



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 PM UTC

PDB ID : 5Z5C / pdb_00005z5c
Title : Crystal structure of hydrogen sulfide-producing enzyme (Fn1055) from *Fusobacterium nucleatum*: lysine-dimethylated form
Authors : Kezuka, Y.; Yoshida, Y.; Nonaka, T.
Deposited on : 2018-01-17
Resolution : 2.07 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

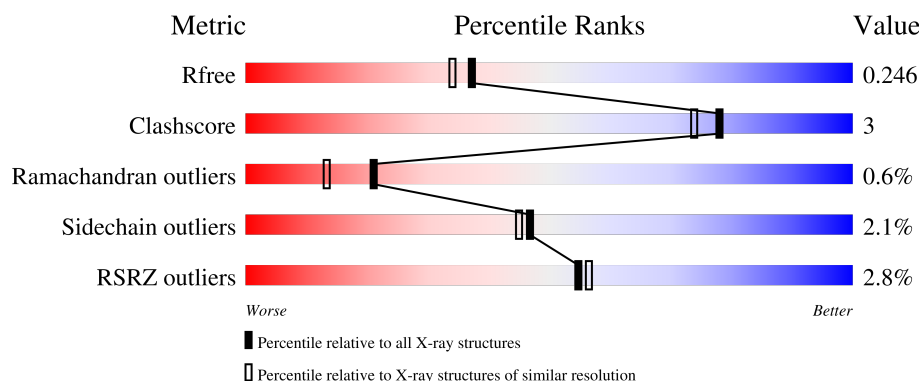
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	340	0% 89% 7% ..
1	B	340	3% 90% 8% ..
1	C	340	3% 91% 6% .
1	D	340	2% 89% 8% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10840 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.

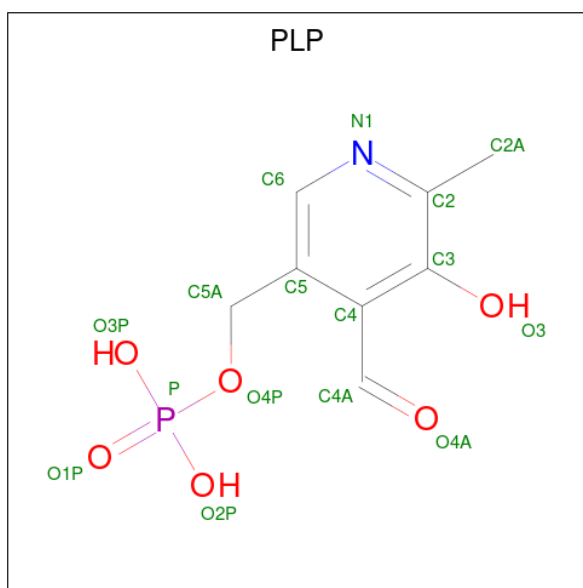
- Molecule 1 is a protein called Cysteine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2590	1663	427	487	13			
1	B	336	Total	C	N	O	S	0	1	0
			2622	1678	434	496	14			
1	C	332	Total	C	N	O	S	0	0	0
			2591	1661	429	488	13			
1	D	332	Total	C	N	O	S	0	0	0
			2601	1671	429	488	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8REP3
A	-2	PRO	-	expression tag	UNP Q8REP3
A	-1	LEU	-	expression tag	UNP Q8REP3
A	0	GLY	-	expression tag	UNP Q8REP3
A	1	SER	-	expression tag	UNP Q8REP3
B	-3	GLY	-	expression tag	UNP Q8REP3
B	-2	PRO	-	expression tag	UNP Q8REP3
B	-1	LEU	-	expression tag	UNP Q8REP3
B	0	GLY	-	expression tag	UNP Q8REP3
B	1	SER	-	expression tag	UNP Q8REP3
C	-3	GLY	-	expression tag	UNP Q8REP3
C	-2	PRO	-	expression tag	UNP Q8REP3
C	-1	LEU	-	expression tag	UNP Q8REP3
C	0	GLY	-	expression tag	UNP Q8REP3
C	1	SER	-	expression tag	UNP Q8REP3
D	-3	GLY	-	expression tag	UNP Q8REP3
D	-2	PRO	-	expression tag	UNP Q8REP3
D	-1	LEU	-	expression tag	UNP Q8REP3
D	0	GLY	-	expression tag	UNP Q8REP3
D	1	SER	-	expression tag	UNP Q8REP3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	68	Total	O	0	0
			68	68		

Continued on next page...

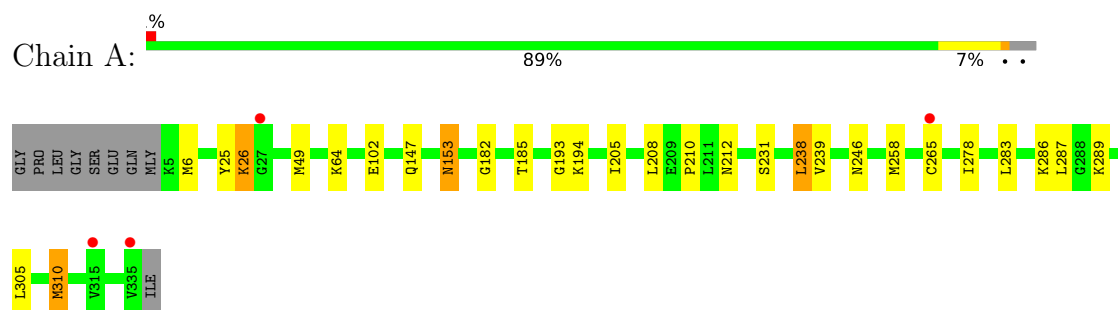
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	99	Total 99	O 99	0	0
4	D	84	Total 84	O 84	0	0

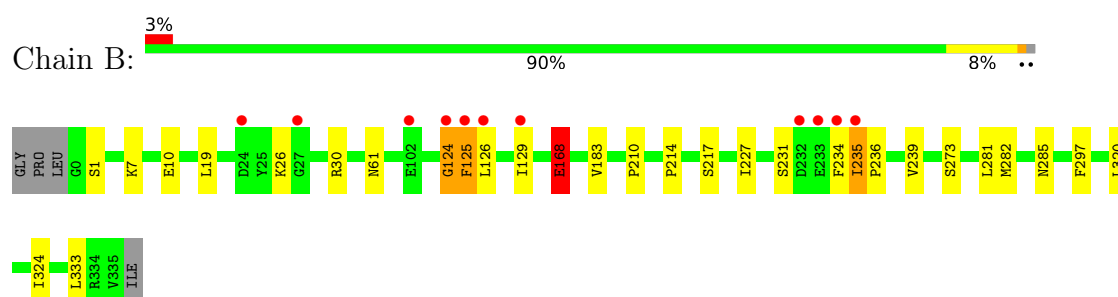
3 Residue-property plots [i](#)

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.

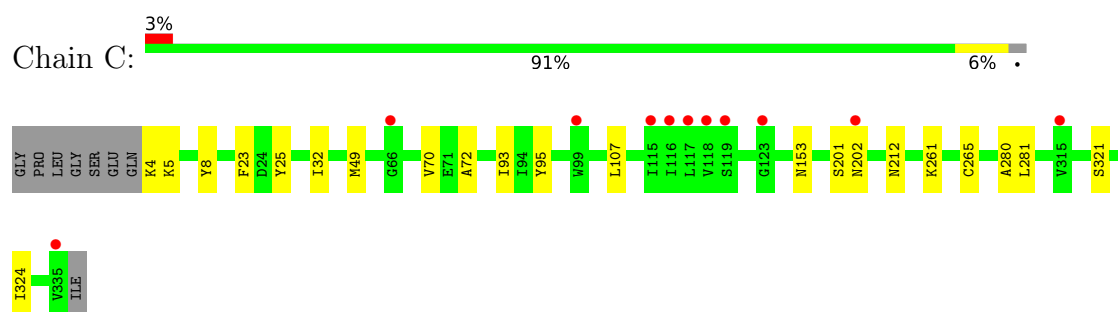
• Molecule 1: Cysteine synthase



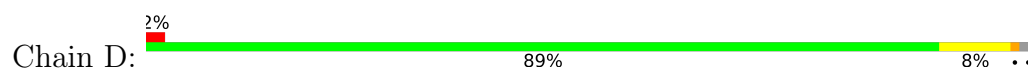
• Molecule 1: Cysteine synthase

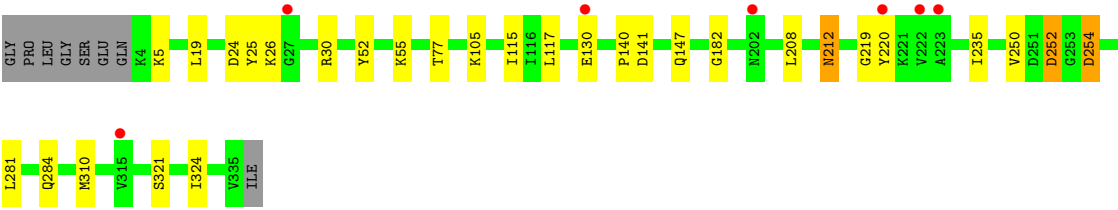


• Molecule 1: Cysteine synthase



• Molecule 1: Cysteine synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	57.76Å 136.16Å 171.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 2.07 40.93 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.93-2.07) 99.5 (40.93-2.07)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.186 , 0.242 0.194 , 0.246	Depositor DCC
R_{free} test set	4180 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10840	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MLY, PLP

