



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 05:38 AM EDT

PDB ID : 2ZZE  
Title : Crystal structure of alanyl-tRNA synthetase without oligomerization domain in lysine-methylated form  
Authors : Sokabe, M.; Ose, T.; Tokunaga, K.; Nakamura, A.; Nureki, O.; Yao, M.; Tanaka, I.  
Deposited on : 2009-02-10  
Resolution : 2.16 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](mailto: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>.

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

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

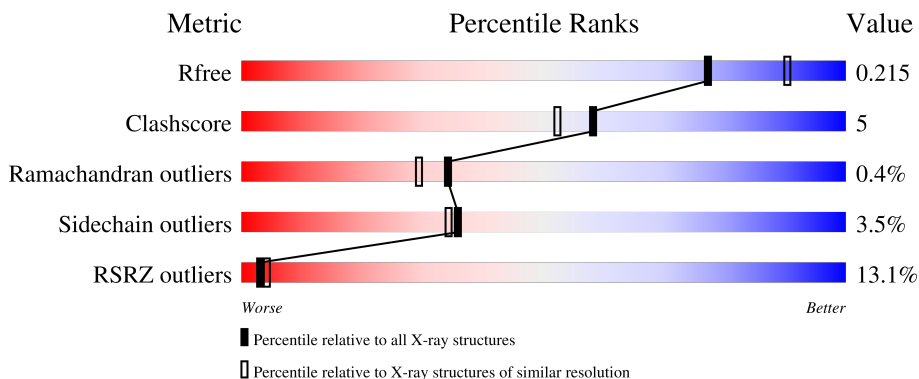
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	752	 15% 82% 14% ..
1	B	752	 10% 84% 13% ..

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	235	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13125 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 Alanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	744	6139	3977	1034	1096	32	0	3	0
1	B	744	6141	3979	1034	1096	32	0	3	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

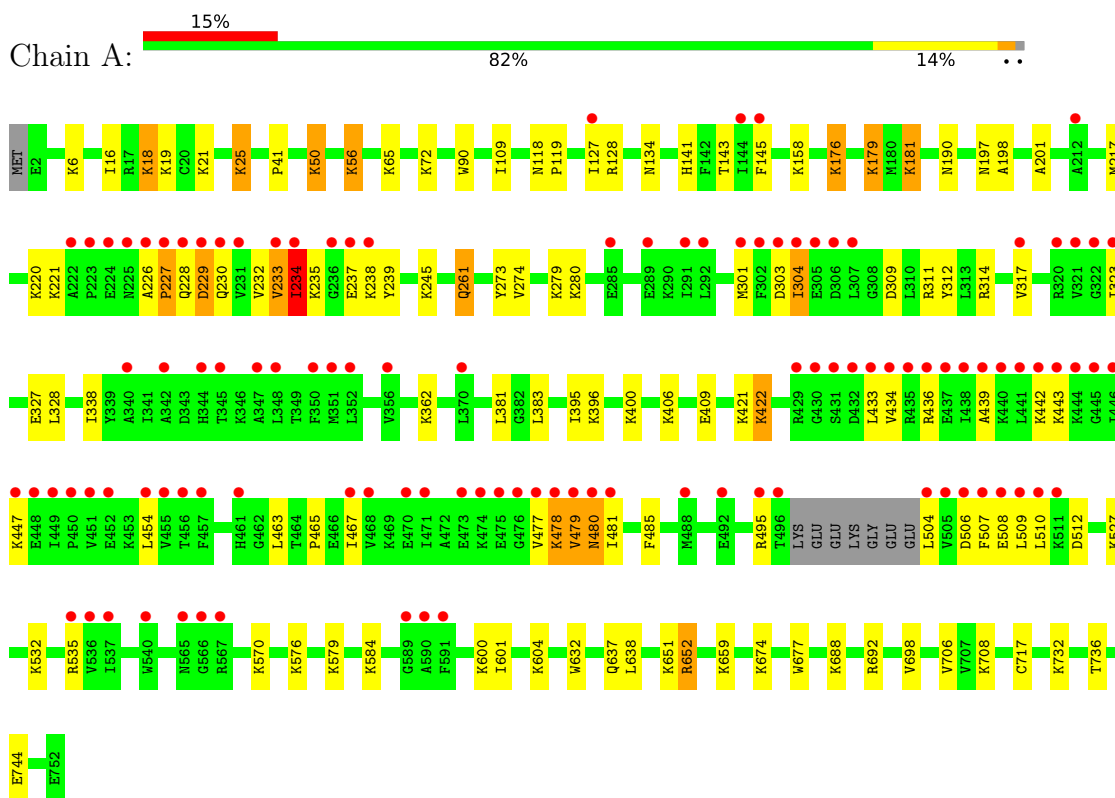
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	414	Total	O	0	0
			414	414		
3	B	429	Total	O	0	0
			429	429		

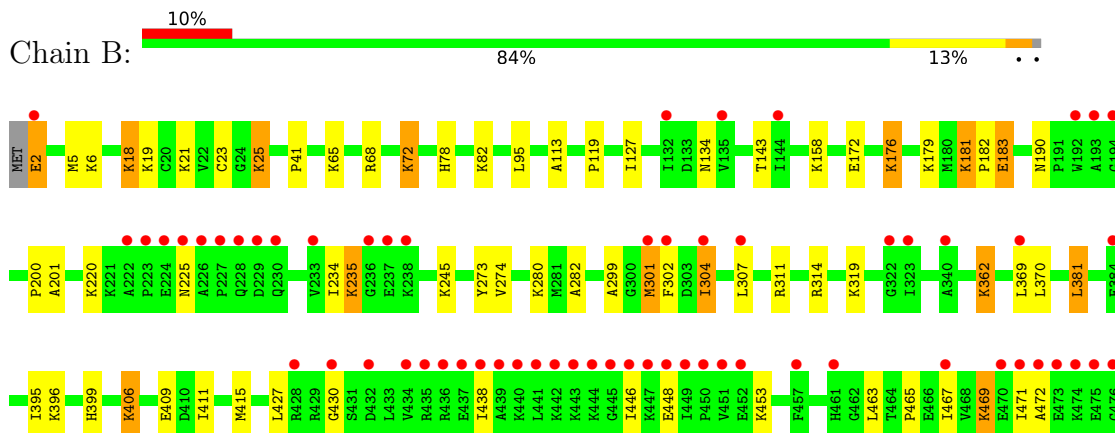
### 3 Residue-property plots [i](#)

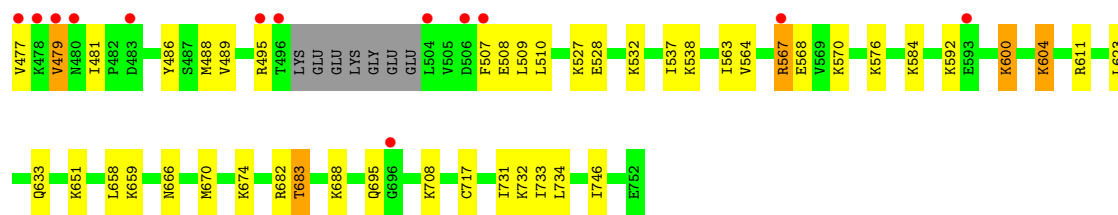
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alanyl-tRNA synthetase



- Molecule 1: Alanyl-tRNA synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.06Å 130.15Å 94.86Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	38.58 – 2.16 38.56 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.58-2.16) 98.0 (38.56-2.16)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.16Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189 , 0.227 0.217 , 0.215	Depositor DCC
$R_{free}$ test set	5053 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtrriage
Anisotropy	0.635	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/5843	0.55	0/7933
1	B	0.41	0/5843	0.53	0/7933
All	All	0.41	0/11686	0.54	0/15866

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	VAL	Peptide
1	B	508	GLU	Peptide

### 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	6139	0	6192	70	0
1	B	6141	0	6200	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	414	0	0	6	0
3	B	429	0	0	2	0
All	All	13125	0	12392	118	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 5.

