Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 09:04 pm GMT

PDB ID	:	2VJ4
Title	:	Methylated Shigella flexneri MxiC
Authors	:	Deane, J.E.; Roversi, P.; King, C.; Johnson, S.; Lea, S.M.
Deposited on	:	2007-12-06
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.286
Clashscore		15
Ramachandran outliers		2.2%
Sidechain outliers		11.1%
RSRZ outliers		5.1%

Worse ▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬ *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
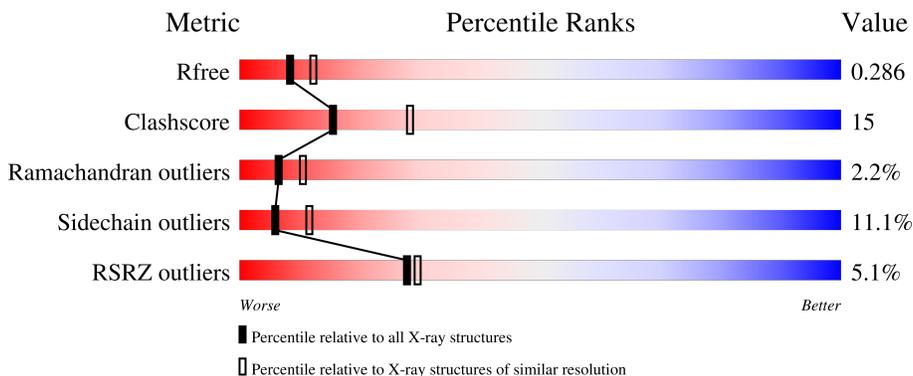
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	294	5% · 68% 27% 5% ·
1	B	294	4% · 66% 27% 5% ··

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	132	-	-	-	X
1	MLY	A	98	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4955 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 PROTEIN MXIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2388	1527	395	458	8			
1	B	292	Total	C	N	O	S	0	0	0
			2388	1527	395	458	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	HIS	-	expression tag	UNP Q04640
A	63	SER	-	expression tag	UNP Q04640
A	64	SER	-	expression tag	UNP Q04640
A	65	GLY	-	expression tag	UNP Q04640
A	66	LEU	-	expression tag	UNP Q04640
A	67	VAL	-	expression tag	UNP Q04640
A	68	PRO	-	expression tag	UNP Q04640
A	69	ARG	-	expression tag	UNP Q04640
A	70	GLY	-	expression tag	UNP Q04640
A	71	SER	-	expression tag	UNP Q04640
A	72	HIS	-	expression tag	UNP Q04640
A	73	MET	-	expression tag	UNP Q04640
B	62	HIS	-	expression tag	UNP Q04640
B	63	SER	-	expression tag	UNP Q04640
B	64	SER	-	expression tag	UNP Q04640
B	65	GLY	-	expression tag	UNP Q04640
B	66	LEU	-	expression tag	UNP Q04640
B	67	VAL	-	expression tag	UNP Q04640
B	68	PRO	-	expression tag	UNP Q04640
B	69	ARG	-	expression tag	UNP Q04640
B	70	GLY	-	expression tag	UNP Q04640
B	71	SER	-	expression tag	UNP Q04640
B	72	HIS	-	expression tag	UNP Q04640
B	73	MET	-	expression tag	UNP Q04640

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	95	Total O 95 95	0	0
2	B	84	Total O 84 84	0	0

3 Residue-property plots ⓘ

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: PROTEIN MXIC

Chain A:

• Molecule 1: PROTEIN MXIC

Chain B:
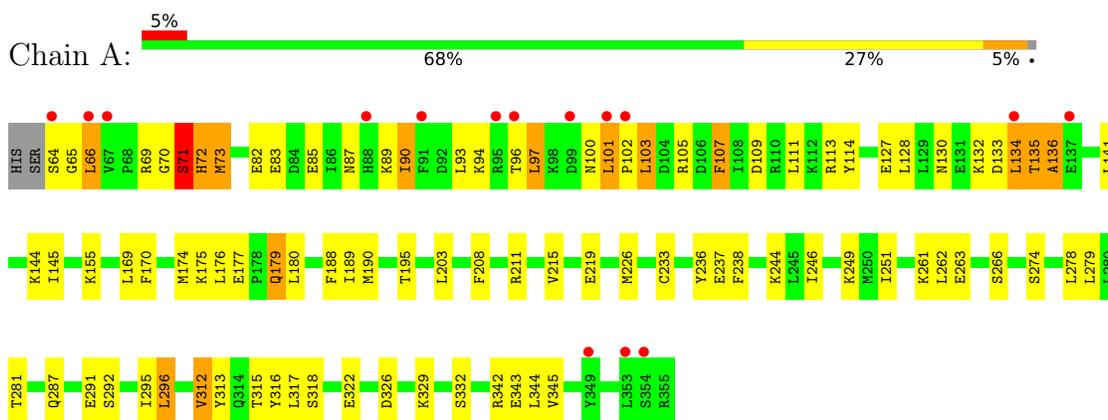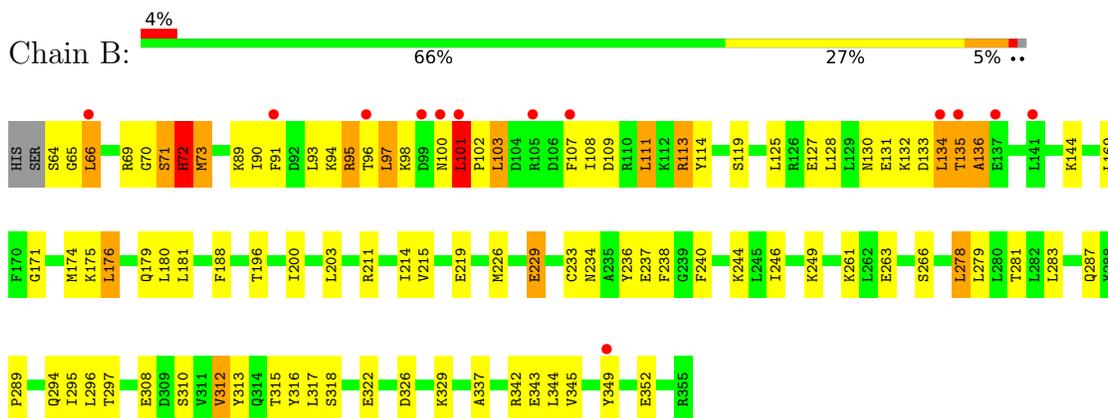
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	83.48Å 83.45Å 117.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 2.50 39.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.00-2.50) 95.7 (39.02-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.39Å)	Xtriage
Refinement program	TNT 5.13.1.0	Depositor
R, R_{free}	0.211 , 0.265 0.231 , 0.286	Depositor DCC
R_{free} test set	1584 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4955	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, 0.333 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	0.29	0/2204	0.56	0/2989
1	B	0.29	0/2204	0.56	1/2989 (0.0%)
All	All	0.29	0/4408	0.56	1/5978 (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	101	LEU	C-N-CD	-5.05	109.48	120.60