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	1.01	0/2299	0.99	1/3128 (0.0%)
1	B	0.88	0/2332	1.00	5/3170 (0.2%)
1	C	1.03	2/2299 (0.1%)	1.04	3/3128 (0.1%)
1	D	0.94	2/2299 (0.1%)	0.96	0/3128
All	All	0.97	4/9229 (0.0%)	1.00	9/12554 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	254	ASP	CA-C	5.54	1.59	1.52
1	D	52	TYR	C-O	-5.43	1.17	1.24
1	C	280	ALA	CA-C	5.13	1.59	1.52
1	C	107	LEU	CA-C	-5.10	1.46	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	ASN	N-CA-C	6.52	119.21	111.71
1	C	201	SER	CA-C-N	5.96	128.87	120.28
1	C	201	SER	C-N-CA	5.96	128.87	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ILE	CA-C-N	-5.61	114.18	119.85
1	B	235	ILE	C-N-CA	-5.61	114.18	119.85
1	B	124	GLY	CA-C-N	5.38	131.38	121.70
1	B	124	GLY	C-N-CA	5.38	131.38	121.70
1	B	168	GLU	CB-CA-C	5.10	120.03	110.70
1	A	102	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	MLY	Peptide
1	B	26	MLY	Peptide

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	2590	0	2590	21	0
1	B	2622	0	2606	11	0
1	C	2591	0	2579	11	0
1	D	2601	0	2607	16	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	7	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	122	0	0	1	0
4	B	68	0	0	0	0
4	C	99	0	0	0	0
4	D	84	0	0	1	0
All	All	10840	0	10407	59	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 3.

All (59) 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:D:105:MLY:HE2	1:D:117:LEU:HD11	1.72	0.71
1:A:153:ASN:C	1:A:153:ASN:HD22	2.08	0.62
1:B:236:PRO:HG2	1:B:239:VAL:HG23	1.82	0.62
1:A:283:LEU:O	1:A:287:LEU:HD12	2.02	0.60
1:D:30:ARG:HH11	1:D:284:GLN:HE21	1.49	0.59
1:A:153:ASN:HB3	1:A:238:LEU:HD11	1.85	0.58
1:C:281:LEU:CD2	1:C:324:ILE:HD11	2.36	0.56
1:B:210:PRO:HB3	1:B:227:ILE:HD12	1.88	0.55
1:A:64:MLY:HE2	4:A:513:HOH:O	2.06	0.55
1:C:5:MLY:HA	1:C:8:TYR:CE2	2.42	0.55
1:D:219:GLY:HA2	1:D:235:ILE:HD11	1.90	0.52
1:A:283:LEU:CD1	1:A:287:LEU:HD11	2.40	0.52
1:A:305:LEU:HA	1:A:310:MET:HG2	1.92	0.52
1:A:25:TYR:O	1:A:26:MLY:C	2.58	0.51
1:C:281:LEU:HD23	1:C:324:ILE:HD11	1.93	0.51
1:A:287:LEU:HD12	1:A:287:LEU:N	2.27	0.50
1:D:141:ASP:N	4:D:502:HOH:O	2.42	0.50
1:B:183:VAL:HG11	1:B:239:VAL:HG21	1.94	0.49
1:D:25:TYR:O	1:D:26:MLY:C	2.60	0.49
1:D:30:ARG:HH11	1:D:284:GLN:NE2	2.10	0.49
1:D:208:LEU:HD11	1:D:250:VAL:HG21	1.95	0.48
1:C:70:VAL:HG22	1:C:93:ILE:HB	1.94	0.48
1:D:30:ARG:HB3	1:D:284:GLN:HE22	1.79	0.48
1:D:105:MLY:CE	1:D:117:LEU:HD11	2.42	0.48
1:A:283:LEU:HG	1:A:287:LEU:CD1	2.44	0.47
1:B:168:GLU:HB2	1:B:333:LEU:HD13	1.96	0.47
1:B:124:GLY:CA	1:B:125:PHE:HB2	2.45	0.47
1:D:182:GLY:HA2	1:D:208:LEU:HB3	1.97	0.47
1:A:283:LEU:O	1:A:287:LEU:CD1	2.62	0.46
1:A:182:GLY:HA2	1:A:208:LEU:HB3	1.98	0.46
1:A:258:MET:HB2	1:A:278:ILE:HD11	1.99	0.45
1:B:281:LEU:CD2	1:B:324:ILE:HD11	2.46	0.45
1:C:23:PHE:CE1	1:C:32:ILE:HD12	2.51	0.45
1:B:214:PRO:HB2	1:B:217:SER:OG	2.17	0.45
1:D:254:ASP:OD1	1:D:321:SER:OG	2.31	0.44
1:C:72:ALA:HA	1:C:95:TYR:O	2.17	0.44
1:A:193:GLY:HA3	1:A:205:ILE:HG21	2.00	0.44
1:A:210:PRO:HD3	1:A:231:SER:HB2	2.00	0.44
1:A:49:MET:HG3	1:A:153:ASN:ND2	2.33	0.43
1:C:261:MLY:HE2	1:C:321:SER:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:SER:HB3	1:B:297:PHE:CD1	2.54	0.42
1:B:30:ARG:HH22	1:B:285:ASN:ND2	2.17	0.42
1:C:49:MET:HE3	1:C:49:MET:HB3	1.94	0.42
1:A:246:ASN:HB2	1:A:286:MLY:HH11	2.02	0.42
1:D:281:LEU:CD2	1:D:324:ILE:HD11	2.50	0.42
1:C:23:PHE:CZ	1:C:32:ILE:HD12	2.54	0.42
1:A:289:MLY:N	1:A:289:MLY:HE2	2.35	0.42
1:B:7:MLY:O	1:B:10:GLU:HG2	2.20	0.42
1:A:153:ASN:C	1:A:153:ASN:ND2	2.76	0.41
1:D:212:ASN:HD21	1:D:252:ASP:HB2	1.85	0.41
1:A:147:GLN:NE2	1:A:185:THR:HG21	2.35	0.41
1:A:194:MLY:HD2	1:A:194:MLY:HH22	1.77	0.40
1:A:49:MET:HE3	1:A:49:MET:HB3	1.83	0.40
1:B:282:MET:HE3	1:B:320:LEU:HD13	2.03	0.40
1:C:25:TYR:CD1	1:C:281:LEU:HD21	2.57	0.40
1:D:77:THR:HG21	1:D:147:GLN:NE2	2.36	0.40
1:D:281:LEU:HD23	1:D:324:ILE:HD11	2.03	0.40
1:C:49:MET:HG3	1:C:153:ASN:OD1	2.22	0.40
1:D:5:MLY:HH12	1:D:5:MLY:HD3	1.87	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	295/340 (87%)	281 (95%)	14 (5%)	0	100	100
1	B	299/340 (88%)	284 (95%)	11 (4%)	4 (1%)	9	3
1	C	295/340 (87%)	287 (97%)	8 (3%)	0	100	100
1	D	295/340 (87%)	279 (95%)	13 (4%)	3 (1%)	12	5
All	All	1184/1360 (87%)	1131 (96%)	46 (4%)	7 (1%)	21	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	PHE
1	D	252	ASP
1	B	1	SER
1	B	61	ASN
1	B	231	SER
1	D	220	TYR
1	D	140	PRO