All (118) 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:477:VAL:HG22	1:A:478:LYS:H	1.39	0.88
1:B:134:ASN:HD21	1:B:304:ILE:H	1.25	0.84
1:A:507:PHE:CD2	1:A:508:GLU:N	2.46	0.83
1:B:666:ASN:HD21	1:B:731:ILE:H	1.22	0.82
1:A:234:ILE:O	1:A:235:MLY:HB3	1.83	0.77
1:A:198:ALA:HB1	1:A:233:VAL:HG21	1.73	0.71
1:A:400:LYS:HG2	3:A:828:HOH:O	1.92	0.68
1:A:506:ASP:CG	1:A:507:PHE:H	1.98	0.67
1:A:652:ARG:NE	1:A:652:ARG:HA	2.10	0.66
1:B:604:MLY:HH21	1:B:611:ARG:HH22	1.59	0.66
1:A:309:ASP:HB2	1:A:312:TYR:HD2	1.61	0.65
1:B:430:GLY:HA3	1:B:463:LEU:HD21	1.80	0.63
1:A:233:VAL:HG23	1:A:234:ILE:HG23	1.82	0.62
1:B:68:ARG:HD2	1:B:72:MLY:HG2	1.82	0.61
1:A:41:PRO:HB3	1:A:301[B]:MET:HG3	1.82	0.61
1:B:486:TYR:HA	1:B:489:VAL:HG22	1.82	0.61
1:A:479:VAL:HG13	1:A:480:ASN:H	1.68	0.59
1:B:563:ILE:HG12	1:B:568:GLU:HG2	1.85	0.57
1:A:317:VAL:HG13	1:A:328:LEU:HD21	1.86	0.56
1:A:56:MLY:HH23	1:A:261:GLN:HG3	1.89	0.55
1:B:472:ALA:HB1	1:B:477:VAL:HG13	1.88	0.55
1:A:395:ILE:HD13	1:A:409:GLU:HG3	1.88	0.55
1:A:507:PHE:HD2	1:A:508:GLU:N	1.99	0.54
1:A:134:ASN:ND2	1:A:304:ILE:HG12	2.23	0.54
1:B:623:LEU:HD21	1:B:746:ILE:HD12	1.89	0.54
1:A:323:ILE:HB	1:A:327:GLU:HG3	1.90	0.54
1:A:652:ARG:HA	1:A:652:ARG:HE	1.72	0.54
1:B:564:VAL:HG13	1:B:567:ARG:HE	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:217:MET:CE	2.38	0.53
1:A:477:VAL:HG22	1:A:478:LYS:N	2.16	0.53
1:B:564:VAL:O	1:B:567:ARG:HG2	2.09	0.53
1:A:434:VAL:HG21	1:A:463:LEU:HD11	1.90	0.52
1:A:232:VAL:HG13	1:A:237:GLU:HA	1.92	0.52
1:B:411:ILE:HG22	1:B:415:MET:HE2	1.92	0.52
1:A:506:ASP:OD2	1:A:507:PHE:N	2.44	0.51
1:A:176:LYS:HE2	3:A:840:HOH:O	2.10	0.51
1:A:465:PRO:HD3	1:A:485:PHE:CE2	2.46	0.51
1:A:512:ASP:OD1	1:A:512:ASP:N	2.42	0.51
1:B:282:ALA:HB2	1:B:381:LEU:HD13	1.92	0.51
1:A:314:ARG:HA	1:A:317:VAL:HG12	1.93	0.51
1:A:25:MLY:HH23	1:A:190:ASN:OD1	2.10	0.50
1:A:127:ILE:HA	1:A:143:THR:O	2.11	0.50
1:A:237:GLU:O	1:A:239:TYR:CD1	2.64	0.50
1:A:507:PHE:C	1:A:509:LEU:H	2.14	0.50
1:B:467:ILE:O	1:B:471:ILE:HG12	2.12	0.50
1:A:506:ASP:CG	1:A:507:PHE:N	2.64	0.49
1:A:477:VAL:CG2	1:A:478:LYS:H	2.17	0.49
1:B:2:GLU:N	3:B:842:HOH:O	2.46	0.49
1:A:465:PRO:HB2	1:A:481:ILE:HG12	1.95	0.49
1:B:282:ALA:CB	1:B:381:LEU:HD13	2.43	0.48
1:B:395:ILE:HD13	1:B:409:GLU:HG3	1.94	0.48
1:A:652:ARG:NE	1:A:744:GLU:OE1	2.46	0.48
1:B:438:ILE:HD12	1:B:472:ALA:HA	1.95	0.48
1:B:469:MLY:HG3	1:B:479:VAL:HG22	1.94	0.48
1:A:197:ASN:HB3	1:A:217:MET:HE3	1.96	0.48
1:A:233:VAL:HB	1:A:234:ILE:HG22	1.96	0.48
1:B:41:PRO:HB3	1:B:301[B]:MET:HG3	1.96	0.48
1:B:113:ALA:HB1	1:B:683:THR:HG23	1.95	0.47
1:B:299:ALA:HA	1:B:302:PHE:HB2	1.97	0.47
1:A:134:ASN:ND2	1:A:304:ILE:CG1	2.78	0.47
1:A:400:LYS:HG3	3:A:785:HOH:O	2.16	0.46
1:B:633:GLN:H	1:B:695:GLN:NE2	2.14	0.46
1:B:666:ASN:ND2	1:B:731:ILE:H	2.03	0.46
1:B:172:GLU:HG3	1:B:176:LYS:HG3	1.98	0.46
1:A:109:ILE:HD13	1:A:217:MET:HE1	1.97	0.46
1:A:226:ALA:HA	1:A:227:PRO:HD3	1.79	0.46
1:A:632:TRP:CH2	1:A:692:ARG:HA	2.51	0.46
1:B:68:ARG:HD2	1:B:72:MLY:CG	2.44	0.46
1:A:228:GLN:HG3	1:A:229:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MLY:HH23	3:A:1015:HOH:O	2.15	0.46
1:B:528:GLU:CD	1:B:600:MLY:HE2	2.37	0.46
1:B:78:HIS:CD2	1:B:119:PRO:HB2	2.52	0.45
1:A:134:ASN:HB3	1:A:141:HIS:CD2	2.51	0.45
1:B:95:LEU:HD22	1:B:362:MLY:HB2	1.97	0.45
1:A:479:VAL:CG2	1:A:481:ILE:HG13	2.46	0.45
1:A:128:ARG:HG3	1:A:145:PHE:HE2	1.80	0.45
1:A:234:ILE:O	1:A:235:MLY:CB	2.61	0.45
1:B:5:MET:HE3	1:B:200:PRO:HB2	1.99	0.45
1:B:234:ILE:HG22	1:B:235:MLY:HG3	1.98	0.45
1:B:682:ARG:HD3	3:B:1025:HOH:O	2.17	0.45
1:A:50:LYS:HA	1:A:50:LYS:HD2	1.77	0.44
1:A:16:ILE:HG21	1:A:18:MLY:HH23	1.99	0.44
1:A:637:GLN:NE2	3:A:1035:HOH:O	2.50	0.44
1:B:319:LYS:N	1:B:319:LYS:HD2	2.32	0.44
1:A:176:LYS:HA	1:A:179:MLY:HH13	2.00	0.44
1:A:134:ASN:HD21	1:A:304:ILE:CG1	2.31	0.43
1:A:232:VAL:HG13	1:A:237:GLU:HG2	2.00	0.43
1:A:237:GLU:HB3	1:A:238:LYS:H	1.50	0.43
1:A:439:ALA:O	1:A:443:LYS:HB2	2.19	0.43
1:B:369:LEU:C	1:B:369:LEU:HD23	2.39	0.43
1:B:623:LEU:HD21	1:B:746:ILE:CD1	2.49	0.43
1:B:273:TYR:CD1	1:B:274:VAL:HG23	2.54	0.43
1:A:677:TRP:HA	1:A:706:VAL:O	2.18	0.42
1:A:433:LEU:HA	1:A:436:ARG:HE	1.85	0.42
1:A:338:ILE:HG13	1:A:381:LEU:HD11	2.01	0.42
1:A:233:VAL:HB	1:A:234:ILE:CG2	2.49	0.42
1:B:183:GLU:H	1:B:183:GLU:CD	2.23	0.42
1:A:90:TRP:O	1:A:698:VAL:HG11	2.20	0.42
1:A:190:ASN:O	1:A:201:ALA:HB3	2.19	0.42
1:B:411:ILE:HG22	1:B:415:MET:CE	2.48	0.42
1:B:127:ILE:HA	1:B:143:THR:O	2.20	0.42
1:A:463:LEU:HD12	1:A:467:ILE:HG22	2.02	0.41
1:A:652:ARG:HH22	1:A:736:THR:HG23	1.84	0.41
1:B:95:LEU:HD21	1:B:362:MLY:HH23	2.01	0.41
1:A:228:GLN:HG3	1:A:229:ASP:N	2.35	0.41
1:B:399:HIS:HB2	1:B:406:MLY:HB3	2.03	0.41
1:A:317:VAL:HG13	1:A:328:LEU:CD2	2.50	0.41
1:A:422:MLY:HE2	3:A:951:HOH:O	2.20	0.41
1:B:510:LEU:HD21	1:B:537:ILE:HD12	2.03	0.41
1:B:465:PRO:HB2	1:B:481:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:CB	1:A:217:MET:CE	2.99	0.41
1:B:18:MLY:HH12	1:B:18:MLY:HD2	1.84	0.41
1:B:190:ASN:O	1:B:201:ALA:HB3	2.21	0.41
1:A:273:TYR:CD1	1:A:274:VAL:HG23	2.56	0.40
1:A:118:ASN:HA	1:A:119:PRO:HA	1.94	0.40
1:B:23:CYS:SG	1:B:25:MLY:HB3	2.62	0.40
1:B:181:MLY:HA	1:B:182:PRO:HD3	1.96	0.40
1:B:658:LEU:HG	1:B:733:ILE:HG21	2.03	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	702/752 (93%)	679 (97%)	19 (3%)	4 (1%)	25 18
1	B	702/752 (93%)	686 (98%)	14 (2%)	2 (0%)	41 37
All	All	1404/1504 (93%)	1365 (97%)	33 (2%)	6 (0%)	34 29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	PRO
1	A	234	ILE
1	A	478	LYS
1	B	448	GLU
1	B	446	ILE
1	A	479	VAL