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	2388	0	2425	76	0
1	B	2388	0	2425	79	0
2	A	95	0	0	2	0
2	B	84	0	0	4	0
All	All	4955	0	4850	142	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 15.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

All (142) 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:66:LEU:HG	1:B:66:LEU:HD12	1.28	1.13
1:A:66:LEU:HD12	1:B:66:LEU:HG	1.29	1.05
1:A:102:PRO:HB3	1:A:103:LEU:HB3	1.40	1.04
1:B:102:PRO:HB3	1:B:103:LEU:HB3	1.40	1.02
1:A:64:SER:HB3	1:A:65:GLY:HA2	1.46	0.97
1:B:96:THR:HA	1:B:97:LEU:HB2	1.43	0.96
1:A:96:THR:HA	1:A:97:LEU:HB2	1.50	0.93
1:B:102:PRO:CB	1:B:103:LEU:HB3	2.10	0.80
1:B:64:SER:HB3	1:B:65:GLY:HA2	1.64	0.80
1:B:133:ASP:HB2	1:B:134:LEU:HA	1.64	0.80
1:A:102:PRO:CB	1:A:103:LEU:HB3	2.11	0.80
1:B:89:MLY:HD2	1:B:114:TYR:HB3	1.63	0.79
1:B:233:CYS:HB3	1:B:237:GLU:HB2	1.69	0.75
1:A:89:MLY:HD2	1:A:114:TYR:HB3	1.69	0.75
1:A:97:LEU:HB3	1:A:102:PRO:HG2	1.68	0.74
1:A:133:ASP:HB2	1:A:134:LEU:HA	1.68	0.74
1:A:233:CYS:HB3	1:A:237:GLU:HB2	1.71	0.71
1:A:188:PHE:O	1:A:244:MLY:HH22	1.90	0.71
1:B:188:PHE:O	1:B:244:MLY:HH22	1.90	0.70
1:B:97:LEU:HB3	1:B:102:PRO:HG2	1.78	0.66
1:B:66:LEU:O	1:B:66:LEU:HD13	1.98	0.64
1:A:66:LEU:CG	1:B:66:LEU:HD12	2.18	0.64
1:B:226:MET:CE	1:B:238:PHE:HB3	2.28	0.64
1:B:281:THR:HG23	1:B:295:ILE:HG22	1.81	0.63
1:A:66:LEU:HD12	1:B:66:LEU:CG	2.18	0.63
1:A:64:SER:CB	1:A:65:GLY:HA2	2.23	0.63
1:A:72:HIS:O	1:A:73:MET:HB2	1.99	0.63
1:B:97:LEU:HD21	1:B:100:ASN:HB2	1.81	0.63
1:A:66:LEU:HD13	1:A:66:LEU:O	1.99	0.62
1:B:174:MET:HB2	2:B:2033:HOH:O	2.00	0.62
1:A:66:LEU:CD1	1:B:66:LEU:HG	2.18	0.62
1:A:96:THR:CA	1:A:97:LEU:HB2	2.27	0.61
1:A:281:THR:HG23	1:A:295:ILE:HG22	1.83	0.61
1:B:226:MET:HE3	1:B:238:PHE:HB3	1.83	0.60
1:A:66:LEU:HG	1:B:66:LEU:CD1	2.18	0.60
1:B:219:GLU:OE2	1:B:249:MLY:HH22	2.02	0.60
1:B:181:LEU:HD11	2:B:2033:HOH:O	2.02	0.59
1:A:226:MET:CE	1:A:238:PHE:HB3	2.33	0.59
1:B:93:LEU:HB3	1:B:128:LEU:HD21	1.85	0.59
1:B:96:THR:CA	1:B:97:LEU:HB2	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:CD2	1:B:100:ASN:HB2	2.33	0.57
1:B:176:LEU:HB2	2:B:2033:HOH:O	2.04	0.57
1:A:100:ASN:O	1:A:101:LEU:HB2	2.05	0.56
1:B:219:GLU:OE2	1:B:249:MLY:HE2	2.06	0.55
1:B:100:ASN:O	1:B:101:LEU:HB2	2.05	0.55
1:A:261:MLY:HB2	1:A:315:THR:HG23	1.89	0.55
1:A:292:SER:O	1:A:296:LEU:HD22	2.06	0.54
1:A:219:GLU:OE2	1:A:249:MLY:HH22	2.07	0.54
1:A:73:MET:HA	2:A:2007:HOH:O	2.07	0.54
1:B:130:ASN:O	1:B:132:MLY:HE3	2.09	0.53
1:B:261:MLY:HB2	1:B:315:THR:HG23	1.89	0.53
1:A:226:MET:HE1	1:A:238:PHE:HB3	1.90	0.53
1:B:133:ASP:HB2	1:B:134:LEU:CA	2.39	0.52
1:A:66:LEU:HB3	1:B:66:LEU:HB3	1.92	0.51
1:A:219:GLU:OE2	1:A:249:MLY:HE2	2.09	0.51
1:A:130:ASN:O	1:A:132:MLY:HE3	2.10	0.51
1:A:135:THR:CA	1:A:136:ALA:HB2	2.41	0.51
1:B:109:ASP:O	1:B:113:ARG:HB2	2.10	0.51
1:B:72:HIS:O	1:B:73:MET:HB2	2.12	0.50
1:A:97:LEU:HD21	1:A:100:ASN:HB2	1.93	0.50
1:A:93:LEU:HB3	1:A:128:LEU:HD21	1.93	0.49
1:A:135:THR:CB	1:A:136:ALA:HB2	2.42	0.49
1:A:318:SER:O	1:A:322:GLU:HG2	2.13	0.49
1:B:98:MLY:HE3	1:B:131:GLU:HB2	1.94	0.49
1:B:313:TYR:HB3	1:B:345:VAL:HG23	1.94	0.49
1:A:133:ASP:CB	1:A:134:LEU:HA	2.33	0.48
1:A:262:LEU:HD23	1:A:315:THR:HG21	1.96	0.48
1:B:135:THR:CA	1:B:136:ALA:HB2	2.43	0.48
1:B:246:ILE:CD1	1:B:249:MLY:HH12	2.43	0.48
1:A:97:LEU:HD21	1:A:100:ASN:OD1	2.13	0.48
1:A:70:GLY:HA3	1:A:71:SER:CB	2.44	0.47
1:B:312:VAL:O	1:B:316:TYR:HD2	1.97	0.47