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	248/254 (98%)	241 (97%)	7 (3%)	38	34
1	B	252/254 (99%)	246 (98%)	6 (2%)	43	40
1	C	248/254 (98%)	246 (99%)	2 (1%)	73	77
1	D	248/254 (98%)	242 (98%)	6 (2%)	43	40
All	All	996/1016 (98%)	975 (98%)	21 (2%)	47	45

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	153	ASN
1	A	212	ASN
1	A	238	LEU
1	A	239	VAL
1	A	265	CYS
1	A	310	MET
1	B	19	LEU
1	B	126	LEU
1	B	129	ILE
1	B	168	GLU
1	B	234	PHE
1	B	235	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	212	ASN
1	C	265	CYS
1	D	19	LEU
1	D	24	ASP
1	D	115	ILE
1	D	130	GLU
1	D	212	ASN
1	D	310	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	147	GLN
1	A	153	ASN
1	A	199	ASN
1	B	147	GLN
1	B	285	ASN
1	C	138	ASN
1	C	139	ASN
1	C	147	GLN
1	D	147	GLN
1	D	260	GLN
1	D	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

143 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	289	1	7,8,11	0.47	0	3,8,13	0.47	0
1	MLY	A	264	1	7,8,11	0.51	0	3,8,13	0.61	0
1	MLY	B	35	1	7,8,11	0.69	0	3,8,13	0.41	0
1	MLY	D	302	1	7,8,11	0.50	0	3,8,13	0.69	0
1	MLY	C	330	1	7,8,11	0.36	0	3,8,13	0.42	0
1	MLY	A	15	1	9,10,11	0.66	0	6,11,13	0.83	0
1	MLY	A	322	1	7,8,11	0.49	0	3,8,13	0.43	0
1	MLY	A	35	1	7,8,11	0.53	0	3,8,13	0.39	0
1	MLY	B	327	1	7,8,11	0.75	0	3,8,13	0.42	0
1	MLY	C	15	1	7,8,11	0.62	0	3,8,13	0.39	0
1	MLY	B	204	1	7,8,11	0.47	0	3,8,13	0.47	0
1	MLY	B	224	1	7,8,11	0.45	0	3,8,13	0.30	0
1	MLY	B	322	1	7,8,11	0.36	0	3,8,13	0.47	0
1	MLY	D	286	1	9,10,11	0.40	0	6,11,13	0.76	0
1	MLY	A	330	1	7,8,11	0.43	0	3,8,13	0.39	0
1	MLY	D	314	1	7,8,11	0.52	0	3,8,13	0.43	0
1	MLY	D	243	1	7,8,11	0.53	0	3,8,13	0.47	0
1	MLY	C	105	1	7,8,11	0.61	0	3,8,13	0.39	0
1	MLY	D	197	1	7,8,11	0.37	0	3,8,13	0.39	0
1	MLY	B	26	1	7,8,11	0.49	0	3,8,13	0.51	0
1	MLY	B	131	1	7,8,11	0.37	0	3,8,13	0.50	0
1	MLY	C	121	1	7,8,11	0.41	0	3,8,13	0.44	0
1	MLY	C	4	1	7,8,11	0.83	1 (14%)	3,8,13	0.39	0
1	MLY	A	316	1	7,8,11	0.46	0	3,8,13	0.53	0
1	MLY	C	133	1	9,10,11	0.42	0	6,11,13	0.81	0
1	MLY	B	137	1	7,8,11	0.37	0	3,8,13	0.40	0
1	MLY	C	264	1	7,8,11	0.53	0	3,8,13	0.29	0
1	MLY	B	55	1	9,10,11	0.63	0	6,11,13	0.47	0
1	MLY	B	240	1	7,8,11	0.71	0	3,8,13	0.28	0
1	MLY	C	322	1	7,8,11	0.23	0	3,8,13	0.64	0
1	MLY	D	15	1	9,10,11	0.46	0	6,11,13	0.72	0
1	MLY	D	137	1	9,10,11	0.42	0	6,11,13	0.61	0
1	MLY	B	15	1	7,8,11	0.44	0	3,8,13	0.45	0
1	MLY	B	114	1	7,8,11	0.53	0	3,8,13	0.40	0
1	MLY	D	264	1	7,8,11	0.29	0	3,8,13	0.38	0
1	MLY	D	26	1	9,10,11	0.64	0	6,11,13	0.59	0
1	MLY	D	4	1	7,8,11	0.33	0	3,8,13	0.49	0
1	MLY	B	5	1	7,8,11	0.50	0	3,8,13	0.34	0
1	MLY	B	121	1	7,8,11	0.56	0	3,8,13	0.36	0
1	MLY	A	26	1	9,10,11	0.51	0	6,11,13	0.72	0
1	MLY	C	240	1	7,8,11	0.59	0	3,8,13	0.33	0
1	MLY	C	316	1	7,8,11	0.53	0	3,8,13	0.46	0
1	MLY	D	289	1	7,8,11	0.52	0	3,8,13	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	240	1	9,10,11	0.57	0	6,11,13	0.49	0
1	MLY	B	60	1	7,8,11	0.42	0	3,8,13	0.36	0
1	MLY	B	286	1	7,8,11	0.54	0	3,8,13	0.35	0
1	MLY	B	314	1	7,8,11	0.51	0	3,8,13	0.30	0
1	MLY	A	121	1	7,8,11	0.59	0	3,8,13	0.65	0
1	MLY	C	197	1	7,8,11	0.38	0	3,8,13	0.49	0
1	MLY	B	133	1	7,8,11	0.48	0	3,8,13	0.45	0
1	MLY	C	327	1	7,8,11	0.42	0	3,8,13	0.46	0
1	MLY	B	194	1	9,10,11	0.51	0	6,11,13	0.42	0
1	MLY	A	60	1	9,10,11	0.58	0	6,11,13	0.30	0
1	MLY	D	194	1	9,10,11	0.65	0	6,11,13	0.50	0
1	MLY	B	316	1	7,8,11	0.46	0	3,8,13	0.39	0
1	MLY	A	289	1	7,8,11	0.51	0	3,8,13	0.39	0
1	MLY	B	243	1	7,8,11	0.51	0	3,8,13	0.36	0
1	MLY	D	204	1	7,8,11	0.51	0	3,8,13	0.40	0
1	MLY	C	114	1	7,8,11	0.50	0	3,8,13	0.36	0
1	MLY	C	221	1	7,8,11	0.54	0	3,8,13	0.47	0
1	MLY	D	221	1	7,8,11	0.40	0	3,8,13	0.61	0
1	MLY	A	327	1	7,8,11	0.52	0	3,8,13	0.31	0
1	MLY	A	7	1	7,8,11	0.75	0	3,8,13	0.54	0
1	MLY	C	7	1	7,8,11	0.72	0	3,8,13	0.50	0
1	MLY	B	56	1	9,10,11	0.68	0	6,11,13	0.60	0
1	MLY	A	204	1	7,8,11	0.68	0	3,8,13	0.09	0
1	MLY	A	221	1	7,8,11	0.53	0	3,8,13	0.37	0
1	MLY	D	131	1	7,8,11	0.49	0	3,8,13	0.48	0
1	MLY	D	133	1	7,8,11	0.36	0	3,8,13	0.43	0
1	MLY	B	197	1	7,8,11	0.40	0	3,8,13	0.42	0
1	MLY	D	55	1	7,8,11	0.81	1 (14%)	3,8,13	0.50	0
1	MLY	D	56	1	9,10,11	0.59	0	6,11,13	0.62	0
1	MLY	C	60	1	7,8,11	0.48	0	3,8,13	0.34	0
1	MLY	A	5	1	7,8,11	0.87	0	3,8,13	0.35	0
1	MLY	D	60	1	7,8,11	0.56	0	3,8,13	0.36	0
1	MLY	C	289	1	7,8,11	0.51	0	3,8,13	0.52	0
1	MLY	C	35	1	7,8,11	0.46	0	3,8,13	0.59	0