### 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	610/614 (99%)	588 (96%)	22 (4%)	35	33
1	B	610/614 (99%)	587 (96%)	23 (4%)	33	31
All	All	1220/1228 (99%)	1175 (96%)	45 (4%)	36	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	176	LYS
1	A	229	ASP
1	A	230	GLN
1	A	234	ILE
1	A	261	GLN
1	A	303	ASP
1	A	304	ILE
1	A	311	ARG
1	A	383	LEU
1	A	421	LYS
1	A	442	LYS
1	A	447	LYS
1	A	454	LEU
1	A	480	ASN
1	A	495	ARG
1	A	504	LEU
1	A	510	LEU
1	A	535	ARG
1	A	601	ILE
1	A	638	LEU
1	A	652	ARG
1	B	2	GLU
1	B	176	LYS
1	B	183	GLU
1	B	225	ASN
1	B	301[A]	MET

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Mol	Chain	Res	Type
1	B	301[B]	MET
1	B	304	ILE
1	B	307	LEU
1	B	311	ARG
1	B	314	ARG
1	B	370	LEU
1	B	381	LEU
1	B	427	LEU
1	B	479	VAL
1	B	488[A]	MET
1	B	488[B]	MET
1	B	495	ARG
1	B	507	PHE
1	B	509	LEU
1	B	567	ARG
1	B	670	MET
1	B	683	THR
1	B	734	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	141	HIS
1	A	565	ASN
1	A	608	GLN
1	A	633	GLN
1	A	740	GLN
1	B	134	ASN
1	B	608	GLN
1	B	666	ASN
1	B	687	GLN
1	B	695	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

82 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	406	1	9,10,11	0.52	0	6,11,13	2.37	4 (66%)
1	MLY	A	181	1	9,10,11	0.37	0	6,11,13	2.08	2 (33%)
1	MLY	B	56	1	7,8,11	0.47	0	3,8,13	0.32	0
1	MLY	A	220	1	9,10,11	0.46	0	6,11,13	2.25	3 (50%)
1	MLY	A	18	1	9,10,11	0.51	0	6,11,13	2.29	2 (33%)
1	MLY	A	708	1	9,10,11	0.50	0	6,11,13	2.04	2 (33%)
1	MLY	B	158	1	9,10,11	0.36	0	6,11,13	2.46	4 (66%)
1	MLY	A	688	1	9,10,11	0.47	0	6,11,13	2.15	3 (50%)
1	MLY	B	362	1	9,10,11	0.30	0	6,11,13	2.32	4 (66%)
1	MLY	A	82	1	7,8,11	0.61	0	3,8,13	0.06	0
1	MLY	A	279	1	9,10,11	0.42	0	6,11,13	2.28	3 (50%)
1	MLY	B	584	1	9,10,11	0.45	0	6,11,13	2.29	3 (50%)
1	MLY	B	220	1	9,10,11	0.42	0	6,11,13	2.15	2 (33%)
1	MLY	B	453	1	9,10,11	0.41	0	6,11,13	2.27	4 (66%)
1	MLY	A	674	1	9,10,11	0.39	0	6,11,13	2.32	4 (66%)
1	MLY	A	579	1	9,10,11	0.44	0	6,11,13	2.41	4 (66%)
1	MLY	B	469	1	9,10,11	0.39	0	6,11,13	2.32	4 (66%)
1	MLY	A	235	1	7,8,11	0.59	0	3,8,13	0.48	0
1	MLY	A	659	1	9,10,11	0.42	0	6,11,13	2.30	4 (66%)
1	MLY	B	6	1	9,10,11	0.53	0	6,11,13	2.29	4 (66%)
1	MLY	A	732	1	9,10,11	0.49	0	6,11,13	2.16	3 (50%)
1	MLY	B	280	1	9,10,11	0.40	0	6,11,13	2.43	4 (66%)
1	MLY	B	532	1	9,10,11	0.46	0	6,11,13	2.12	3 (50%)
1	OCS	A	717	1	7,8,9	1.00	0	6,11,13	2.24	1 (16%)
1	MLY	A	221	1	9,10,11	0.39	0	6,11,13	2.21	3 (50%)
1	MLY	B	708	1	9,10,11	0.45	0	6,11,13	2.14	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	21	1	9,10,11	0.43	0	6,11,13	2.30	4 (66%)
1	MLY	B	21	1	9,10,11	0.41	0	6,11,13	2.15	2 (33%)
1	MLY	B	732	1	9,10,11	0.46	0	6,11,13	2.09	2 (33%)
1	MLY	A	362	1	9,10,11	0.38	0	6,11,13	2.21	3 (50%)
1	MLY	A	396	1	9,10,11	0.42	0	6,11,13	2.20	3 (50%)
1	MLY	B	245	1	9,10,11	0.43	0	6,11,13	2.39	4 (66%)
1	MLY	B	422	1	7,8,11	0.52	0	3,8,13	0.24	0
1	MLY	A	25	1	9,10,11	0.45	0	6,11,13	2.19	4 (66%)
1	OCS	B	717	1	7,8,9	1.11	0	6,11,13	1.83	2 (33%)
1	MLY	B	527	1	9,10,11	0.35	0	6,11,13	2.28	4 (66%)
1	MLY	B	674	1	9,10,11	0.42	0	6,11,13	2.24	3 (50%)
1	MLY	B	659	1	9,10,11	0.34	0	6,11,13	2.26	3 (50%)
1	MLY	A	592	1	7,8,11	0.49	0	3,8,13	0.30	0
1	MLY	B	65	1	9,10,11	0.40	0	6,11,13	2.26	3 (50%)
1	MLY	B	538	1	9,10,11	0.34	0	6,11,13	2.22	3 (50%)
1	MLY	A	19	1	9,10,11	0.49	0	6,11,13	2.22	3 (50%)
1	MLY	A	245	1	9,10,11	0.44	0	6,11,13	2.29	3 (50%)
1	MLY	A	72	1	9,10,11	0.39	0	6,11,13	2.31	4 (66%)
1	MLY	B	235	1	9,10,11	0.43	0	6,11,13	2.26	3 (50%)
1	MLY	A	600	1	9,10,11	0.42	0	6,11,13	2.24	4 (66%)
1	MLY	B	181	1	9,10,11	0.44	0	6,11,13	2.09	2 (33%)
1	MLY	B	19	1	9,10,11	0.52	0	6,11,13	2.34	4 (66%)
1	MLY	A	280	1	9,10,11	0.41	0	6,11,13	2.36	4 (66%)
1	MLY	A	469	1	7,8,11	0.50	0	3,8,13	0.39	0
1	MLY	B	221	1	7,8,11	0.47	0	3,8,13	0.53	0
1	MLY	A	570	1	9,10,11	0.47	0	6,11,13	2.32	4 (66%)
1	MLY	A	651	1	9,10,11	0.48	0	6,11,13	2.06	2 (33%)
1	MLY	A	406	1	9,10,11	0.43	0	6,11,13	2.31	4 (66%)
1	MLY	A	538	1	7,8,11	0.63	0	3,8,13	0.28	0
1	MLY	A	6	1	9,10,11	0.49	0	6,11,13	2.19	3 (50%)
1	MLY	B	18	1	9,10,11	0.47	0	6,11,13	2.23	2 (33%)
1	MLY	A	584	1	9,10,11	0.40	0	6,11,13	2.31	4 (66%)
1	MLY	B	82	1	9,10,11	0.45	0	6,11,13	2.25	4 (66%)
1	MLY	B	592	1	9,10,11	0.38	0	6,11,13	2.17	3 (50%)
1	MLY	A	56	1	9,10,11	0.44	0	6,11,13	2.39	4 (66%)
1	MLY	B	179	1	9,10,11	0.32	0	6,11,13	2.48	4 (66%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	579	1	7,8,11	0.56	0	3,8,13	0.30	0
1	MLY	A	422	1	9,10,11	0.40	0	6,11,13	2.42	4 (66%)
1	MLY	A	604	1	9,10,11	0.41	0	6,11,13	2.22	4 (66%)
1	MLY	A	158	1	9,10,11	0.40	0	6,11,13	2.08	3 (50%)
1	MLY	A	65	1	9,10,11	0.37	0	6,11,13	2.25	4 (66%)
1	MLY	A	453	1	7,8,11	0.51	0	3,8,13	0.18	0
1	MLY	A	527	1	9,10,11	0.40	0	6,11,13	2.25	4 (66%)
1	MLY	B	25	1	9,10,11	0.60	0	6,11,13	2.48	4 (66%)
1	MLY	A	532	1	9,10,11	0.44	0	6,11,13	2.33	4 (66%)
1	MLY	B	72	1	9,10,11	0.38	0	6,11,13	2.28	4 (66%)
1	MLY	B	600	1	9,10,11	0.39	0	6,11,13	2.24	3 (50%)
1	MLY	B	651	1	9,10,11	0.43	0	6,11,13	2.12	2 (33%)
1	MLY	B	604	1	9,10,11	0.49	0	6,11,13	2.06	2 (33%)
1	MLY	A	179	1	9,10,11	0.39	0	6,11,13	2.53	4 (66%)
1	MLY	B	279	1	7,8,11	0.51	0	3,8,13	0.21	0
1	MLY	B	570	1	9,10,11	0.48	0	6,11,13	2.11	3 (50%)
1	MLY	B	688	1	9,10,11	0.43	0	6,11,13	2.36	4 (66%)
1	MLY	B	576	1	9,10,11	0.50	0	6,11,13	2.34	4 (66%)
1	MLY	A	576	1	9,10,11	0.45	0	6,11,13	2.29	4 (66%)
1	MLY	B	396	1	9,10,11	0.43	0	6,11,13	2.24	4 (66%)