1:B:317:LEU:HD21	1:B:342:ARG:HD3	1.96	0.47
1:A:246:ILE:HG21	1:B:240:PHE:CE2	2.49	0.47
1:B:310:SER:HB2	1:B:349:TYR:CE2	2.50	0.47
1:A:82:GLU:H	1:A:85:GLU:HB3	1.80	0.47
1:A:66:LEU:HB3	1:B:66:LEU:CB	2.45	0.47
1:A:208:PHE:O	1:A:211:ARG:HG2	2.15	0.47
1:B:66:LEU:HD22	1:B:66:LEU:HA	1.61	0.47
1:B:127:GLU:O	1:B:130:ASN:HB2	2.15	0.46
1:A:195:THR:HG22	1:A:251:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:CB	1:B:136:ALA:HB2	2.45	0.46
1:B:287:GLN:O	1:B:329:MLY:HH13	2.14	0.46
1:A:127:GLU:O	1:A:130:ASN:HB2	2.15	0.46
1:A:135:THR:HA	1:A:136:ALA:HB2	1.95	0.46
1:B:234:ASN:OD1	1:B:237:GLU:HG3	2.15	0.46
1:B:318:SER:O	1:B:322:GLU:HG2	2.15	0.46
1:B:135:THR:HA	1:B:136:ALA:HB2	1.97	0.46
1:A:97:LEU:CD2	1:A:100:ASN:HB2	2.46	0.46
1:A:177:GLU:HG3	1:A:179:GLN:HG3	1.98	0.46
1:A:312:VAL:O	1:A:316:TYR:HD2	1.99	0.46
1:B:97:LEU:HD21	1:B:100:ASN:OD1	2.16	0.46
1:B:98:MLY:HH13	1:B:133:ASP:HB2	1.98	0.46
1:B:111:LEU:HD11	1:B:125:LEU:HD11	1.98	0.46
1:B:289:PRO:HB3	1:B:337:ALA:HB2	1.98	0.46
1:A:287:GLN:O	1:A:329:MLY:HH13	2.16	0.46
1:A:109:ASP:O	1:A:113:ARG:HB2	2.16	0.45
1:A:69:ARG:HA	1:A:70:GLY:HA2	1.72	0.45
1:A:226:MET:HE2	1:A:238:PHE:HB3	1.99	0.45
1:B:175:MLY:HH22	1:B:175:MLY:HD3	1.70	0.45
1:A:66:LEU:CB	1:B:66:LEU:HB3	2.47	0.45
1:A:261:MLY:HE2	1:A:318:SER:OG	2.17	0.45
1:A:249:MLY:HH13	1:B:236:TYR:CZ	2.52	0.45
1:A:141:LEU:O	1:A:145:ILE:HG13	2.17	0.44
1:A:236:TYR:CD1	1:B:246:ILE:HD13	2.52	0.44
1:B:94:MLY:HH23	1:B:131:GLU:OE1	2.17	0.44
1:B:294:GLN:O	1:B:297:THR:OG1	2.29	0.44
1:A:135:THR:OG1	1:A:136:ALA:HB2	2.18	0.44
1:A:155:MLY:HE3	1:A:190:MET:HG2	1.99	0.44
1:A:132:MLY:HH11	2:A:2028:HOH:O	2.18	0.43
1:A:189:ILE:HG13	1:A:190:MET:HG3	1.99	0.43
1:B:69:ARG:HB2	1:B:229:GLU:HB2	2.00	0.43
1:B:171:GLY:HA2	2:B:2033:HOH:O	2.18	0.43
1:B:234:ASN:ND2	1:B:237:GLU:HG3	2.32	0.43
1:A:83:GLU:O	1:A:87:ASN:HB2	2.18	0.43
1:A:246:ILE:HD13	1:B:236:TYR:CD1	2.54	0.43
1:B:102:PRO:CA	1:B:103:LEU:CB	2.97	0.43
1:B:69:ARG:HA	1:B:70:GLY:HA2	1.67	0.42
1:B:234:ASN:CG	1:B:237:GLU:HG3	2.39	0.42
1:A:102:PRO:CA	1:A:103:LEU:CB	2.97	0.42
1:B:211:ARG:O	1:B:214:ILE:HG22	2.19	0.42
1:A:144:MLY:HH13	1:A:144:MLY:HD3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD21	1:A:342:ARG:HD3	2.01	0.42
1:B:97:LEU:HG	1:B:100:ASN:H	1.83	0.42
1:B:196:THR:HG23	1:B:283:LEU:HD22	2.01	0.42
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.42
1:A:105:ARG:C	1:A:107:PHE:H	2.23	0.42
1:A:70:GLY:CA	1:A:71:SER:CB	2.98	0.41
1:A:175:MLY:HH22	1:A:175:MLY:HD3	1.68	0.41
1:B:133:ASP:CB	1:B:134:LEU:HA	2.32	0.41
1:A:97:LEU:HB3	1:A:102:PRO:CG	2.43	0.41
1:A:170:PHE:HB3	1:A:174:MET:CE	2.50	0.41
1:A:313:TYR:HB3	1:A:345:VAL:HG23	2.02	0.41
1:B:102:PRO:CA	1:B:103:LEU:HB3	2.50	0.41
1:B:308:GLU:HG3	1:B:352:GLU:OE1	2.20	0.41
1:B:101:LEU:N	1:B:102:PRO:CD	2.84	0.41
1:A:133:ASP:CB	1:A:134:LEU:CA	2.98	0.40
1:B:200:ILE:HG13	1:B:283:LEU:HD13	2.02	0.40
1:B:278:LEU:HD12	1:B:278:LEU:HA	1.94	0.40
1:B:144:MLY:HH13	1:B:144:MLY:HD3	1.67	0.40
1:A:90:ILE:CG2	1:A:94:MLY:HE2	2.51	0.40
1:B:91:PHE:O	1:B:95:ARG:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	270/294 (92%)	255 (94%)	9 (3%)	6 (2%)	6	10
1	B	270/294 (92%)	256 (95%)	8 (3%)	6 (2%)	6	10
All	All	540/588 (92%)	511 (95%)	17 (3%)	12 (2%)	6	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	103	LEU
1	B	72	HIS
1	B	101	LEU
1	B	103	LEU
1	A	71	SER
1	A	73	MET
1	A	136	ALA
1	B	71	SER
1	B	136	ALA
1	B	97	LEU
1	A	97	LEU