1	MLY	B	264	1	7,8,11	0.27	0	3,8,13	0.61	0
1	MLY	D	303	1	7,8,11	0.69	0	3,8,13	0.30	0
1	MLY	D	240	1	9,10,11	0.55	0	6,11,13	0.43	0
1	MLY	A	56	1	7,8,11	0.29	0	3,8,13	0.28	0
1	MLY	B	330	1	7,8,11	0.37	0	3,8,13	0.46	0
1	MLY	A	114	1	7,8,11	0.46	0	3,8,13	0.26	0
1	MLY	A	303	1	7,8,11	0.48	0	3,8,13	0.29	0
1	MLY	C	243	1	7,8,11	0.33	0	3,8,13	0.48	0
1	MLY	C	204	1	9,10,11	0.79	0	6,11,13	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	64	1	7,8,11	0.59	0	3,8,13	0.17	0
1	MLY	C	131	1	7,8,11	0.27	0	3,8,13	0.37	0
1	MLY	D	224	1	7,8,11	0.56	0	3,8,13	0.51	0
1	MLY	A	286	1	9,10,11	0.51	0	6,11,13	0.47	0
1	MLY	B	221	1	7,8,11	0.60	0	3,8,13	0.39	0
1	MLY	B	4	1	7,8,11	0.37	0	3,8,13	0.53	0
1	MLY	C	55	1	7,8,11	0.73	0	3,8,13	0.59	0
1	MLY	A	133	1	7,8,11	0.33	0	3,8,13	0.60	0
1	MLY	D	35	1	7,8,11	0.34	0	3,8,13	0.33	0
1	MLY	A	224	1	7,8,11	0.55	0	3,8,13	0.48	0
1	MLY	D	322	1	7,8,11	0.43	0	3,8,13	0.48	0
1	MLY	A	261	1	9,10,11	0.58	0	6,11,13	0.50	0
1	MLY	C	26	1	7,8,11	0.26	0	3,8,13	0.44	0
1	MLY	A	137	1	7,8,11	0.33	0	3,8,13	0.44	0
1	MLY	A	55	1	7,8,11	0.40	0	3,8,13	0.58	0
1	MLY	D	327	1	7,8,11	0.37	0	3,8,13	0.47	0
1	MLY	B	170	1	7,8,11	0.36	0	3,8,13	0.37	0
1	MLY	D	330	1	7,8,11	0.43	0	3,8,13	0.52	0
1	MLY	D	7	1	7,8,11	0.54	0	3,8,13	0.26	0
1	MLY	A	194	1	9,10,11	0.69	0	6,11,13	0.59	0
1	MLY	B	64	1	7,8,11	0.36	0	3,8,13	0.60	0
1	MLY	C	56	1	7,8,11	0.74	0	3,8,13	0.42	0
1	MLY	C	303	1	7,8,11	0.59	0	3,8,13	0.13	0
1	MLY	B	105	1	9,10,11	0.60	0	6,11,13	0.44	0
1	MLY	A	170	1	7,8,11	0.66	0	3,8,13	0.62	0
1	MLY	A	314	1	7,8,11	0.46	0	3,8,13	0.43	0
1	MLY	D	114	1	9,10,11	0.57	0	6,11,13	0.54	0
1	MLY	C	261	1	9,10,11	0.48	0	6,11,13	0.65	0
1	MLY	A	65	1	7,8,11	0.34	0	3,8,13	0.43	0
1	MLY	C	286	1	9,10,11	0.49	0	6,11,13	0.66	0
1	MLY	D	64	1	7,8,11	0.66	0	3,8,13	0.26	0
1	MLY	C	5	1	7,8,11	0.50	0	3,8,13	0.58	0
1	MLY	D	65	1	7,8,11	0.47	0	3,8,13	0.40	0
1	MLY	B	65	1	7,8,11	0.33	0	3,8,13	0.48	0
1	MLY	C	170	1	7,8,11	0.64	0	3,8,13	0.30	0
1	MLY	B	302	1	7,8,11	0.27	0	3,8,13	0.46	0
1	MLY	C	137	1	7,8,11	0.26	0	3,8,13	0.46	0
1	MLY	D	316	1	7,8,11	0.56	0	3,8,13	0.55	0
1	MLY	B	261	1	9,10,11	0.57	0	6,11,13	0.60	0
1	MLY	C	64	1	7,8,11	0.59	0	3,8,13	0.36	0
1	MLY	D	261	1	9,10,11	0.60	0	6,11,13	0.50	0
1	MLY	C	302	1	7,8,11	0.60	0	3,8,13	0.53	0
1	MLY	D	105	1	7,8,11	0.65	0	3,8,13	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	121	1	7,8,11	0.34	0	3,8,13	0.63	0
1	MLY	C	194	1	9,10,11	0.48	0	6,11,13	0.83	0
1	MLY	A	243	1	7,8,11	0.25	0	3,8,13	0.47	0
1	MLY	C	224	1	7,8,11	0.48	0	3,8,13	0.52	0
1	MLY	A	197	1	7,8,11	0.55	0	3,8,13	0.57	0
1	MLY	C	314	1	7,8,11	0.48	0	3,8,13	0.29	0
1	MLY	A	105	1	9,10,11	0.75	0	6,11,13	0.46	0
1	MLY	A	131	1	9,10,11	0.64	0	6,11,13	0.59	0
1	MLY	D	170	1	7,8,11	0.51	0	3,8,13	0.37	0
1	MLY	B	303	1	7,8,11	0.42	0	3,8,13	0.41	0
1	MLY	B	7	1	7,8,11	0.67	0	3,8,13	0.36	0
1	MLY	A	302	1	7,8,11	0.25	0	3,8,13	0.52	0
1	MLY	C	65	1	7,8,11	0.39	0	3,8,13	0.45	0
1	MLY	D	5	1	9,10,11	0.67	0	6,11,13	0.47	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	289	1	-	2/6/7/11	-
1	MLY	A	264	1	-	2/6/7/11	-
1	MLY	B	35	1	-	1/6/7/11	-
1	MLY	D	302	1	-	1/6/7/11	-
1	MLY	C	330	1	-	1/6/7/11	-
1	MLY	A	15	1	-	0/8/9/11	-
1	MLY	A	322	1	-	4/6/7/11	-
1	MLY	A	35	1	-	1/6/7/11	-
1	MLY	B	327	1	-	2/6/7/11	-
1	MLY	C	15	1	-	1/6/7/11	-
1	MLY	B	204	1	-	0/6/7/11	-
1	MLY	B	224	1	-	2/6/7/11	-
1	MLY	B	322	1	-	2/6/7/11	-
1	MLY	D	286	1	-	1/8/9/11	-
1	MLY	A	330	1	-	2/6/7/11	-
1	MLY	D	314	1	-	3/6/7/11	-
1	MLY	D	243	1	-	1/6/7/11	-
1	MLY	C	105	1	-	1/6/7/11	-
1	MLY	D	197	1	-	3/6/7/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	26	1	-	2/6/7/11	-
1	MLY	B	131	1	-	0/6/7/11	-
1	MLY	C	121	1	-	3/6/7/11	-
1	MLY	C	4	1	-	3/6/7/11	-
1	MLY	A	316	1	-	2/6/7/11	-
1	MLY	C	133	1	-	2/8/9/11	-
1	MLY	B	137	1	-	2/6/7/11	-
1	MLY	C	264	1	-	2/6/7/11	-
1	MLY	B	55	1	-	0/8/9/11	-
1	MLY	B	240	1	-	3/6/7/11	-
1	MLY	C	322	1	-	2/6/7/11	-
1	MLY	D	15	1	-	1/8/9/11	-
1	MLY	D	137	1	-	5/8/9/11	-
1	MLY	B	15	1	-	2/6/7/11	-
1	MLY	B	114	1	-	2/6/7/11	-
1	MLY	D	264	1	-	2/6/7/11	-
1	MLY	D	26	1	-	3/8/9/11	-
1	MLY	D	4	1	-	3/6/7/11	-
1	MLY	B	5	1	-	1/6/7/11	-
1	MLY	B	121	1	-	2/6/7/11	-
1	MLY	A	26	1	-	3/8/9/11	-
1	MLY	C	240	1	-	1/6/7/11	-
1	MLY	C	316	1	-	1/6/7/11	-
1	MLY	D	289	1	-	3/6/7/11	-
1	MLY	A	240	1	-	3/8/9/11	-
1	MLY	B	60	1	-	3/6/7/11	-
1	MLY	B	286	1	-	1/6/7/11	-