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	406	1	-	5/8/9/11	-
1	MLY	A	181	1	-	2/8/9/11	-
1	MLY	B	56	1	-	1/6/7/11	-
1	MLY	A	220	1	-	2/8/9/11	-
1	MLY	A	18	1	-	3/8/9/11	-
1	MLY	A	708	1	-	1/8/9/11	-
1	MLY	B	158	1	-	3/8/9/11	-
1	MLY	A	688	1	-	6/8/9/11	-
1	MLY	B	362	1	-	5/8/9/11	-
1	MLY	A	82	1	-	2/6/7/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	279	1	-	1/8/9/11	-
1	MLY	B	584	1	-	3/8/9/11	-
1	MLY	B	220	1	-	1/8/9/11	-
1	MLY	B	453	1	-	3/8/9/11	-
1	MLY	A	674	1	-	2/8/9/11	-
1	MLY	A	579	1	-	2/8/9/11	-
1	MLY	B	469	1	-	4/8/9/11	-
1	MLY	A	235	1	-	2/6/7/11	-
1	MLY	A	659	1	-	1/8/9/11	-
1	MLY	B	6	1	-	3/8/9/11	-
1	MLY	A	732	1	-	1/8/9/11	-
1	MLY	B	280	1	-	2/8/9/11	-
1	MLY	B	532	1	-	2/8/9/11	-
1	OCS	A	717	1	-	3/4/7/9	-
1	MLY	A	221	1	-	2/8/9/11	-
1	MLY	B	708	1	-	1/8/9/11	-
1	MLY	A	21	1	-	4/8/9/11	-
1	MLY	B	21	1	-	1/8/9/11	-
1	MLY	B	732	1	-	3/8/9/11	-
1	MLY	A	362	1	-	3/8/9/11	-
1	MLY	A	396	1	-	1/8/9/11	-
1	MLY	B	245	1	-	1/8/9/11	-
1	MLY	B	422	1	-	3/6/7/11	-
1	MLY	A	25	1	-	3/8/9/11	-
1	OCS	B	717	1	-	1/4/7/9	-
1	MLY	B	527	1	-	3/8/9/11	-
1	MLY	B	674	1	-	4/8/9/11	-
1	MLY	B	659	1	-	2/8/9/11	-
1	MLY	A	592	1	-	0/6/7/11	-
1	MLY	B	65	1	-	1/8/9/11	-
1	MLY	B	538	1	-	3/8/9/11	-
1	MLY	A	19	1	-	2/8/9/11	-
1	MLY	A	245	1	-	2/8/9/11	-
1	MLY	A	72	1	-	3/8/9/11	-
1	MLY	B	235	1	-	5/8/9/11	-
1	MLY	A	600	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	181	1	-	1/8/9/11	-
1	MLY	B	19	1	-	1/8/9/11	-
1	MLY	A	280	1	-	2/8/9/11	-
1	MLY	A	469	1	-	1/6/7/11	-
1	MLY	B	221	1	-	0/6/7/11	-
1	MLY	A	570	1	-	4/8/9/11	-
1	MLY	A	651	1	-	1/8/9/11	-
1	MLY	A	406	1	-	3/8/9/11	-
1	MLY	A	538	1	-	2/6/7/11	-
1	MLY	A	6	1	-	2/8/9/11	-
1	MLY	B	18	1	-	3/8/9/11	-
1	MLY	A	584	1	-	3/8/9/11	-
1	MLY	B	82	1	-	6/8/9/11	-
1	MLY	B	592	1	-	6/8/9/11	-
1	MLY	A	56	1	-	3/8/9/11	-
1	MLY	B	179	1	-	1/8/9/11	-
1	MLY	B	579	1	-	2/6/7/11	-
1	MLY	A	422	1	-	5/8/9/11	-
1	MLY	A	604	1	-	3/8/9/11	-
1	MLY	A	158	1	-	1/8/9/11	-
1	MLY	A	65	1	-	2/8/9/11	-
1	MLY	A	453	1	-	0/6/7/11	-
1	MLY	A	527	1	-	5/8/9/11	-
1	MLY	B	25	1	-	3/8/9/11	-
1	MLY	A	532	1	-	2/8/9/11	-
1	MLY	B	72	1	-	4/8/9/11	-
1	MLY	B	600	1	-	1/8/9/11	-
1	MLY	B	651	1	-	1/8/9/11	-
1	MLY	B	604	1	-	5/8/9/11	-
1	MLY	A	179	1	-	1/8/9/11	-
1	MLY	B	279	1	-	2/6/7/11	-
1	MLY	B	570	1	-	1/8/9/11	-
1	MLY	B	688	1	-	4/8/9/11	-
1	MLY	B	576	1	-	4/8/9/11	-
1	MLY	A	576	1	-	2/8/9/11	-
1	MLY	B	396	1	-	3/8/9/11	-

There are no bond length outliers.