5.3.2 Protein sidechains ⓘ

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	248/250 (99%)	222 (90%)	26 (10%)	7	13
1	B	248/250 (99%)	219 (88%)	29 (12%)	5	10
All	All	496/500 (99%)	441 (89%)	55 (11%)	6	11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	71	SER
1	A	72	HIS
1	A	90	ILE
1	A	107	PHE
1	A	111	LEU
1	A	134	LEU
1	A	135	THR
1	A	169	LEU
1	A	176	LEU
1	A	179	GLN
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	215	VAL
1	A	263	GLU
1	A	266	SER
1	A	274	SER
1	A	278	LEU
1	A	279	LEU
1	A	291	GLU
1	A	296	LEU
1	A	312	VAL
1	A	326	ASP
1	A	332	SER
1	A	343	GLU
1	A	344	LEU
1	B	66	LEU
1	B	71	SER
1	B	72	HIS
1	B	73	MET
1	B	90	ILE
1	B	95	ARG
1	B	107	PHE
1	B	108	ILE
1	B	111	LEU
1	B	113	ARG
1	B	119	SER
1	B	134	LEU
1	B	135	THR
1	B	169	LEU
1	B	176	LEU
1	B	179	GLN
1	B	180	LEU
1	B	203	LEU
1	B	215	VAL
1	B	229	GLU
1	B	263	GLU
1	B	266	SER
1	B	278	LEU
1	B	279	LEU
1	B	296	LEU
1	B	312	VAL
1	B	326	ASP
1	B	343	GLU

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Mol	Chain	Res	Type
1	B	344	LEU