1	MLY	B	314	1	-	1/6/7/11	-
1	MLY	A	121	1	-	3/6/7/11	-
1	MLY	C	197	1	-	3/6/7/11	-
1	MLY	B	133	1	-	1/6/7/11	-
1	MLY	C	327	1	-	3/6/7/11	-
1	MLY	B	194	1	-	0/8/9/11	-
1	MLY	A	60	1	-	2/8/9/11	-
1	MLY	D	194	1	-	1/8/9/11	-
1	MLY	B	316	1	-	1/6/7/11	-
1	MLY	A	289	1	-	1/6/7/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	243	1	-	2/6/7/11	-
1	MLY	D	204	1	-	1/6/7/11	-
1	MLY	C	114	1	-	0/6/7/11	-
1	MLY	C	221	1	-	3/6/7/11	-
1	MLY	D	221	1	-	0/6/7/11	-
1	MLY	A	327	1	-	3/6/7/11	-
1	MLY	A	7	1	-	0/6/7/11	-
1	MLY	C	7	1	-	1/6/7/11	-
1	MLY	B	56	1	-	0/8/9/11	-
1	MLY	A	204	1	-	3/6/7/11	-
1	MLY	A	221	1	-	1/6/7/11	-
1	MLY	D	131	1	-	0/6/7/11	-
1	MLY	D	133	1	-	0/6/7/11	-
1	MLY	B	197	1	-	2/6/7/11	-
1	MLY	D	55	1	-	0/6/7/11	-
1	MLY	D	56	1	-	0/8/9/11	-
1	MLY	C	60	1	-	0/6/7/11	-
1	MLY	A	5	1	-	3/6/7/11	-
1	MLY	D	60	1	-	0/6/7/11	-
1	MLY	C	289	1	-	0/6/7/11	-
1	MLY	C	35	1	-	1/6/7/11	-
1	MLY	B	264	1	-	2/6/7/11	-
1	MLY	D	303	1	-	0/6/7/11	-
1	MLY	D	240	1	-	2/8/9/11	-
1	MLY	A	56	1	-	0/6/7/11	-
1	MLY	B	330	1	-	0/6/7/11	-
1	MLY	A	114	1	-	5/6/7/11	-
1	MLY	A	303	1	-	1/6/7/11	-
1	MLY	C	243	1	-	1/6/7/11	-
1	MLY	C	204	1	-	1/8/9/11	-
1	MLY	A	64	1	-	1/6/7/11	-
1	MLY	C	131	1	-	3/6/7/11	-
1	MLY	D	224	1	-	3/6/7/11	-
1	MLY	A	286	1	-	2/8/9/11	-
1	MLY	B	221	1	-	2/6/7/11	-
1	MLY	B	4	1	-	3/6/7/11	-
1	MLY	C	55	1	-	0/6/7/11	-
1	MLY	A	133	1	-	0/6/7/11	-
1	MLY	D	35	1	-	1/6/7/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	224	1	-	2/6/7/11	-
1	MLY	D	322	1	-	2/6/7/11	-
1	MLY	A	261	1	-	2/8/9/11	-
1	MLY	C	26	1	-	1/6/7/11	-
1	MLY	A	137	1	-	3/6/7/11	-
1	MLY	A	55	1	-	0/6/7/11	-
1	MLY	D	327	1	-	4/6/7/11	-
1	MLY	B	170	1	-	2/6/7/11	-
1	MLY	D	330	1	-	0/6/7/11	-
1	MLY	D	7	1	-	3/6/7/11	-
1	MLY	A	194	1	-	2/8/9/11	-
1	MLY	B	64	1	-	1/6/7/11	-
1	MLY	C	56	1	-	0/6/7/11	-
1	MLY	C	303	1	-	1/6/7/11	-
1	MLY	B	105	1	-	0/8/9/11	-
1	MLY	A	170	1	-	4/6/7/11	-
1	MLY	A	314	1	-	2/6/7/11	-
1	MLY	D	114	1	-	2/8/9/11	-
1	MLY	C	261	1	-	2/8/9/11	-
1	MLY	A	65	1	-	2/6/7/11	-
1	MLY	C	286	1	-	0/8/9/11	-
1	MLY	D	64	1	-	4/6/7/11	-
1	MLY	C	5	1	-	1/6/7/11	-
1	MLY	D	65	1	-	1/6/7/11	-
1	MLY	B	65	1	-	1/6/7/11	-
1	MLY	C	170	1	-	2/6/7/11	-
1	MLY	B	302	1	-	0/6/7/11	-
1	MLY	C	137	1	-	2/6/7/11	-
1	MLY	D	316	1	-	0/6/7/11	-
1	MLY	B	261	1	-	2/8/9/11	-
1	MLY	C	64	1	-	2/6/7/11	-
1	MLY	D	261	1	-	2/8/9/11	-
1	MLY	C	302	1	-	1/6/7/11	-
1	MLY	D	105	1	-	1/6/7/11	-
1	MLY	D	121	1	-	2/6/7/11	-
1	MLY	C	194	1	-	0/8/9/11	-
1	MLY	A	243	1	-	2/6/7/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	224	1	-	4/6/7/11	-
1	MLY	A	197	1	-	3/6/7/11	-
1	MLY	C	314	1	-	2/6/7/11	-
1	MLY	A	105	1	-	1/8/9/11	-
1	MLY	A	131	1	-	1/8/9/11	-
1	MLY	D	170	1	-	2/6/7/11	-
1	MLY	B	303	1	-	0/6/7/11	-
1	MLY	B	7	1	-	1/6/7/11	-
1	MLY	A	302	1	-	0/6/7/11	-
1	MLY	C	65	1	-	2/6/7/11	-
1	MLY	D	5	1	-	3/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	MLY	O-C	2.07	1.27	1.20
1	D	55	MLY	O-C	2.00	1.27	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	60	MLY	O-C-CA-CB
1	A	64	MLY	C-CA-CB-CG
1	A	114	MLY	C-CA-CB-CG
1	A	121	MLY	N-CA-CB-CG
1	A	121	MLY	C-CA-CB-CG
1	A	137	MLY	N-CA-CB-CG
1	A	137	MLY	C-CA-CB-CG
1	A	170	MLY	N-CA-CB-CG
1	A	170	MLY	C-CA-CB-CG
1	A	197	MLY	C-CA-CB-CG
1	A	197	MLY	O-C-CA-CB
1	A	224	MLY	O-C-CA-CB
1	A	240	MLY	O-C-CA-CB
1	A	243	MLY	C-CA-CB-CG
1	A	264	MLY	C-CA-CB-CG
1	A	322	MLY	O-C-CA-CB
1	B	4	MLY	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	4	MLY	C-CA-CB-CG
1	B	26	MLY	O-C-CA-CB
1	B	60	MLY	O-C-CA-CB
1	B	221	MLY	O-C-CA-CB
1	B	240	MLY	C-CA-CB-CG
1	B	322	MLY	O-C-CA-CB
1	C	137	MLY	O-C-CA-CB
1	C	197	MLY	O-C-CA-CB
1	C	224	MLY	N-CA-CB-CG
1	C	224	MLY	C-CA-CB-CG
1	C	240	MLY	O-C-CA-CB
1	C	302	MLY	O-C-CA-CB
1	C	322	MLY	C-CA-CB-CG
1	D	4	MLY	N-CA-CB-CG
1	D	4	MLY	C-CA-CB-CG
1	D	4	MLY	O-C-CA-CB
1	D	5	MLY	C-CA-CB-CG
1	D	7	MLY	N-CA-CB-CG
1	D	7	MLY	C-CA-CB-CG
1	D	26	MLY	O-C-CA-CB
1	D	137	MLY	C-CA-CB-CG
1	D	224	MLY	C-CA-CB-CG
1	D	240	MLY	O-C-CA-CB
1	D	289	MLY	C-CA-CB-CG
1	D	302	MLY	O-C-CA-CB
1	D	314	MLY	O-C-CA-CB
1	D	327	MLY	N-CA-CB-CG
1	D	327	MLY	C-CA-CB-CG
1	C	133	MLY	CD-CE-NZ-CH1
1	C	261	MLY	CD-CE-NZ-CH1
1	A	204	MLY	CE-CD-CG-CB
1	D	137	MLY	CG-CD-CE-NZ
1	A	194	MLY	CD-CE-NZ-CH2
1	C	133	MLY	CD-CE-NZ-CH2
1	D	114	MLY	CD-CE-NZ-CH2
1	D	240	MLY	CD-CE-NZ-CH1
1	D	261	MLY	CD-CE-NZ-CH1
1	B	261	MLY	CG-CD-CE-NZ
1	A	26	MLY	CG-CD-CE-NZ
1	A	261	MLY	CG-CD-CE-NZ