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	OCS	OD3-SG-CB	4.83	112.67	106.94
1	B	25	MLY	CH2-NZ-CH1	4.32	120.91	109.73
1	B	245	MLY	CH2-NZ-CH1	4.06	120.23	109.73
1	B	600	MLY	CH2-NZ-CH1	4.03	120.15	109.73
1	B	659	MLY	CH2-NZ-CH1	3.98	120.03	109.73
1	A	18	MLY	CH2-NZ-CH1	3.95	119.95	109.73
1	B	179	MLY	CH2-NZ-CH1	3.93	119.89	109.73
1	A	72	MLY	CH2-NZ-CH1	3.92	119.88	109.73
1	B	362	MLY	CH2-NZ-CH1	3.91	119.83	109.73
1	A	659	MLY	CH2-NZ-CH1	3.89	119.80	109.73
1	A	179	MLY	CH2-NZ-CH1	3.89	119.79	109.73
1	A	56	MLY	CH2-NZ-CH1	3.89	119.78	109.73
1	A	576	MLY	CH2-NZ-CH1	3.88	119.75	109.73
1	A	579	MLY	CH2-NZ-CH1	3.88	119.75	109.73
1	B	688	MLY	CH2-NZ-CH1	3.87	119.75	109.73
1	B	584	MLY	CH2-NZ-CH1	3.86	119.71	109.73
1	A	220	MLY	CH2-NZ-CH1	3.83	119.64	109.73
1	A	279	MLY	CH2-NZ-CH1	3.82	119.61	109.73
1	B	406	MLY	CH2-NZ-CH1	3.82	119.60	109.73
1	B	674	MLY	CH2-NZ-CH1	3.81	119.57	109.73
1	B	469	MLY	CH2-NZ-CH1	3.81	119.57	109.73
1	A	245	MLY	CH2-NZ-CH1	3.80	119.56	109.73
1	A	527	MLY	CH2-NZ-CH1	3.80	119.56	109.73
1	B	235	MLY	CH2-NZ-CH1	3.80	119.55	109.73
1	B	65	MLY	CH2-NZ-CH1	3.79	119.54	109.73
1	B	18	MLY	CH2-NZ-CH1	3.78	119.51	109.73
1	A	280	MLY	CH2-NZ-CH1	3.77	119.49	109.73
1	A	362	MLY	CH2-NZ-CH1	3.76	119.44	109.73
1	A	65	MLY	CH2-NZ-CH1	3.74	119.41	109.73
1	B	453	MLY	CH2-NZ-CH1	3.73	119.37	109.73
1	A	406	MLY	CH2-NZ-CH1	3.72	119.35	109.73
1	B	158	MLY	CH2-NZ-CH1	3.72	119.34	109.73
1	B	72	MLY	CH2-NZ-CH1	3.72	119.34	109.73
1	A	732	MLY	CH2-NZ-CH1	3.71	119.33	109.73
1	A	570	MLY	CH2-NZ-CH1	3.70	119.30	109.73
1	A	532	MLY	CH2-NZ-CH1	3.70	119.30	109.73
1	A	584	MLY	CH2-NZ-CH1	3.69	119.27	109.73
1	A	600	MLY	CH2-NZ-CH1	3.68	119.25	109.73
1	B	576	MLY	CH2-NZ-CH1	3.68	119.25	109.73
1	A	422	MLY	CH2-NZ-CH1	3.67	119.22	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	MLY	CH2-NZ-CH1	3.67	119.22	109.73
1	A	674	MLY	CH2-NZ-CH1	3.65	119.17	109.73
1	A	604	MLY	CH2-NZ-CH1	3.64	119.15	109.73
1	A	221	MLY	CH2-NZ-CH1	3.64	119.13	109.73
1	A	396	MLY	CH2-NZ-CH1	3.63	119.12	109.73
1	B	396	MLY	CH2-NZ-CH1	3.62	119.10	109.73
1	B	708	MLY	CH2-NZ-CH1	3.62	119.09	109.73
1	B	19	MLY	CH2-NZ-CH1	3.61	119.07	109.73
1	B	82	MLY	CH2-NZ-CH1	3.60	119.03	109.73
1	B	6	MLY	CH2-NZ-CH1	3.59	119.00	109.73
1	B	538	MLY	CH2-NZ-CH1	3.58	118.98	109.73
1	A	21	MLY	CH2-NZ-CH1	3.57	118.96	109.73
1	A	6	MLY	CH2-NZ-CH1	3.57	118.95	109.73
1	B	527	MLY	CH2-NZ-CH1	3.55	118.90	109.73
1	A	688	MLY	CH2-NZ-CH1	3.52	118.84	109.73
1	B	21	MLY	CH2-NZ-CH1	3.49	118.76	109.73
1	B	592	MLY	CH2-NZ-CH1	3.49	118.75	109.73
1	B	220	MLY	CH2-NZ-CH1	3.44	118.62	109.73
1	A	19	MLY	CH2-NZ-CH1	3.42	118.58	109.73
1	B	570	MLY	CH2-NZ-CH1	3.39	118.50	109.73
1	B	732	MLY	CH2-NZ-CH1	3.39	118.50	109.73
1	B	651	MLY	CH2-NZ-CH1	3.38	118.47	109.73
1	A	651	MLY	CH1-NZ-CE	3.34	123.97	110.74
1	A	25	MLY	CH2-NZ-CH1	3.33	118.34	109.73
1	B	532	MLY	CH2-NZ-CH1	3.32	118.32	109.73
1	B	181	MLY	CH2-NZ-CH1	3.31	118.28	109.73
1	B	604	MLY	CH1-NZ-CE	3.28	123.73	110.74
1	B	651	MLY	CH2-NZ-CE	3.28	123.73	110.74
1	B	604	MLY	CH2-NZ-CH1	3.28	118.20	109.73
1	A	179	MLY	CD-CE-NZ	-3.28	104.92	113.79
1	A	708	MLY	CH2-NZ-CH1	3.27	118.19	109.73
1	A	181	MLY	CH2-NZ-CH1	3.26	118.17	109.73
1	B	181	MLY	CH1-NZ-CE	3.22	123.50	110.74
1	B	717	OCS	OD3-SG-CB	3.21	110.75	106.94
1	A	181	MLY	CH1-NZ-CE	3.19	123.39	110.74
1	A	708	MLY	CH1-NZ-CE	3.14	123.16	110.74
1	B	220	MLY	CH1-NZ-CE	3.12	123.12	110.74
1	A	158	MLY	CH2-NZ-CE	3.11	123.06	110.74
1	B	158	MLY	CD-CE-NZ	-3.10	105.39	113.79
1	B	708	MLY	CH1-NZ-CE	3.09	122.99	110.74
1	B	732	MLY	CH1-NZ-CE	3.09	122.98	110.74
1	B	21	MLY	CH1-NZ-CE	3.06	122.87	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	MLY	CH2-NZ-CH1	3.03	117.57	109.73
1	B	179	MLY	CD-CE-NZ	-3.01	105.64	113.79
1	A	19	MLY	CH1-NZ-CE	3.00	122.62	110.74
1	A	158	MLY	CH2-NZ-CH1	3.00	117.48	109.73
1	B	532	MLY	CH2-NZ-CE	2.99	122.59	110.74
1	B	18	MLY	CH1-NZ-CE	2.99	122.56	110.74
1	A	422	MLY	CD-CE-NZ	-2.97	105.74	113.79
1	B	570	MLY	CH1-NZ-CE	2.96	122.47	110.74
1	A	245	MLY	CH1-NZ-CE	2.94	122.40	110.74
1	B	538	MLY	CH2-NZ-CE	2.93	122.35	110.74
1	B	280	MLY	CD-CE-NZ	-2.92	105.88	113.79
1	A	18	MLY	CH1-NZ-CE	2.89	122.19	110.74
1	A	688	MLY	CH2-NZ-CE	2.88	122.16	110.74
1	B	19	MLY	CH2-NZ-CE	2.88	122.16	110.74
1	A	396	MLY	CH2-NZ-CE	2.84	121.97	110.74
1	A	25	MLY	CH2-NZ-CE	2.80	121.83	110.74
1	A	579	MLY	CD-CE-NZ	-2.76	106.32	113.79
1	B	82	MLY	CH2-NZ-CE	2.75	121.61	110.74
1	A	21	MLY	CH1-NZ-CE	2.74	121.61	110.74
1	A	279	MLY	CH1-NZ-CE	2.73	121.54	110.74
1	A	732	MLY	CH2-NZ-CE	2.71	121.47	110.74
1	A	600	MLY	CH2-NZ-CE	2.71	121.47	110.74
1	A	65	MLY	CH1-NZ-CE	2.71	121.46	110.74
1	A	72	MLY	CH2-NZ-CE	2.70	121.44	110.74
1	A	604	MLY	CH1-NZ-CE	2.70	121.42	110.74
1	B	717	OCS	OD2-SG-CB	2.68	110.01	105.74
1	B	527	MLY	CH2-NZ-CE	2.66	121.27	110.74
1	B	72	MLY	CH1-NZ-CE	2.63	121.15	110.74
1	A	6	MLY	CH2-NZ-CE	2.62	121.14	110.74
1	A	280	MLY	CD-CE-NZ	-2.62	106.69	113.79
1	B	235	MLY	CH2-NZ-CE	2.62	121.11	110.74
1	A	56	MLY	CD-CE-NZ	-2.61	106.72	113.79
1	B	576	MLY	CD-CE-NZ	-2.60	106.76	113.79
1	A	674	MLY	CD-CE-NZ	-2.59	106.77	113.79