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

Mol	Chain	Res	Type
1	B	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 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	260	1	9,10,11	0.60	0	6,11,13	0.37	0
1	MLY	B	155	1	9,10,11	0.53	0	6,11,13	0.68	0
1	MLY	B	350	1	9,10,11	0.52	0	6,11,13	0.48	0
1	MLY	A	89	1	9,10,11	0.52	0	6,11,13	0.62	0
1	MLY	B	116	1	9,10,11	0.57	0	6,11,13	0.52	0
1	MLY	B	249	1	9,10,11	0.59	0	6,11,13	0.49	0
1	MLY	B	175	1	9,10,11	0.62	0	6,11,13	0.40	0
1	MLY	B	244	1	9,10,11	0.73	0	6,11,13	0.42	0
1	MLY	A	94	1	9,10,11	0.60	0	6,11,13	0.54	0
1	MLY	B	112	1	9,10,11	0.50	0	6,11,13	0.51	0
1	MLY	B	168	1	9,10,11	0.50	0	6,11,13	0.53	0
1	MLY	A	244	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	A	329	1	9,10,11	0.48	0	6,11,13	0.52	0
1	MLY	A	350	1	9,10,11	0.49	0	6,11,13	0.54	0
1	MLY	A	173	1	9,10,11	0.55	0	6,11,13	0.44	0
1	MLY	A	116	1	9,10,11	0.55	0	6,11,13	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MLY	B	89	1	9,10,11	0.54	0	6,11,13	0.63	0
1	MLY	B	351	1	9,10,11	0.51	0	6,11,13	0.58	0
1	MLY	A	249	1	9,10,11	0.52	0	6,11,13	0.56	0
1	MLY	A	98	1	9,10,11	0.50	0	6,11,13	0.67	0
1	MLY	B	260	1	9,10,11	0.57	0	6,11,13	0.43	0
1	MLY	A	351	1	9,10,11	0.51	0	6,11,13	0.61	0
1	MLY	A	230	1	9,10,11	0.54	0	6,11,13	0.37	0
1	MLY	B	94	1	9,10,11	0.59	0	6,11,13	0.54	0
1	MLY	A	269	1	9,10,11	0.52	0	6,11,13	0.47	0
1	MLY	B	132	1	9,10,11	0.65	0	6,11,13	0.49	0
1	MLY	A	261	1	9,10,11	0.53	0	6,11,13	0.50	0
1	MLY	B	329	1	9,10,11	0.50	0	6,11,13	0.48	0
1	MLY	A	175	1	9,10,11	0.57	0	6,11,13	0.41	0
1	MLY	A	155	1	9,10,11	0.50	0	6,11,13	0.64	0
1	MLY	B	144	1	9,10,11	0.58	0	6,11,13	0.41	0
1	MLY	A	168	1	9,10,11	0.53	0	6,11,13	0.51	0
1	MLY	B	98	1	9,10,11	0.54	0	6,11,13	0.58	0
1	MLY	B	230	1	9,10,11	0.49	0	6,11,13	0.38	0
1	MLY	A	132	1	9,10,11	0.62	0	6,11,13	0.47	0
1	MLY	A	144	1	9,10,11	0.56	0	6,11,13	0.47	0
1	MLY	B	261	1	9,10,11	0.55	0	6,11,13	0.43	0
1	MLY	A	112	1	9,10,11	0.51	0	6,11,13	0.51	0
1	MLY	B	269	1	9,10,11	0.46	0	6,11,13	0.51	0
1	MLY	B	173	1	9,10,11	0.55	0	6,11,13	0.48	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	260	1	-	4/8/9/11	-
1	MLY	B	155	1	-	4/8/9/11	-
1	MLY	B	350	1	-	6/8/9/11	-
1	MLY	A	89	1	-	3/8/9/11	-
1	MLY	B	116	1	-	5/8/9/11	-
1	MLY	B	249	1	-	3/8/9/11	-
1	MLY	B	175	1	-	7/8/9/11	-
1	MLY	B	244	1	-	5/8/9/11	-
1	MLY	A	94	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	112	1	-	5/8/9/11	-
1	MLY	B	168	1	-	3/8/9/11	-
1	MLY	A	244	1	-	4/8/9/11	-
1	MLY	A	329	1	-	4/8/9/11	-
1	MLY	A	350	1	-	7/8/9/11	-
1	MLY	A	173	1	-	7/8/9/11	-
1	MLY	A	116	1	-	5/8/9/11	-
1	MLY	B	89	1	-	2/8/9/11	-
1	MLY	B	351	1	-	5/8/9/11	-
1	MLY	A	249	1	-	4/8/9/11	-
1	MLY	A	98	1	-	6/8/9/11	-
1	MLY	B	260	1	-	2/8/9/11	-
1	MLY	A	351	1	-	5/8/9/11	-