1	D	5	MLY	CG-CD-CE-NZ
1	A	114	MLY	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	60	MLY	CD-CE-NZ-CH2
1	D	137	MLY	CD-CE-NZ-CH1
1	D	137	MLY	CD-CE-NZ-CH2
1	D	26	MLY	CG-CD-CE-NZ
1	A	240	MLY	CD-CE-NZ-CH2
1	A	194	MLY	CG-CD-CE-NZ
1	A	204	MLY	CA-CB-CG-CD
1	A	243	MLY	CA-CB-CG-CD
1	A	289	MLY	CA-CB-CG-CD
1	C	261	MLY	CD-CE-NZ-CH2
1	D	170	MLY	CE-CD-CG-CB
1	A	114	MLY	CE-CD-CG-CB
1	A	327	MLY	CE-CD-CG-CB
1	A	65	MLY	CA-CB-CG-CD
1	B	121	MLY	CA-CB-CG-CD
1	A	26	MLY	CE-CD-CG-CB
1	A	322	MLY	CE-CD-CG-CB
1	D	289	MLY	CE-CD-CG-CB
1	A	314	MLY	CE-CD-CG-CB
1	D	105	MLY	CE-CD-CG-CB
1	D	64	MLY	CE-CD-CG-CB
1	C	264	MLY	CA-CB-CG-CD
1	B	15	MLY	CE-CD-CG-CB
1	A	197	MLY	CA-CB-CG-CD
1	B	114	MLY	CA-CB-CG-CD
1	B	4	MLY	CE-CD-CG-CB
1	D	261	MLY	CD-CE-NZ-CH2
1	D	314	MLY	CG-CD-CE-NZ
1	B	60	MLY	CA-CB-CG-CD
1	A	5	MLY	CE-CD-CG-CB
1	B	197	MLY	CA-CB-CG-CD
1	A	105	MLY	CG-CD-CE-NZ
1	D	137	MLY	CE-CD-CG-CB
1	B	114	MLY	CE-CD-CG-CB
1	B	197	MLY	CE-CD-CG-CB
1	C	170	MLY	CE-CD-CG-CB
1	A	224	MLY	CE-CD-CG-CB
1	C	121	MLY	CA-CB-CG-CD
1	C	105	MLY	CE-CD-CG-CB
1	A	286	MLY	CE-CD-CG-CB
1	B	224	MLY	CE-CD-CG-CB
1	B	327	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	286	MLY	CE-CD-CG-CB
1	A	170	MLY	CA-CB-CG-CD
1	D	322	MLY	CA-CB-CG-CD
1	A	65	MLY	CE-CD-CG-CB
1	D	224	MLY	CE-CD-CG-CB
1	C	4	MLY	CE-CD-CG-CB
1	B	322	MLY	CE-CD-CG-CB
1	C	221	MLY	CE-CD-CG-CB
1	C	65	MLY	CE-CD-CG-CB
1	C	316	MLY	CE-CD-CG-CB
1	D	26	MLY	CA-CB-CG-CD
1	B	289	MLY	CA-CB-CG-CD
1	D	194	MLY	CD-CE-NZ-CH1
1	B	221	MLY	CA-CB-CG-CD
1	C	314	MLY	CA-CB-CG-CD
1	B	5	MLY	CE-CD-CG-CB
1	A	316	MLY	CA-CB-CG-CD
1	A	327	MLY	CA-CB-CG-CD
1	C	224	MLY	CA-CB-CG-CD
1	D	314	MLY	CA-CB-CG-CD
1	B	170	MLY	CG-CD-CE-NZ
1	C	15	MLY	CG-CD-CE-NZ
1	D	243	MLY	CG-CD-CE-NZ
1	C	65	MLY	CA-CB-CG-CD
1	D	65	MLY	CA-CB-CG-CD
1	B	137	MLY	CE-CD-CG-CB
1	D	327	MLY	CE-CD-CG-CB
1	C	327	MLY	CA-CB-CG-CD
1	D	15	MLY	CG-CD-CE-NZ
1	D	64	MLY	CA-CB-CG-CD
1	B	65	MLY	CE-CD-CG-CB
1	D	204	MLY	CE-CD-CG-CB
1	B	60	MLY	CG-CD-CE-NZ
1	C	5	MLY	CG-CD-CE-NZ
1	C	7	MLY	CG-CD-CE-NZ
1	D	121	MLY	CG-CD-CE-NZ
1	A	286	MLY	C-CA-CB-CG
1	A	322	MLY	C-CA-CB-CG
1	B	7	MLY	C-CA-CB-CG
1	B	243	MLY	C-CA-CB-CG
1	B	261	MLY	C-CA-CB-CG
1	D	121	MLY	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	170	MLY	C-CA-CB-CG
1	D	264	MLY	C-CA-CB-CG
1	D	322	MLY	C-CA-CB-CG
1	C	303	MLY	CE-CD-CG-CB
1	A	261	MLY	CD-CE-NZ-CH1
1	B	243	MLY	CE-CD-CG-CB
1	C	131	MLY	CA-CB-CG-CD
1	A	314	MLY	N-CA-CB-CG
1	B	240	MLY	N-CA-CB-CG
1	C	4	MLY	N-CA-CB-CG
1	C	221	MLY	N-CA-CB-CG
1	D	224	MLY	N-CA-CB-CG
1	D	289	MLY	N-CA-CB-CG
1	C	131	MLY	CE-CD-CG-CB
1	B	121	MLY	CG-CD-CE-NZ
1	B	224	MLY	CG-CD-CE-NZ
1	C	64	MLY	CG-CD-CE-NZ
1	C	314	MLY	CG-CD-CE-NZ
1	D	64	MLY	CG-CD-CE-NZ
1	A	264	MLY	CE-CD-CG-CB
1	B	133	MLY	CE-CD-CG-CB
1	C	26	MLY	CE-CD-CG-CB
1	B	64	MLY	CE-CD-CG-CB
1	C	204	MLY	CA-CB-CG-CD
1	A	137	MLY	CG-CD-CE-NZ
1	A	221	MLY	CG-CD-CE-NZ
1	A	327	MLY	CG-CD-CE-NZ
1	A	330	MLY	CG-CD-CE-NZ
1	B	314	MLY	CG-CD-CE-NZ
1	C	131	MLY	CG-CD-CE-NZ
1	C	221	MLY	CG-CD-CE-NZ
1	C	224	MLY	CG-CD-CE-NZ
1	C	243	MLY	CG-CD-CE-NZ
1	D	7	MLY	CG-CD-CE-NZ
1	D	327	MLY	CA-CB-CG-CD
1	D	197	MLY	CA-CB-CG-CD
1	A	303	MLY	CE-CD-CG-CB
1	B	170	MLY	CE-CD-CG-CB
1	C	197	MLY	CE-CD-CG-CB
1	D	197	MLY	CE-CD-CG-CB
1	C	35	MLY	CE-CD-CG-CB
1	B	240	MLY	CG-CD-CE-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	137	MLY	CG-CD-CE-NZ
1	C	170	MLY	CG-CD-CE-NZ
1	C	264	MLY	CG-CD-CE-NZ
1	A	121	MLY	CE-CD-CG-CB
1	A	330	MLY	CE-CD-CG-CB
1	D	35	MLY	CE-CD-CG-CB
1	B	15	MLY	CG-CD-CE-NZ
1	A	170	MLY	CE-CD-CG-CB
1	B	316	MLY	CA-CB-CG-CD
1	A	5	MLY	CG-CD-CE-NZ
1	C	327	MLY	CG-CD-CE-NZ
1	C	121	MLY	CE-CD-CG-CB
1	D	286	MLY	CE-CD-CG-CB
1	C	64	MLY	CE-CD-CG-CB
1	D	114	MLY	CE-CD-CG-CB
1	A	114	MLY	CG-CD-CE-NZ
1	A	322	MLY	CG-CD-CE-NZ
1	B	264	MLY	CG-CD-CE-NZ
1	B	327	MLY	CG-CD-CE-NZ
1	C	4	MLY	CG-CD-CE-NZ
1	C	322	MLY	CG-CD-CE-NZ
1	D	264	MLY	CG-CD-CE-NZ
1	A	131	MLY	C-CA-CB-CG
1	A	204	MLY	C-CA-CB-CG
1	A	316	MLY	C-CA-CB-CG
1	B	137	MLY	C-CA-CB-CG
1	B	264	MLY	C-CA-CB-CG
1	C	121	MLY	C-CA-CB-CG
1	C	197	MLY	C-CA-CB-CG
1	C	327	MLY	C-CA-CB-CG
1	D	197	MLY	C-CA-CB-CG
1	B	35	MLY	CE-CD-CG-CB
1	D	5	MLY	CA-CB-CG-CD
1	C	330	MLY	CE-CD-CG-CB
1	A	240	MLY	CA-CB-CG-CD
1	B	289	MLY	CG-CD-CE-NZ
1	A	5	MLY	N-CA-CB-CG
1	A	26	MLY	N-CA-CB-CG
1	A	114	MLY	N-CA-CB-CG
1	B	26	MLY	N-CA-CB-CG
1	D	64	MLY	N-CA-CB-CG
1	A	35	MLY	CE-CD-CG-CB