1	A	570	MLY	CH2-NZ-CE	2.59	120.99	110.74
1	B	396	MLY	CH1-NZ-CE	2.58	120.98	110.74
1	B	592	MLY	CH2-NZ-CE	2.58	120.97	110.74
1	B	674	MLY	CH2-NZ-CE	2.56	120.89	110.74
1	A	532	MLY	CH1-NZ-CE	2.55	120.83	110.74
1	B	6	MLY	CH1-NZ-CE	2.54	120.80	110.74
1	A	406	MLY	CH1-NZ-CE	2.54	120.80	110.74
1	B	65	MLY	CH2-NZ-CE	2.54	120.78	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	MLY	CH1-NZ-CE	2.53	120.76	110.74
1	A	220	MLY	CH2-NZ-CE	2.53	120.74	110.74
1	B	584	MLY	CH2-NZ-CE	2.52	120.74	110.74
1	A	584	MLY	CH1-NZ-CE	2.52	120.72	110.74
1	B	576	MLY	CH2-NZ-CE	2.51	120.70	110.74
1	A	674	MLY	CH1-NZ-CE	2.51	120.70	110.74
1	B	245	MLY	CD-CE-NZ	-2.51	106.98	113.79
1	B	406	MLY	CH2-NZ-CE	2.51	120.68	110.74
1	B	688	MLY	CH1-NZ-CE	2.51	120.68	110.74
1	B	406	MLY	CD-CE-NZ	-2.50	107.01	113.79
1	B	25	MLY	CD-CE-NZ	-2.50	107.02	113.79
1	A	422	MLY	CH2-NZ-CE	2.50	120.64	110.74
1	B	600	MLY	CH2-NZ-CE	2.49	120.60	110.74
1	A	579	MLY	CH1-NZ-CE	2.49	120.59	110.74
1	B	280	MLY	CH2-NZ-CE	2.48	120.55	110.74
1	A	576	MLY	CH1-NZ-CE	2.47	120.54	110.74
1	B	179	MLY	CH1-NZ-CE	2.47	120.54	110.74
1	A	362	MLY	CH2-NZ-CE	2.47	120.53	110.74
1	B	659	MLY	CH2-NZ-CE	2.47	120.53	110.74
1	B	688	MLY	CD-CE-NZ	-2.47	107.11	113.79
1	B	362	MLY	CH1-NZ-CE	2.46	120.49	110.74
1	B	245	MLY	CH2-NZ-CE	2.46	120.49	110.74
1	B	469	MLY	CD-CE-NZ	-2.46	107.13	113.79
1	A	527	MLY	CH2-NZ-CE	2.46	120.47	110.74
1	A	280	MLY	CH1-NZ-CE	2.45	120.45	110.74
1	A	570	MLY	CD-CE-NZ	-2.44	107.17	113.79
1	B	158	MLY	CH2-NZ-CE	2.44	120.39	110.74
1	A	179	MLY	CH2-NZ-CE	2.44	120.39	110.74
1	B	453	MLY	CH1-NZ-CE	2.43	120.36	110.74
1	B	469	MLY	CH2-NZ-CE	2.42	120.33	110.74
1	A	532	MLY	CD-CE-NZ	-2.42	107.24	113.79
1	A	56	MLY	CH2-NZ-CE	2.42	120.31	110.74
1	B	453	MLY	CH2-NZ-CE	2.41	120.27	110.74
1	B	158	MLY	CH1-NZ-CE	2.41	120.27	110.74
1	B	592	MLY	CH1-NZ-CE	2.40	120.26	110.74
1	B	280	MLY	CH1-NZ-CE	2.40	120.23	110.74
1	B	19	MLY	CD-CE-NZ	-2.39	107.32	113.79
1	B	6	MLY	CH2-NZ-CE	2.39	120.19	110.74
1	A	659	MLY	CH1-NZ-CE	2.38	120.17	110.74
1	A	422	MLY	CH1-NZ-CE	2.37	120.14	110.74
1	A	674	MLY	CH2-NZ-CE	2.37	120.13	110.74
1	A	221	MLY	CH2-NZ-CE	2.36	120.10	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	MLY	CH1-NZ-CE	2.36	120.09	110.74
1	B	25	MLY	CH1-NZ-CE	2.35	120.06	110.74
1	A	280	MLY	CH2-NZ-CE	2.35	120.06	110.74
1	B	576	MLY	CH1-NZ-CE	2.35	120.05	110.74
1	A	584	MLY	CD-CE-NZ	-2.35	107.43	113.79
1	A	659	MLY	CH2-NZ-CE	2.34	120.02	110.74
1	A	362	MLY	CH1-NZ-CE	2.34	120.02	110.74
1	A	584	MLY	CH2-NZ-CE	2.34	120.01	110.74
1	A	527	MLY	CH1-NZ-CE	2.33	119.96	110.74
1	A	659	MLY	CD-CE-NZ	-2.32	107.50	113.79
1	B	396	MLY	CH2-NZ-CE	2.32	119.92	110.74
1	A	56	MLY	CH1-NZ-CE	2.31	119.91	110.74
1	A	6	MLY	CH1-NZ-CE	2.31	119.91	110.74
1	A	406	MLY	CD-CE-NZ	-2.31	107.55	113.79
1	A	532	MLY	CH2-NZ-CE	2.31	119.87	110.74
1	A	406	MLY	CH2-NZ-CE	2.30	119.84	110.74
1	B	453	MLY	CD-CE-NZ	-2.29	107.58	113.79
1	B	527	MLY	CH1-NZ-CE	2.29	119.83	110.74
1	A	25	MLY	CH1-NZ-CE	2.29	119.83	110.74
1	A	179	MLY	CH1-NZ-CE	2.29	119.82	110.74
1	A	21	MLY	CD-CE-NZ	-2.29	107.59	113.79
1	B	406	MLY	CH1-NZ-CE	2.27	119.72	110.74
1	A	576	MLY	CH2-NZ-CE	2.26	119.71	110.74
1	A	570	MLY	CH1-NZ-CE	2.26	119.70	110.74
1	B	65	MLY	CH1-NZ-CE	2.25	119.67	110.74
1	A	579	MLY	CH2-NZ-CE	2.25	119.66	110.74
1	B	362	MLY	CH2-NZ-CE	2.25	119.66	110.74
1	A	576	MLY	CD-CE-NZ	-2.25	107.69	113.79
1	A	220	MLY	CH1-NZ-CE	2.24	119.60	110.74
1	B	82	MLY	CD-CE-NZ	-2.23	107.75	113.79
1	B	688	MLY	CH2-NZ-CE	2.23	119.58	110.74
1	B	179	MLY	CH2-NZ-CE	2.23	119.56	110.74
1	B	6	MLY	CD-CE-NZ	-2.22	107.77	113.79
1	B	584	MLY	CH1-NZ-CE	2.22	119.55	110.74
1	B	72	MLY	CD-CE-NZ	-2.22	107.77	113.79
1	B	674	MLY	CH1-NZ-CE	2.22	119.52	110.74
1	B	72	MLY	CH2-NZ-CE	2.21	119.50	110.74
1	A	158	MLY	CH1-NZ-CE	2.20	119.45	110.74
1	A	21	MLY	CH2-NZ-CE	2.19	119.42	110.74
1	A	604	MLY	CH2-NZ-CE	2.19	119.42	110.74
1	B	659	MLY	CH1-NZ-CE	2.19	119.42	110.74
1	B	82	MLY	CH1-NZ-CE	2.17	119.35	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	MLY	CH1-NZ-CE	2.17	119.33	110.74
1	B	396	MLY	CD-CE-NZ	-2.17	107.92	113.79
1	B	245	MLY	CH1-NZ-CE	2.16	119.28	110.74
1	A	600	MLY	CH1-NZ-CE	2.15	119.28	110.74
1	B	362	MLY	CD-CE-NZ	-2.15	107.95	113.79
1	B	600	MLY	CH1-NZ-CE	2.14	119.23	110.74
1	A	732	MLY	CH1-NZ-CE	2.13	119.17	110.74
1	A	527	MLY	CD-CE-NZ	-2.12	108.05	113.79
1	A	65	MLY	CH2-NZ-CE	2.12	119.13	110.74
1	B	527	MLY	CD-CE-NZ	-2.11	108.06	113.79
1	B	532	MLY	CH1-NZ-CE	2.11	119.09	110.74
1	A	72	MLY	CD-CE-NZ	-2.10	108.11	113.79
1	B	25	MLY	CH2-NZ-CE	2.09	119.02	110.74
1	B	570	MLY	CH2-NZ-CE	2.09	119.02	110.74
1	A	245	MLY	CD-CE-NZ	-2.09	108.14	113.79
1	A	688	MLY	CH1-NZ-CE	2.08	118.99	110.74
1	A	25	MLY	CD-CE-NZ	-2.07	108.17	113.79
1	A	396	MLY	CH1-NZ-CE	2.06	118.91	110.74
1	A	279	MLY	CH2-NZ-CE	2.04	118.84	110.74
1	A	600	MLY	CD-CE-NZ	-2.04	108.27	113.79
1	A	19	MLY	CH2-NZ-CE	2.03	118.79	110.74
1	B	19	MLY	CH1-NZ-CE	2.03	118.78	110.74
1	A	604	MLY	CD-CE-NZ	-2.03	108.30	113.79
1	A	65	MLY	CD-CE-NZ	-2.01	108.33	113.79
1	B	538	MLY	CH1-NZ-CE	2.00	118.67	110.74
1	A	72	MLY	CH1-NZ-CE	2.00	118.67	110.74