1	MLY	A	230	1	-	4/8/9/11	-
1	MLY	B	94	1	-	5/8/9/11	-
1	MLY	A	269	1	-	5/8/9/11	-
1	MLY	B	132	1	-	6/8/9/11	-
1	MLY	A	261	1	-	5/8/9/11	-
1	MLY	B	329	1	-	4/8/9/11	-
1	MLY	A	175	1	-	7/8/9/11	-
1	MLY	A	155	1	-	4/8/9/11	-
1	MLY	B	144	1	-	7/8/9/11	-
1	MLY	A	168	1	-	3/8/9/11	-
1	MLY	B	98	1	-	6/8/9/11	-
1	MLY	B	230	1	-	4/8/9/11	-
1	MLY	A	132	1	-	6/8/9/11	-
1	MLY	A	144	1	-	6/8/9/11	-
1	MLY	B	261	1	-	6/8/9/11	-
1	MLY	A	112	1	-	3/8/9/11	-
1	MLY	B	269	1	-	5/8/9/11	-
1	MLY	B	173	1	-	6/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	94	MLY	C-CA-CB-CG
1	A	98	MLY	N-CA-CB-CG
1	A	98	MLY	C-CA-CB-CG
1	A	98	MLY	O-C-CA-CB
1	A	116	MLY	O-C-CA-CB
1	A	132	MLY	C-CA-CB-CG
1	A	144	MLY	C-CA-CB-CG
1	A	173	MLY	N-CA-CB-CG
1	A	175	MLY	C-CA-CB-CG
1	A	244	MLY	N-CA-CB-CG
1	A	244	MLY	C-CA-CB-CG
1	A	249	MLY	O-C-CA-CB
1	A	260	MLY	C-CA-CB-CG
1	A	261	MLY	N-CA-CB-CG
1	A	261	MLY	C-CA-CB-CG
1	A	350	MLY	C-CA-CB-CG
1	A	350	MLY	O-C-CA-CB
1	A	351	MLY	C-CA-CB-CG
1	B	94	MLY	C-CA-CB-CG
1	B	98	MLY	N-CA-CB-CG
1	B	98	MLY	C-CA-CB-CG
1	B	132	MLY	C-CA-CB-CG
1	B	144	MLY	C-CA-CB-CG
1	B	173	MLY	N-CA-CB-CG
1	B	173	MLY	C-CA-CB-CG
1	B	175	MLY	C-CA-CB-CG
1	B	244	MLY	N-CA-CB-CG
1	B	244	MLY	C-CA-CB-CG
1	B	261	MLY	N-CA-CB-CG
1	B	261	MLY	C-CA-CB-CG
1	B	350	MLY	C-CA-CB-CG
1	A	89	MLY	CD-CE-NZ-CH1
1	B	94	MLY	CD-CE-NZ-CH1
1	A	89	MLY	CD-CE-NZ-CH2
1	A	94	MLY	CD-CE-NZ-CH2
1	A	132	MLY	CD-CE-NZ-CH1
1	A	132	MLY	CD-CE-NZ-CH2
1	A	144	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CD-CE-NZ-CH1
1	A	173	MLY	CD-CE-NZ-CH2
1	A	261	MLY	CD-CE-NZ-CH1
1	A	269	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	350	MLY	CD-CE-NZ-CH1
1	A	351	MLY	CD-CE-NZ-CH1
1	A	351	MLY	CD-CE-NZ-CH2
1	B	89	MLY	CD-CE-NZ-CH1
1	B	89	MLY	CD-CE-NZ-CH2
1	B	94	MLY	CD-CE-NZ-CH2
1	B	98	MLY	CD-CE-NZ-CH2
1	B	144	MLY	CD-CE-NZ-CH2
1	B	155	MLY	CD-CE-NZ-CH2
1	B	261	MLY	CD-CE-NZ-CH1
1	B	261	MLY	CD-CE-NZ-CH2
1	B	269	MLY	CD-CE-NZ-CH1
1	B	269	MLY	CD-CE-NZ-CH2
1	B	350	MLY	CD-CE-NZ-CH1
1	B	350	MLY	CD-CE-NZ-CH2
1	B	351	MLY	CD-CE-NZ-CH1
1	B	351	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CG-CD-CE-NZ
1	A	175	MLY	CG-CD-CE-NZ
1	B	173	MLY	CG-CD-CE-NZ
1	A	329	MLY	CG-CD-CE-NZ
1	B	112	MLY	CG-CD-CE-NZ
1	B	175	MLY	CG-CD-CE-NZ
1	B	116	MLY	CG-CD-CE-NZ
1	A	112	MLY	CG-CD-CE-NZ
1	A	116	MLY	CG-CD-CE-NZ
1	B	98	MLY	CG-CD-CE-NZ
1	B	329	MLY	CG-CD-CE-NZ
1	A	132	MLY	CG-CD-CE-NZ
1	A	249	MLY	CG-CD-CE-NZ
1	B	249	MLY	CG-CD-CE-NZ
1	B	351	MLY	CG-CD-CE-NZ
1	A	94	MLY	CD-CE-NZ-CH1
1	A	144	MLY	CD-CE-NZ-CH1
1	A	155	MLY	CD-CE-NZ-CH2
1	A	175	MLY	CD-CE-NZ-CH2
1	A	260	MLY	CD-CE-NZ-CH2
1	A	261	MLY	CD-CE-NZ-CH2
1	A	269	MLY	CD-CE-NZ-CH1
1	A	350	MLY	CD-CE-NZ-CH2
1	B	132	MLY	CD-CE-NZ-CH1
1	B	132	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	175	MLY	CD-CE-NZ-CH2
