Some 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	A	14	1	8,10,11	0.53	0	9,11,13	0.88	0
1	MLY	A	1783	1	8,10,11	0.49	0	9,11,13	0.96	0
1	MLY	A	1784	1	8,10,11	0.54	0	9,11,13	0.94	0
1	MLY	A	1791	1	8,10,11	0.47	0	9,11,13	0.99	1 (11%)
1	MLY	A	1806	1	8,10,11	0.51	0	9,11,13	0.89	0
1	MLY	A	1809	1	8,10,11	0.52	0	9,11,13	0.85	0
1	MLY	A	1810	1	8,10,11	0.51	0	9,11,13	0.99	1 (11%)
1	MLY	A	1814	1	8,10,11	0.51	0	9,11,13	0.92	0
1	MLY	A	1831	1	8,10,11	0.58	0	9,11,13	0.93	0
1	MLY	A	1838	1	8,10,11	0.67	0	9,11,13	0.82	0
1	MLY	A	1842	1	8,10,11	0.56	0	9,11,13	1.31	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
1	MLY	A	1848	1	8,10,11	0.51	0	9,11,13	0.88	0
1	MLY	A	212	1	8,10,11	0.57	0	9,11,13	0.97	1 (11%)
1	MLY	A	220	1	8,10,11	0.57	0	9,11,13	0.82	0
1	MLY	A	4	1	8,10,11	0.55	0	9,11,13	0.94	1 (11%)
1	MLY	A	48	1	8,10,11	0.64	0	9,11,13	0.93	0
1	MLY	B	14	1	8,10,11	0.51	0	9,11,13	0.85	0
1	MLY	B	1783	1	8,10,11	0.52	0	9,11,13	0.85	0
1	MLY	B	1784	1	8,10,11	0.50	0	9,11,13	0.92	0
1	MLY	B	1791	1	8,10,11	0.47	0	9,11,13	0.98	1 (11%)
1	MLY	B	1806	1	8,10,11	0.50	0	9,11,13	0.98	1 (11%)
1	MLY	B	1809	1	8,10,11	0.50	0	9,11,13	0.88	0
1	MLY	B	1810	1	8,10,11	0.48	0	9,11,13	0.91	0
1	MLY	B	1814	1	8,10,11	0.56	0	9,11,13	0.88	0
1	MLY	B	1831	1	8,10,11	0.52	0	9,11,13	0.93	0
1	MLY	B	1838	1	8,10,11	0.47	0	9,11,13	0.94	0
1	MLY	B	1842	1	8,10,11	0.57	0	9,11,13	0.83	0
1	MLY	B	1848	1	8,10,11	0.50	0	9,11,13	0.95	0
1	MLY	B	212	1	8,10,11	0.53	0	9,11,13	0.96	0
1	MLY	B	220	1	8,10,11	0.55	0	9,11,13	0.90	0
1	MLY	B	4	1	8,10,11	0.47	0	9,11,13	1.01	1 (11%)
1	MLY	B	48	1	8,10,11	0.56	0	9,11,13	0.89	0
1	MLY	C	1783	1	8,10,11	0.65	0	9,11,13	0.82	0
1	MLY	C	1784	1	8,10,11	0.45	0	9,11,13	0.87	0
1	MLY	C	1791	1	8,10,11	0.48	0	9,11,13	0.94	1 (11%)
1	MLY	C	1806	1	8,10,11	0.52	0	9,11,13	0.94	0
1	MLY	C	1809	1	8,10,11	0.53	0	9,11,13	0.86	0
1	MLY	C	1810	1	8,10,11	0.56	0	9,11,13	0.89	0
1	MLY	C	1814	1	8,10,11	0.56	0	9,11,13	0.89	0
1	MLY	C	1831	1	8,10,11	0.55	0	9,11,13	0.90	0
1	MLY	C	1838	1	8,10,11	0.65	0	9,11,13	0.84	0
1	MLY	C	1842	1	8,10,11	0.57	0	9,11,13	0.92	1 (11%)
1	MLY	C	1848	1	8,10,11	0.52	0	9,11,13	0.89	0
1	MLY	C	212	1	8,10,11	0.55	0	9,11,13	0.89	0
1	MLY	C	220	1	8,10,11	0.62	0	9,11,13	1.02	0
1	MLY	D	1791	1	8,10,11	0.60	0	9,11,13	0.82	0
1	MLY	D	1806	1	8,10,11	0.53	0	9,11,13	0.88	0
1	MLY	D	1809	1	8,10,11	0.51	0	9,11,13	0.91	0
1	MLY	D	1810	1	8,10,11	0.56	0	9,11,13	0.83	0
1	MLY	D	1814	1	8,10,11	0.60	0	9,11,13	0.76	0
1	MLY	D	1831	1	8,10,11	0.48	0	9,11,13	0.88	0
1	MLY	D	1838	1	8,10,11	0.53	0	9,11,13	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
1	MLY	D	1842	1	8,10,11	0.58	0	9,11,13	0.76	0
1	MLY	D	1848	1	8,10,11	0.54	0	9,11,13	0.97	1 (11%)
1	MLY	D	212	1	8,10,11	0.65	0	9,11,13	0.89	0
1	MLY	D	220	1	8,10,11	0.55	0	9,11,13	0.90	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	14	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1783	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1784	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1791	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1806	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1809	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1810	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1814	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1831	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1838	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1842	1	-	0/7/9/11	0/0/0/0