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	26	MLY	1	0
1	A	26	MLY	1	0
1	A	289	MLY	1	0
1	A	64	MLY	1	0
1	A	286	MLY	1	0
1	A	194	MLY	1	0
1	C	261	MLY	1	0
1	C	5	MLY	1	0
1	D	105	MLY	2	0
1	B	7	MLY	1	0
1	D	5	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
2	PLP	C	401	1	15,15,16	3.01	3 (20%)	21,22,23	1.39	4 (19%)
2	PLP	B	401	1	15,15,16	2.74	3 (20%)	21,22,23	1.39	3 (14%)
2	PLP	D	401	1	15,15,16	3.04	3 (20%)	21,22,23	1.58	4 (19%)
2	PLP	A	401	1	15,15,16	2.75	4 (26%)	21,22,23	1.62	4 (19%)

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
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PLP	C3-C2	7.92	1.49	1.41
2	C	401	PLP	C3-C2	7.50	1.48	1.41
2	C	401	PLP	C5-C4	7.47	1.48	1.40
2	A	401	PLP	C5-C4	7.22	1.48	1.40
2	D	401	PLP	C5-C4	7.22	1.48	1.40
2	B	401	PLP	C5-C4	6.65	1.48	1.40
2	B	401	PLP	C3-C2	6.58	1.47	1.41
2	A	401	PLP	C3-C2	6.47	1.47	1.41
2	C	401	PLP	C3-C4	4.22	1.48	1.40
2	B	401	PLP	C3-C4	4.15	1.48	1.40
2	D	401	PLP	C3-C4	3.91	1.47	1.40
2	A	401	PLP	C3-C4	3.16	1.46	1.40
2	A	401	PLP	C4A-C4	-2.39	1.46	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLP	O3-C3-C2	3.20	124.21	117.58
2	A	401	PLP	O3-C3-C2	2.97	123.74	117.58
2	D	401	PLP	C6-N1-C2	2.75	124.19	119.20
2	A	401	PLP	C6-N1-C2	2.72	124.13	119.20
2	D	401	PLP	O4P-C5A-C5	2.68	114.39	109.36
2	A	401	PLP	O4P-C5A-C5	2.64	114.30	109.36
2	A	401	PLP	C4A-C4-C5	2.62	123.64	120.94
2	D	401	PLP	C4A-C4-C5	2.62	123.64	120.94
2	C	401	PLP	C6-C5-C4	2.60	120.23	118.10
2	B	401	PLP	C2A-C2-N1	2.31	121.99	117.64
2	B	401	PLP	C6-N1-C2	2.22	123.22	119.20
2	C	401	PLP	C6-N1-C2	2.17	123.13	119.20
2	C	401	PLP	O3P-P-O2P	2.14	115.83	107.80
2	B	401	PLP	O4P-C5A-C5	2.08	113.25	109.36
2	C	401	PLP	C4A-C4-C5	2.07	123.07	120.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	296/340 (87%)	-0.21	4 (1%) 73 75	20, 30, 47, 72	0
1	B	300/340 (88%)	0.29	11 (3%) 45 46	23, 42, 70, 92	1 (0%)
1	C	296/340 (87%)	0.02	11 (3%) 45 46	21, 35, 54, 66	0
1	D	296/340 (87%)	0.21	7 (2%) 59 61	23, 39, 61, 78	0
All	All	1188/1360 (87%)	0.08	33 (2%) 55 56	20, 36, 61, 92	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	PHE	4.7
1	D	315	VAL	4.1
1	A	315	VAL	3.8
1	C	116	ILE	3.2
1	B	232	ASP	3.1
1	B	126	LEU	3.1
1	B	125	PHE	2.9
1	B	124	GLY	2.9
1	C	315	VAL	2.9
1	C	117	LEU	2.8
1	C	202	ASN	2.8
1	C	118	VAL	2.8
1	D	202	ASN	2.7
1	A	265	CYS	2.7
1	A	335	VAL	2.6
1	C	119	SER	2.6
1	C	115	ILE	2.6
1	C	335	VAL	2.5
1	C	123	GLY	2.5
1	B	129	ILE	2.4
1	D	222	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	2.4
1	B	27	GLY	2.4
1	B	235	ILE	2.3
1	D	220	TYR	2.3
1	B	233	GLU	2.2
1	C	99	TRP	2.2
1	B	24	ASP	2.2
1	D	27	GLY	2.1
1	B	102	GLU	2.1
1	C	66	GLY	2.1
1	D	223	ALA	2.1
1	D	130	GLU	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	5	9/12	0.47	0.23	58,63,65,67	0
1	MLY	C	4	9/12	0.52	0.22	62,64,65,66	0
1	MLY	B	121	9/12	0.68	0.16	83,87,92,92	0
1	MLY	D	4	9/12	0.69	0.18	45,47,48,48	0
1	MLY	D	314	9/12	0.71	0.18	72,77,83,83	0
1	MLY	D	316	9/12	0.74	0.17	73,76,77,77	0
1	MLY	C	121	9/12	0.76	0.17	55,58,65,66	0
1	MLY	A	7	9/12	0.77	0.18	43,50,56,57	0
1	MLY	D	224	9/12	0.77	0.17	55,59,68,68	0
1	MLY	C	7	9/12	0.78	0.16	46,51,54,55	0
1	MLY	D	26	11/12	0.78	0.20	70,75,82,83	0
1	MLY	D	221	9/12	0.78	0.14	62,65,75,77	0
1	MLY	D	121	9/12	0.79	0.13	57,59,67,69	0
1	MLY	D	64	9/12	0.81	0.15	48,52,64,66	0
1	MLY	A	286	11/12	0.81	0.14	42,44,46,46	0
1	MLY	A	289	9/12	0.82	0.17	45,49,60,63	0
1	MLY	B	286	9/12	0.82	0.12	44,47,53,54	0
1	MLY	B	26	9/12	0.82	0.12	47,51,55,57	0
1	MLY	D	137	11/12	0.82	0.13	54,59,64,64	0
1	MLY	A	114	9/12	0.83	0.15	29,31,41,41	0
1	MLY	D	7	9/12	0.83	0.16	31,34,42,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	B	60	9/12	0.83	0.14	61,63,66,66	0
1	MLY	A	264	9/12	0.83	0.13	35,42,51,54	0
1	MLY	B	137	9/12	0.83	0.15	68,72,76,79	0
1	MLY	D	322	9/12	0.83	0.17	58,60,70,71	0
1	MLY	A	204	9/12	0.84	0.13	33,36,39,40	0
1	MLY	C	243	9/12	0.84	0.10	45,47,52,52	0
1	MLY	C	286	11/12	0.84	0.13	47,48,48,49	0
1	MLY	B	289	9/12	0.84	0.14	41,46,56,56	0
1	MLY	D	243	9/12	0.84	0.10	51,53,59,63	0
1	MLY	A	243	9/12	0.84	0.15	42,43,55,56	0
1	MLY	A	26	11/12	0.84	0.12	52,55,61,61	0
1	MLY	C	114	9/12	0.84	0.14	44,48,60,62	0
1	MLY	A	60	11/12	0.85	0.12	35,39,48,48	0
1	MLY	C	26	9/12	0.85	0.12	49,53,55,56	0
1	MLY	D	286	11/12	0.85	0.12	53,55,58,58	0
1	MLY	C	314	9/12	0.85	0.13	59,61,70,71	0
1	MLY	B	322	9/12	0.85	0.12	38,40,45,45	0
1	MLY	A	170	9/12	0.85	0.14	38,42,52,53	0
1	MLY	D	131	9/12	0.86	0.12	44,46,50,50	0
1	MLY	C	5	9/12	0.86	0.11	56,60,63,63	0
1	MLY	B	243	9/12	0.86	0.12	57,58,67,69	0
1	MLY	C	322	9/12	0.86	0.11	48,52,59,60	0
1	MLY	D	240	11/12	0.86	0.12	45,48,54,54	0