1	B	260	MLY	CD-CE-NZ-CH2
1	A	261	MLY	CG-CD-CE-NZ
1	B	144	MLY	CG-CD-CE-NZ
1	A	175	MLY	CA-CB-CG-CD
1	B	175	MLY	CA-CB-CG-CD
1	A	155	MLY	CD-CE-NZ-CH1
1	A	329	MLY	CD-CE-NZ-CH2
1	B	144	MLY	CD-CE-NZ-CH1
1	B	173	MLY	CD-CE-NZ-CH2
1	B	244	MLY	CD-CE-NZ-CH2
1	B	230	MLY	CG-CD-CE-NZ
1	B	350	MLY	CG-CD-CE-NZ
1	B	173	MLY	CA-CB-CG-CD
1	A	230	MLY	CG-CD-CE-NZ
1	A	244	MLY	CG-CD-CE-NZ
1	A	351	MLY	CG-CD-CE-NZ
1	B	244	MLY	CG-CD-CE-NZ
1	A	175	MLY	CD-CE-NZ-CH1
1	A	329	MLY	CD-CE-NZ-CH1
1	B	98	MLY	CD-CE-NZ-CH1
1	B	155	MLY	CD-CE-NZ-CH1
1	B	175	MLY	CD-CE-NZ-CH1
1	A	144	MLY	CA-CB-CG-CD
1	B	144	MLY	CA-CB-CG-CD
1	A	168	MLY	CD-CE-NZ-CH1
1	A	168	MLY	CD-CE-NZ-CH2
1	A	260	MLY	CD-CE-NZ-CH1
1	B	112	MLY	CD-CE-NZ-CH1
1	B	168	MLY	CD-CE-NZ-CH2
1	A	173	MLY	CA-CB-CG-CD
1	B	132	MLY	CE-CD-CG-CB
1	B	168	MLY	CE-CD-CG-CB
1	A	269	MLY	CE-CD-CG-CB
1	A	329	MLY	CE-CD-CG-CB
1	A	98	MLY	CD-CE-NZ-CH1
1	B	132	MLY	CG-CD-CE-NZ
1	A	116	MLY	CE-CD-CG-CB
1	A	132	MLY	CE-CD-CG-CB
1	B	269	MLY	CE-CD-CG-CB
1	A	249	MLY	CE-CD-CG-CB
1	A	175	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	350	MLY	CE-CD-CG-CB
1	B	175	MLY	CE-CD-CG-CB
1	B	116	MLY	CA-CB-CG-CD
1	B	249	MLY	CE-CD-CG-CB
1	A	168	MLY	CE-CD-CG-CB
1	A	132	MLY	CA-CB-CG-CD
1	A	350	MLY	CA-CB-CG-CD
1	B	269	MLY	CA-CB-CG-CD
1	A	94	MLY	CE-CD-CG-CB
1	B	329	MLY	CD-CE-NZ-CH1
1	A	269	MLY	CA-CB-CG-CD
1	B	132	MLY	CA-CB-CG-CD
1	A	173	MLY	C-CA-CB-CG
1	B	351	MLY	C-CA-CB-CG
1	A	173	MLY	CE-CD-CG-CB
1	B	112	MLY	CE-CD-CG-CB
1	B	350	MLY	CE-CD-CG-CB
1	A	98	MLY	CD-CE-NZ-CH2
1	B	112	MLY	CD-CE-NZ-CH2
1	B	168	MLY	CD-CE-NZ-CH1
1	A	350	MLY	CG-CD-CE-NZ
1	A	351	MLY	CE-CD-CG-CB
1	B	94	MLY	CE-CD-CG-CB
1	B	173	MLY	CE-CD-CG-CB
1	A	155	MLY	CE-CD-CG-CB
1	B	116	MLY	CE-CD-CG-CB
1	B	144	MLY	CE-CD-CG-CB
1	A	155	MLY	CA-CB-CG-CD
1	B	155	MLY	CA-CB-CG-CD
1	A	112	MLY	CE-CD-CG-CB
1	B	351	MLY	CE-CD-CG-CB
1	A	144	MLY	CG-CD-CE-NZ
1	A	112	MLY	CD-CE-NZ-CH1
1	B	116	MLY	CD-CE-NZ-CH1
1	B	329	MLY	CE-CD-CG-CB
1	B	260	MLY	CD-CE-NZ-CH1
1	A	98	MLY	CE-CD-CG-CB
1	B	155	MLY	CE-CD-CG-CB
1	A	116	MLY	CA-CB-CG-CD
1	A	144	MLY	CE-CD-CG-CB
1	B	329	MLY	CD-CE-NZ-CH2
1	A	94	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	175	MLY	N-CA-CB-CG
1	B	144	MLY	N-CA-CB-CG
1	B	175	MLY	N-CA-CB-CG
1	B	244	MLY	CE-CD-CG-CB
1	A	230	MLY	C-CA-CB-CG
1	A	249	MLY	C-CA-CB-CG
1	B	230	MLY	C-CA-CB-CG
1	B	249	MLY	C-CA-CB-CG
1	A	260	MLY	CE-CD-CG-CB
1	A	244	MLY	CD-CE-NZ-CH2
1	A	230	MLY	CE-CD-CG-CB
1	A	116	MLY	CD-CE-NZ-CH1
1	B	350	MLY	CA-CB-CG-CD
1	B	98	MLY	CE-CD-CG-CB
1	A	230	MLY	CA-CB-CG-CD
1	B	112	MLY	CA-CB-CG-CD
1	B	230	MLY	CA-CB-CG-CD
1	B	230	MLY	CE-CD-CG-CB
1	B	261	MLY	CA-CB-CG-CD
1	B	269	MLY	CG-CD-CE-NZ
1	A	269	MLY	CG-CD-CE-NZ
1	B	261	MLY	CG-CD-CE-NZ
1	A	89	MLY	CE-CD-CG-CB
1	B	94	MLY	N-CA-CB-CG
1	B	116	MLY	CD-CE-NZ-CH2