There are no chirality outliers.

All (203) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	56	MLY	O-C-CA-CB
1	A	72	MLY	O-C-CA-CB
1	A	235	MLY	N-CA-CB-CG
1	A	235	MLY	C-CA-CB-CG
1	A	362	MLY	O-C-CA-CB
1	A	422	MLY	C-CA-CB-CG
1	A	527	MLY	N-CA-CB-CG
1	A	527	MLY	C-CA-CB-CG
1	A	538	MLY	O-C-CA-CB
1	A	570	MLY	C-CA-CB-CG
1	A	600	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	600	MLY	C-CA-CB-CG
1	A	688	MLY	C-CA-CB-CG
1	A	717	OCS	N-CA-CB-SG
1	B	25	MLY	C-CA-CB-CG
1	B	56	MLY	O-C-CA-CB
1	B	72	MLY	O-C-CA-CB
1	B	82	MLY	N-CA-CB-CG
1	B	82	MLY	C-CA-CB-CG
1	B	235	MLY	N-CA-CB-CG
1	B	279	MLY	C-CA-CB-CG
1	B	362	MLY	O-C-CA-CB
1	B	406	MLY	N-CA-CB-CG
1	B	406	MLY	C-CA-CB-CG
1	B	422	MLY	C-CA-CB-CG
1	B	422	MLY	O-C-CA-CB
1	B	469	MLY	C-CA-CB-CG
1	B	527	MLY	N-CA-CB-CG
1	B	527	MLY	C-CA-CB-CG
1	B	538	MLY	O-C-CA-CB
1	B	576	MLY	C-CA-CB-CG
1	B	579	MLY	O-C-CA-CB
1	B	592	MLY	C-CA-CB-CG
1	B	604	MLY	N-CA-CB-CG
1	B	674	MLY	O-C-CA-CB
1	B	717	OCS	N-CA-CB-SG
1	A	19	MLY	CD-CE-NZ-CH2
1	A	21	MLY	CD-CE-NZ-CH2
1	A	65	MLY	CD-CE-NZ-CH2
1	A	72	MLY	CD-CE-NZ-CH1
1	A	179	MLY	CD-CE-NZ-CH1
1	A	220	MLY	CD-CE-NZ-CH1
1	A	279	MLY	CD-CE-NZ-CH2
1	A	406	MLY	CD-CE-NZ-CH2
1	A	422	MLY	CD-CE-NZ-CH1
1	A	532	MLY	CD-CE-NZ-CH2
1	A	576	MLY	CD-CE-NZ-CH2
1	A	579	MLY	CD-CE-NZ-CH2
1	A	600	MLY	CD-CE-NZ-CH1
1	A	688	MLY	CD-CE-NZ-CH1
1	B	6	MLY	CD-CE-NZ-CH2
1	B	19	MLY	CD-CE-NZ-CH2
1	B	65	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	B	72	MLY	CD-CE-NZ-CH2
1	B	158	MLY	CD-CE-NZ-CH2
1	B	179	MLY	CD-CE-NZ-CH2
1	B	235	MLY	CD-CE-NZ-CH1
1	B	245	MLY	CD-CE-NZ-CH1
1	B	280	MLY	CD-CE-NZ-CH1
1	B	396	MLY	CD-CE-NZ-CH2
1	B	527	MLY	CD-CE-NZ-CH1
1	B	538	MLY	CD-CE-NZ-CH2
1	B	570	MLY	CD-CE-NZ-CH2
1	B	576	MLY	CD-CE-NZ-CH1
1	B	659	MLY	CD-CE-NZ-CH1
1	B	674	MLY	CD-CE-NZ-CH1
1	B	688	MLY	CD-CE-NZ-CH2
1	B	732	MLY	CD-CE-NZ-CH2
1	A	674	MLY	CG-CD-CE-NZ
1	B	592	MLY	CG-CD-CE-NZ
1	B	25	MLY	CG-CD-CE-NZ
1	B	18	MLY	CG-CD-CE-NZ
1	A	18	MLY	CG-CD-CE-NZ
1	A	422	MLY	CG-CD-CE-NZ
1	B	396	MLY	CG-CD-CE-NZ
1	B	674	MLY	CG-CD-CE-NZ
1	A	221	MLY	CG-CD-CE-NZ
1	A	576	MLY	CG-CD-CE-NZ
1	A	6	MLY	CD-CE-NZ-CH1
1	A	181	MLY	CD-CE-NZ-CH1
1	A	570	MLY	CD-CE-NZ-CH1
1	A	604	MLY	CD-CE-NZ-CH2
1	A	708	MLY	CD-CE-NZ-CH1
1	A	732	MLY	CD-CE-NZ-CH1
1	B	18	MLY	CD-CE-NZ-CH1
1	B	220	MLY	CD-CE-NZ-CH1
1	B	532	MLY	CD-CE-NZ-CH2
1	B	708	MLY	CD-CE-NZ-CH1
1	A	584	MLY	CG-CD-CE-NZ
1	A	6	MLY	CG-CD-CE-NZ
1	A	82	MLY	CA-CB-CG-CD
1	B	362	MLY	CA-CB-CG-CD
1	B	406	MLY	CA-CB-CG-CD
1	A	18	MLY	CD-CE-NZ-CH1
1	A	18	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	25	MLY	CD-CE-NZ-CH2
1	A	158	MLY	CD-CE-NZ-CH2
1	A	245	MLY	CD-CE-NZ-CH1
1	B	21	MLY	CD-CE-NZ-CH1
1	B	82	MLY	CD-CE-NZ-CH2
1	B	181	MLY	CD-CE-NZ-CH1
1	B	651	MLY	CD-CE-NZ-CH2
1	B	82	MLY	CG-CD-CE-NZ
1	A	245	MLY	CG-CD-CE-NZ
1	B	235	MLY	CG-CD-CE-NZ
1	A	600	MLY	CG-CD-CE-NZ
1	B	6	MLY	CG-CD-CE-NZ
1	B	688	MLY	CG-CD-CE-NZ
1	A	688	MLY	CG-CD-CE-NZ
1	A	25	MLY	CD-CE-NZ-CH1
1	A	280	MLY	CD-CE-NZ-CH2
1	A	396	MLY	CD-CE-NZ-CH2
1	A	651	MLY	CD-CE-NZ-CH1
1	A	659	MLY	CD-CE-NZ-CH1
1	B	82	MLY	CD-CE-NZ-CH1
1	B	362	MLY	CD-CE-NZ-CH2
1	B	604	MLY	CD-CE-NZ-CH1
1	A	527	MLY	CG-CD-CE-NZ
1	B	158	MLY	CA-CB-CG-CD
1	B	469	MLY	CA-CB-CG-CD
1	A	21	MLY	CD-CE-NZ-CH1
1	A	72	MLY	CD-CE-NZ-CH2
1	A	688	MLY	CD-CE-NZ-CH2
1	B	584	MLY	CD-CE-NZ-CH1
1	B	600	MLY	CD-CE-NZ-CH1
1	A	532	MLY	CE-CD-CG-CB
1	A	406	MLY	CE-CD-CG-CB
1	A	570	MLY	CE-CD-CG-CB
1	A	604	MLY	CE-CD-CG-CB
1	B	604	MLY	CA-CB-CG-CD
1	A	221	MLY	CD-CE-NZ-CH2
1	A	280	MLY	CE-CD-CG-CB
1	B	532	MLY	CE-CD-CG-CB
1	B	158	MLY	CE-CD-CG-CB
1	B	362	MLY	CE-CD-CG-CB
1	A	25	MLY	CA-CB-CG-CD
1	B	592	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	B	538	MLY	CE-CD-CG-CB
1	B	674	MLY	CE-CD-CG-CB
1	A	362	MLY	CD-CE-NZ-CH1
1	A	584	MLY	CD-CE-NZ-CH1
1	A	674	MLY	CD-CE-NZ-CH1
1	A	469	MLY	CA-CB-CG-CD
1	B	235	MLY	CA-CB-CG-CD
1	B	584	MLY	CE-CD-CG-CB
1	A	600	MLY	CE-CD-CG-CB
1	A	688	MLY	CA-CB-CG-CD
1	A	717	OCS	CA-CB-SG-OD3
1	B	72	MLY	CD-CE-NZ-CH1
1	B	453	MLY	CD-CE-NZ-CH1
1	A	21	MLY	CE-CD-CG-CB
1	B	579	MLY	CA-CB-CG-CD
1	A	56	MLY	CG-CD-CE-NZ
1	B	406	MLY	CD-CE-NZ-CH1
1	B	82	MLY	CA-CB-CG-CD
1	B	6	MLY	CE-CD-CG-CB
1	A	56	MLY	CD-CE-NZ-CH2
1	B	732	MLY	CE-CD-CG-CB
1	A	570	MLY	CG-CD-CE-NZ
1	B	453	MLY	CA-CB-CG-CD
1	B	688	MLY	CE-CD-CG-CB
1	A	579	MLY	CE-CD-CG-CB
1	B	453	MLY	CG-CD-CE-NZ
1	A	82	MLY	CG-CD-CE-NZ
1	A	538	MLY	CE-CD-CG-CB
1	B	422	MLY	CE-CD-CG-CB
1	B	732	MLY	CD-CE-NZ-CH1
1	A	181	MLY	CD-CE-NZ-CH2
1	B	25	MLY	CD-CE-NZ-CH2
1	B	469	MLY	CD-CE-NZ-CH2
1	B	592	MLY	CD-CE-NZ-CH1
1	A	21	MLY	CG-CD-CE-NZ
1	B	604	MLY	CG-CD-CE-NZ
1	A	584	MLY	N-CA-CB-CG
1	A	688	MLY	N-CA-CB-CG
1	B	280	MLY	N-CA-CB-CG
1	B	362	MLY	N-CA-CB-CG
1	B	576	MLY	N-CA-CB-CG
1	B	592	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	717	OCS	CA-CB-SG-OD2
1	B	584	MLY	CG-CD-CE-NZ
1	B	688	MLY	C-CA-CB-CG
1	B	659	MLY	CA-CB-CG-CD
1	A	19	MLY	CE-CD-CG-CB
1	A	422	MLY	CD-CE-NZ-CH2
1	B	469	MLY	CE-CD-CG-CB
1	A	406	MLY	CG-CD-CE-NZ
1	B	279	MLY	CE-CD-CG-CB
1	B	18	MLY	CE-CD-CG-CB
1	A	527	MLY	CD-CE-NZ-CH2
1	A	527	MLY	CD-CE-NZ-CH1
1	A	220	MLY	CE-CD-CG-CB
1	B	604	MLY	CE-CD-CG-CB
1	B	235	MLY	C-CA-CB-CG
1	B	396	MLY	CE-CD-CG-CB
1	A	65	MLY	CA-CB-CG-CD
1	A	362	MLY	CE-CD-CG-CB
1	B	576	MLY	CA-CB-CG-CD
1	A	604	MLY	CA-CB-CG-CD
1	B	406	MLY	CG-CD-CE-NZ
1	B	592	MLY	CD-CE-NZ-CH2
1	B	72	MLY	CA-CB-CG-CD
1	A	422	MLY	N-CA-CB-CG

There are no ring outliers.