1	MLY	A	1848	1	-	0/7/9/11	0/0/0/0
1	MLY	A	212	1	-	0/7/9/11	0/0/0/0
1	MLY	A	220	1	-	0/7/9/11	0/0/0/0
1	MLY	A	4	1	-	0/7/9/11	0/0/0/0
1	MLY	A	48	1	-	0/7/9/11	0/0/0/0
1	MLY	B	14	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1783	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1784	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1791	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1806	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1809	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1810	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1814	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1831	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1838	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1842	1	-	0/7/9/11	0/0/0/0
1	MLY	B	1848	1	-	0/7/9/11	0/0/0/0
1	MLY	B	212	1	-	0/7/9/11	0/0/0/0
1	MLY	B	220	1	-	0/7/9/11	0/0/0/0
1	MLY	B	4	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	48	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1783	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1784	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1791	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1806	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1809	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1810	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1814	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1831	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1838	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1842	1	-	0/7/9/11	0/0/0/0
1	MLY	C	1848	1	-	0/7/9/11	0/0/0/0
1	MLY	C	212	1	-	0/7/9/11	0/0/0/0
1	MLY	C	220	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1791	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1806	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1809	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1810	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1814	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1831	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1838	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1842	1	-	0/7/9/11	0/0/0/0
1	MLY	D	1848	1	-	0/7/9/11	0/0/0/0
1	MLY	D	212	1	-	0/7/9/11	0/0/0/0
1	MLY	D	220	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1842	MLY	O-C-CA	-2.63	118.67	125.72
1	B	1791	MLY	O-C-CA	-2.16	119.92	125.72
1	A	4	MLY	O-C-CA	-2.13	120.01	125.72
1	A	212	MLY	O-C-CA	-2.12	120.02	125.72
1	C	1842	MLY	O-C-CA	-2.09	120.12	125.72
1	A	1842	MLY	CH2-NZ-CE	-2.06	102.56	110.77
1	B	1806	MLY	O-C-CA	-2.05	120.24	125.72
1	B	4	MLY	O-C-CA	-2.04	120.24	125.72
1	C	1791	MLY	O-C-CA	-2.02	120.31	125.72
1	A	1810	MLY	O-C-CA	-2.01	120.33	125.72
1	D	1848	MLY	O-C-CA	-2.01	120.34	125.72
1	A	1791	MLY	O-C-CA	-2.00	120.34	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1783	MLY	1	0
1	A	1809	MLY	1	0
1	A	1838	MLY	1	0
1	A	1842	MLY	5	0
1	A	212	MLY	1	0
1	A	220	MLY	1	0
1	B	1783	MLY	1	0
1	B	1810	MLY	1	0