There are no ring outliers.

20 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	89	MLY	1	0
1	B	249	MLY	3	0
1	B	175	MLY	1	0
1	B	244	MLY	1	0
1	A	94	MLY	1	0
1	A	244	MLY	1	0
1	A	329	MLY	1	0
1	B	89	MLY	1	0
1	A	249	MLY	3	0
1	B	94	MLY	1	0
1	B	132	MLY	1	0
1	A	261	MLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	329	MLY	1	0
1	A	175	MLY	1	0
1	A	155	MLY	1	0
1	B	144	MLY	1	0
1	B	98	MLY	2	0
1	A	132	MLY	2	0
1	A	144	MLY	1	0
1	B	261	MLY	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	272/294 (92%)	0.30	15 (5%)	25	26	31, 60, 97, 113	0
1	B	272/294 (92%)	0.25	13 (4%)	30	32	32, 59, 98, 115	0
All	All	544/588 (92%)	0.28	28 (5%)	28	29	31, 59, 97, 115	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	4.7
1	A	134	LEU	4.5
1	B	99	ASP	4.2
1	A	99	ASP	3.9
1	B	134	LEU	3.9
1	A	66	LEU	3.9
1	B	96	THR	3.7
1	B	349	TYR	3.5
1	A	91	PHE	3.4
1	A	102	PRO	3.4
1	A	96	THR	3.3
1	B	137	GLU	3.2
1	A	101	LEU	3.2
1	B	91	PHE	3.1
1	B	135	THR	3.0
1	A	353	LEU	3.0
1	A	95	ARG	3.0
1	B	107	PHE	2.7
1	A	67	VAL	2.6
1	B	101	LEU	2.5
1	A	64	SER	2.5
1	B	100	ASN	2.4
1	A	88	HIS	2.3
1	B	105	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	2.3
1	A	137	GLU	2.1
1	A	354	SER	2.1
1	A	349	TYR	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	A	132	11/12	0.59	0.42	87,93,99,99	0
1	MLY	B	132	11/12	0.74	0.34	86,92,97,100	0
1	MLY	A	98	11/12	0.78	0.42	103,108,117,117	0
1	MLY	B	116	11/12	0.81	0.31	59,65,87,90	0
1	MLY	B	98	11/12	0.83	0.40	105,109,119,119	0
1	MLY	A	94	11/12	0.85	0.24	94,100,101,103	0
1	MLY	B	351	11/12	0.85	0.25	86,91,98,98	0
1	MLY	A	350	11/12	0.86	0.33	82,89,94,97	0
1	MLY	B	94	11/12	0.86	0.24	94,98,101,106	0
1	MLY	A	116	11/12	0.86	0.32	60,62,87,89	0
1	MLY	A	329	11/12	0.87	0.27	60,70,86,86	0
1	MLY	B	89	11/12	0.89	0.19	67,74,84,84	0
1	MLY	A	269	11/12	0.89	0.20	50,58,71,74	0
1	MLY	B	144	11/12	0.89	0.27	65,75,81,93	0
1	MLY	A	351	11/12	0.89	0.24	86,89,96,96	0
1	MLY	A	261	11/12	0.90	0.21	44,56,66,66	0
1	MLY	B	350	11/12	0.90	0.22	83,89,93,100	0
1	MLY	A	112	11/12	0.90	0.20	70,75,78,82	0
1	MLY	B	112	11/12	0.91	0.15	68,75,77,86	0
1	MLY	B	244	11/12	0.91	0.20	39,47,70,72	0
1	MLY	A	144	11/12	0.91	0.22	65,72,80,88	0
1	MLY	A	260	11/12	0.91	0.27	48,60,70,73	0
1	MLY	B	260	11/12	0.92	0.20	50,54,72,72	0
1	MLY	A	89	11/12	0.92	0.17	70,75,82,85	0
1	MLY	A	244	11/12	0.92	0.25	39,43,67,75	0
1	MLY	B	173	11/12	0.93	0.21	47,52,80,89	0
1	MLY	B	329	11/12	0.93	0.21	57,69,83,88	0
1	MLY	B	261	11/12	0.94	0.20	42,56,60,62	0
1	MLY	B	269	11/12	0.94	0.16	55,58,68,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	MLY	B	230	11/12	0.94	0.23	31,40,61,68	0
1	MLY	A	155	11/12	0.94	0.17	37,46,49,51	0
1	MLY	A	249	11/12	0.94	0.17	44,48,52,53	0
1	MLY	B	168	11/12	0.95	0.14	21,42,57,67	0
1	MLY	A	230	11/12	0.95	0.21	21,39,66,70	0
1	MLY	B	175	11/12	0.95	0.15	48,53,67,68	0
1	MLY	A	173	11/12	0.95	0.24	42,52,77,82	0
1	MLY	B	155	11/12	0.95	0.17	43,48,57,57	0
1	MLY	B	249	11/12	0.95	0.15	36,44,53,57	0
1	MLY	A	175	11/12	0.96	0.15	51,55,63,64	0
1	MLY	A	168	11/12	0.96	0.12	29,40,58,66	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.