1	MLY	B	64	9/12	0.86	0.12	62,63,69,71	0
1	MLY	A	64	9/12	0.86	0.14	34,40,50,51	0
1	MLY	A	121	9/12	0.86	0.11	38,39,46,47	0
1	MLY	C	224	9/12	0.86	0.13	39,40,50,51	0
1	MLY	B	170	9/12	0.86	0.13	40,42,55,55	0
1	MLY	C	65	9/12	0.87	0.13	49,54,64,66	0
1	MLY	B	4	9/12	0.87	0.12	52,54,59,59	0
1	MLY	A	137	9/12	0.87	0.11	35,38,47,47	0
1	MLY	B	56	11/12	0.87	0.11	44,48,52,52	0
1	MLY	B	240	9/12	0.87	0.12	55,57,60,60	0
1	MLY	A	240	11/12	0.87	0.12	32,34,42,42	0
1	MLY	A	316	9/12	0.87	0.15	61,63,64,64	0
1	MLY	C	316	9/12	0.87	0.14	59,61,62,63	0
1	MLY	C	221	9/12	0.88	0.11	38,40,51,52	0
1	MLY	C	105	9/12	0.88	0.09	41,43,50,50	0
1	MLY	C	327	9/12	0.88	0.09	38,41,54,56	0
1	MLY	B	114	9/12	0.88	0.13	49,51,58,60	0
1	MLY	B	65	9/12	0.88	0.11	60,64,70,70	0
1	MLY	C	137	9/12	0.88	0.11	41,45,51,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	B	264	9/12	0.89	0.11	31,34,42,43	0
1	MLY	B	5	9/12	0.89	0.12	47,49,51,54	0
1	MLY	B	131	9/12	0.89	0.10	65,66,67,67	0
1	MLY	D	105	9/12	0.89	0.12	37,40,50,50	0
1	MLY	D	114	11/12	0.89	0.11	38,41,50,51	0
1	MLY	C	170	9/12	0.89	0.10	40,42,51,54	0
1	MLY	B	133	9/12	0.89	0.10	64,67,68,71	0
1	MLY	D	133	9/12	0.89	0.12	45,47,48,48	0
1	MLY	B	7	9/12	0.89	0.11	41,45,48,49	0
1	MLY	A	327	9/12	0.89	0.12	43,49,56,57	0
1	MLY	B	221	9/12	0.89	0.13	51,52,53,54	0
1	MLY	B	224	9/12	0.89	0.10	46,51,58,60	0
1	MLY	C	55	9/12	0.89	0.10	35,37,40,41	0
1	MLY	D	261	11/12	0.89	0.13	39,43,51,52	0
1	MLY	C	56	9/12	0.89	0.10	36,37,40,41	0
1	MLY	D	289	9/12	0.89	0.10	50,53,57,57	0
1	MLY	B	105	11/12	0.89	0.11	45,47,53,54	0
1	MLY	C	330	9/12	0.89	0.11	28,31,41,43	0
1	MLY	A	322	9/12	0.89	0.12	46,49,61,62	0
1	MLY	D	327	9/12	0.89	0.12	49,51,61,62	0
1	MLY	C	261	11/12	0.90	0.10	30,35,46,47	0
1	MLY	A	314	9/12	0.90	0.09	53,57,62,63	0
1	MLY	C	289	9/12	0.90	0.09	45,49,57,59	0
1	MLY	B	330	9/12	0.90	0.08	32,34,42,44	0
1	MLY	C	60	9/12	0.90	0.11	42,44,48,51	0
1	MLY	D	60	9/12	0.90	0.10	42,43,47,48	0
1	MLY	D	170	9/12	0.90	0.09	40,42,44,45	0
1	MLY	B	314	9/12	0.90	0.11	52,56,67,68	0
1	MLY	D	65	9/12	0.90	0.11	48,52,61,62	0
1	MLY	B	194	11/12	0.91	0.12	41,44,49,49	0
1	MLY	B	197	9/12	0.91	0.10	43,47,51,51	0
1	MLY	B	204	9/12	0.91	0.11	41,42,46,48	0
1	MLY	D	5	11/12	0.91	0.11	35,43,51,51	0
1	MLY	C	64	9/12	0.91	0.11	47,52,58,59	0
1	MLY	C	197	9/12	0.91	0.10	40,43,47,49	0
1	MLY	B	316	9/12	0.91	0.12	51,54,56,56	0
1	MLY	A	194	11/12	0.91	0.10	27,29,36,36	0
1	MLY	D	194	11/12	0.91	0.12	35,37,43,44	0
1	MLY	D	197	9/12	0.91	0.10	41,43,51,54	0
1	MLY	D	204	9/12	0.91	0.09	38,40,45,46	0
1	MLY	D	330	9/12	0.91	0.11	38,40,51,52	0
1	MLY	C	133	11/12	0.92	0.12	35,37,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	C	264	9/12	0.92	0.12	32,35,49,52	0
1	MLY	B	261	11/12	0.92	0.09	27,30,34,36	0
1	MLY	D	15	11/12	0.92	0.09	25,29,41,42	0
1	MLY	B	15	9/12	0.92	0.10	29,32,41,41	0
1	MLY	D	303	9/12	0.92	0.09	30,30,32,34	0
1	MLY	A	15	11/12	0.92	0.11	25,29,40,41	0
1	MLY	C	204	11/12	0.92	0.10	35,39,49,51	0
1	MLY	A	65	9/12	0.92	0.08	35,39,49,51	0
1	MLY	A	105	11/12	0.92	0.10	28,31,41,42	0
1	MLY	C	131	9/12	0.92	0.09	36,38,45,46	0
1	MLY	D	264	9/12	0.93	0.10	39,41,49,51	0
1	MLY	B	327	9/12	0.93	0.09	35,37,49,52	0
1	MLY	A	131	11/12	0.93	0.09	26,28,35,35	0
1	MLY	B	303	9/12	0.93	0.09	30,32,33,33	0
1	MLY	A	197	9/12	0.93	0.09	34,37,47,50	0
1	MLY	B	55	11/12	0.93	0.10	41,43,45,46	0
1	MLY	D	55	9/12	0.93	0.09	29,29,30,32	0
1	MLY	A	330	9/12	0.93	0.09	39,41,51,53	0
1	MLY	C	194	11/12	0.93	0.09	34,36,42,44	0
1	MLY	C	240	9/12	0.94	0.09	35,37,37,38	0
1	MLY	A	221	9/12	0.94	0.08	34,36,46,49	0
1	MLY	A	133	9/12	0.94	0.08	27,30,33,33	0
1	MLY	A	56	9/12	0.94	0.08	26,27,36,39	0
1	MLY	D	302	9/12	0.95	0.06	28,29,31,32	0
1	MLY	C	303	9/12	0.95	0.07	28,28,30,31	0
1	MLY	A	55	9/12	0.95	0.06	25,27,32,34	0
1	MLY	D	56	11/12	0.95	0.07	31,33,36,37	0
1	MLY	A	302	9/12	0.95	0.07	27,28,31,32	0
1	MLY	B	302	9/12	0.95	0.06	27,28,30,30	0
1	MLY	A	224	9/12	0.95	0.08	33,36,45,49	0
1	MLY	A	261	11/12	0.96	0.08	30,36,46,47	0
1	MLY	B	35	9/12	0.96	0.06	27,27,28,28	0
1	MLY	C	15	9/12	0.96	0.06	22,24,31,33	0
1	MLY	C	302	9/12	0.96	0.06	25,27,27,28	0
1	MLY	A	35	9/12	0.96	0.06	23,24,26,26	0
1	MLY	C	35	9/12	0.97	0.06	23,23,24,24	0
1	MLY	A	303	9/12	0.97	0.05	24,25,26,27	0
1	MLY	D	35	9/12	0.97	0.06	26,28,29,29	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	CL	C	402	1/1	0.94	0.12	48,48,48,48	0
2	PLP	D	401	15/16	0.96	0.07	31,31,32,33	0
2	PLP	B	401	15/16	0.97	0.06	33,35,36,36	0
3	CL	D	402	1/1	0.97	0.07	47,47,47,47	0
2	PLP	C	401	15/16	0.98	0.06	23,24,24,24	0
3	CL	A	402	1/1	0.98	0.05	32,32,32,32	0
2	PLP	A	401	15/16	0.99	0.05	20,20,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.