1	B	1838	MLY	1	0
1	B	1848	MLY	1	0
1	C	1784	MLY	1	0
1	C	220	MLY	2	0
1	D	1848	MLY	3	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	149/175 (85%)	0.04	1 (0%)	89	84	16, 69, 131, 161	0
1	B	146/175 (83%)	0.09	4 (2%)	58	52	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%)	0.08	0	100	100	43, 74, 113, 126	0
All	All	488/700 (69%)	0.06	5 (1%)	84	79	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. 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	B	1783	11/12	0.95	0.25	-	19,27,50,52	0
1	MLY	D	1838	11/12	0.88	0.25	-	72,88,92,92	0
1	MLY	C	1842	11/12	0.91	0.26	-	48,69,91,92	0
1	MLY	A	1791	11/12	0.94	0.22	-	29,47,61,63	0
1	MLY	C	1848	11/12	0.90	0.27	-	78,93,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	MLY	B	1848	11/12	0.87	0.33	-	102,115,123,123	0
1	MLY	D	1848	11/12	0.91	0.24	-	53,64,87,90	0
1	MLY	C	1809	11/12	0.84	0.30	-	81,106,126,126	0
1	MLY	A	1848	11/12	0.86	0.46	-	96,106,112,112	0
1	MLY	B	1842	11/12	0.86	0.22	-	95,106,149,150	0
1	MLY	C	1783	11/12	0.71	0.56	-	75,93,110,115	0
1	MLY	A	1814	11/12	0.90	0.33	-	76,86,115,115	0
1	MLY	B	1784	11/12	0.95	0.22	-	32,48,65,70	0
1	MLY	C	212	11/12	0.91	0.45	-	51,72,104,105	0
1	MLY	C	220	11/12	0.94	0.27	-	37,43,81,83	0
1	MLY	A	1810	11/12	0.86	0.35	-	84,97,112,112	0
1	MLY	A	1783	11/12	0.97	0.20	-	11,37,63,65	0
1	MLY	A	1784	11/12	0.95	0.29	-	42,60,97,97	0
1	MLY	C	1806	11/12	0.94	0.35	-	75,85,95,95	0
1	MLY	A	1842	11/12	0.77	0.59	-	167,172,176,176	0
1	MLY	D	1791	11/12	0.75	0.41	-	52,75,94,94	0
1	MLY	A	48	11/12	0.93	0.28	-	20,41,77,80	0
1	MLY	A	1838	11/12	0.74	0.43	-	105,118,127,131	0
1	MLY	B	1791	11/12	0.96	0.21	-	19,29,51,53	0
1	MLY	C	1791	11/12	0.93	0.24	-	57,63,66,68	0
1	MLY	D	1806	11/12	0.85	0.42	-	70,83,104,107	0
1	MLY	A	1809	11/12	0.91	0.25	-	63,80,87,90	0
1	MLY	B	1809	11/12	0.84	0.32	-	105,119,123,123	0
1	MLY	B	1831	11/12	0.82	0.30	-	111,118,129,130	0
1	MLY	B	48	11/12	0.94	0.23	-	22,29,57,62	0
1	MLY	A	212	11/12	0.90	0.34	-	75,94,120,122	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	D	212	11/12	0.88	0.27	-	62,72,103,106	0
1	MLY	D	1810	11/12	0.86	0.41	-	101,109,117,118	0
1	MLY	D	1814	11/12	0.89	0.27	-	71,88,95,97	0
1	MLY	B	1814	11/12	0.88	0.34	-	70,82,89,100	0
1	MLY	C	1831	11/12	0.89	0.38	-	51,68,74,75	0
1	MLY	C	1838	11/12	0.93	0.39	-	54,78,103,103	0
1	MLY	D	1831	11/12	0.94	0.18	-	50,64,70,77	0
1	MLY	A	1831	11/12	0.85	0.35	-	126,130,133,134	0
1	MLY	C	1814	11/12	0.90	0.39	-	54,61,78,88	0
1	MLY	D	1842	11/12	0.86	0.31	-	74,82,100,100	0
1	MLY	D	220	11/12	0.95	0.17	-	42,56,66,68	0
1	MLY	B	1810	11/12	0.83	0.39	-	115,123,150,151	0
1	MLY	B	1838	11/12	0.84	0.42	-	146,153,162,168	0
1	MLY	A	14	11/12	0.89	0.40	-	71,80,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	MLY	B	4	11/12	0.90	0.29	-	83,109,136,136	0
1	MLY	A	4	11/12	0.86	0.34	-	82,98,106,106	0
1	MLY	D	1809	11/12	0.86	0.31	-	88,96,112,121	0
1	MLY	C	1784	11/12	0.81	0.27	-	102,116,122,123	0
1	MLY	C	1810	11/12	0.88	0.40	-	73,90,110,110	0
1	MLY	B	220	11/12	0.95	0.32	-	52,60,90,92	0
1	MLY	B	1806	11/12	0.86	0.31	-	76,80,107,108	0
1	MLY	B	212	11/12	0.91	0.33	-	70,79,88,89	0
1	MLY	B	14	11/12	0.91	0.26	-	63,84,108,108	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.