17 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	406	MLY	1	0
1	A	181	MLY	1	0
1	A	18	MLY	1	0
1	B	362	MLY	2	0
1	B	469	MLY	1	0
1	A	235	MLY	2	0
1	A	25	MLY	1	0
1	B	235	MLY	1	0
1	B	181	MLY	1	0
1	B	18	MLY	1	0
1	A	56	MLY	1	0
1	A	422	MLY	1	0
1	B	25	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	72	MLY	2	0
1	B	600	MLY	1	0
1	B	604	MLY	1	0
1	A	179	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	703/752 (93%)	0.83	110 (15%) <b>2</b> <b>2</b>	10, 22, 40, 72	0
1	B	703/752 (93%)	0.49	74 (10%) <b>6</b> <b>9</b>	11, 20, 44, 65	0
All	All	1406/1504 (93%)	0.66	184 (13%) <b>3</b> <b>4</b>	10, 21, 44, 72	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	10.4
1	A	438	ILE	10.4
1	A	236	GLY	9.9
1	A	446	ILE	9.2
1	A	441	LEU	8.5
1	A	477	VAL	8.5
1	A	447	LYS	8.4
1	B	441	LEU	8.3
1	B	446	ILE	8.1
1	B	438	ILE	7.9
1	A	449	ILE	7.0
1	B	225	ASN	6.7
1	A	442	LYS	6.7
1	B	507	PHE	6.6
1	A	478	LYS	6.4
1	B	443	LYS	6.2
1	A	504	LEU	6.1
1	A	443	LYS	6.0
1	B	447	LYS	5.9
1	A	444	LYS	5.9
1	A	433	LEU	5.9
1	B	228	GLN	5.7
1	A	445	GLY	5.6
1	A	321	VAL	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	496	THR	5.5
1	A	448	GLU	5.5
1	B	445	GLY	5.5
1	A	234	ILE	5.4
1	A	475	GLU	5.3
1	A	306	ASP	5.3
1	B	477	VAL	5.2
1	B	444	LYS	5.2
1	A	224	GLU	5.2
1	A	230	GLN	5.1
1	B	434	VAL	5.1
1	A	474	LYS	5.1
1	B	476	GLY	5.1
1	B	475	GLU	5.0
1	A	440	LYS	5.0
1	A	567	ARG	5.0
1	A	434	VAL	4.9
1	A	510	LEU	4.9
1	A	471	ILE	4.9
1	A	323	ILE	4.8
1	B	442	LYS	4.8
1	A	439	ALA	4.8
1	A	237	GLU	4.7
1	B	495	ARG	4.7
1	A	303	ASP	4.6
1	A	589	GLY	4.6
1	B	436	ARG	4.6
1	A	590	ALA	4.6
1	A	473	GLU	4.6
1	A	223	PRO	4.6
1	B	193	ALA	4.6
1	A	451	VAL	4.5
1	A	302	PHE	4.5
1	B	304	ILE	4.4
1	B	229	ASP	4.4
1	A	509	LEU	4.3
1	B	440	LYS	4.3
1	A	507	PHE	4.3
1	B	448	GLU	4.2
1	A	454	LEU	4.2
1	B	439	ALA	4.2
1	A	480	ASN	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	228	GLN	4.1
1	A	229	ASP	4.1
1	A	495	ARG	4.0
1	A	436	ARG	4.0
1	A	435	ARG	3.9
1	B	236	GLY	3.9
1	B	496	THR	3.9
1	A	457	PHE	3.9
1	A	450	PRO	3.8
1	A	481	ILE	3.8
1	B	504	LEU	3.8
1	B	471	ILE	3.8
1	A	536	VAL	3.7
1	B	223	PRO	3.6
1	A	455	VAL	3.6
1	B	451	VAL	3.6
1	B	479	VAL	3.6
1	B	478	LYS	3.6
1	A	222	ALA	3.6
1	B	226	ALA	3.5
1	B	472	ALA	3.5
1	B	430	GLY	3.5
1	B	192	TRP	3.5
1	A	322	GLY	3.5
1	B	194	GLY	3.5
1	A	476	GLY	3.5
1	A	347	ALA	3.4
1	B	435	ARG	3.4
1	A	289	GLU	3.4
1	B	450	PRO	3.4
1	A	225	ASN	3.4
1	B	227	PRO	3.4
1	A	508	GLU	3.3
1	A	285	GLU	3.3
1	B	461	HIS	3.3
1	A	470	GLU	3.3
1	A	437	GLU	3.2
1	A	429	ARG	3.2
1	B	437	GLU	3.2
1	A	320	ARG	3.2
1	A	506	ASP	3.2
1	A	540	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	431	SER	3.1
1	A	340	ALA	3.1
1	A	307	LEU	3.1
1	B	473	GLU	3.0
1	B	432	ASP	3.0
1	A	430	GLY	2.9
1	A	461	HIS	2.9
1	A	351	MET	2.9
1	A	127	ILE	2.9
1	A	348	LEU	2.9
1	B	301[A]	MET	2.8
1	B	480	ASN	2.8
1	B	224	GLU	2.8
1	A	233	VAL	2.8
1	A	304	ILE	2.8
1	B	340	ALA	2.8
1	B	467	ILE	2.8
1	A	350	PHE	2.8
1	B	384	GLU	2.8
1	A	566	GLY	2.8
1	B	144	ILE	2.8
1	B	428	ARG	2.7
1	A	144	ILE	2.7
1	A	301[A]	MET	2.7
1	A	565	ASN	2.7
1	B	470	GLU	2.6
1	A	342	ALA	2.6
1	B	307	LEU	2.6
1	B	323	ILE	2.6
1	A	467	ILE	2.6
1	B	2	GLU	2.6
1	A	591	PHE	2.6
1	B	322	GLY	2.6
1	A	468	VAL	2.6
1	A	505	VAL	2.6
1	B	449	ILE	2.5
1	B	506	ASP	2.5
1	A	452	GLU	2.5
1	B	230	GLN	2.5
1	A	344	HIS	2.5
1	B	302	PHE	2.5
1	A	492	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	LEU	2.4
1	A	317	VAL	2.4
1	A	305	GLU	2.4
1	A	488[A]	MET	2.4
1	A	231	VAL	2.4
1	A	238	LYS	2.4
1	B	135	VAL	2.4
1	A	226	ALA	2.4
1	A	432	ASP	2.4
1	B	483	ASP	2.4
1	B	237	GLU	2.3
1	A	352	LEU	2.3
1	A	537	ILE	2.3
1	A	292	LEU	2.3
1	B	132	ILE	2.3
1	A	291	ILE	2.3
1	B	233	VAL	2.2
1	B	696	GLY	2.2
1	B	567	ARG	2.2
1	A	456	THR	2.2
1	A	145	PHE	2.1
1	B	457	PHE	2.1
1	A	511	LYS	2.1
1	A	227	PRO	2.1
1	A	356	VAL	2.1
1	B	474	LYS	2.1
1	B	369	LEU	2.1
1	A	535	ARG	2.1
1	A	345	THR	2.1
1	B	452	GLU	2.1
1	B	222	ALA	2.1
1	A	212	ALA	2.0
1	B	593	GLU	2.0
1	B	238	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MLY	A	235	9/12	0.39	0.54	48,48,50,50	0
1	MLY	B	538	11/12	0.77	0.29	24,24,29,30	0
1	MLY	A	469	9/12	0.78	0.35	38,38,39,39	0
1	MLY	B	453	11/12	0.80	0.33	40,41,43,43	0
1	MLY	A	579	11/12	0.81	0.18	30,30,34,34	0
1	MLY	B	406	11/12	0.82	0.23	25,27,32,32	0
1	MLY	A	538	9/12	0.82	0.34	29,29,30,31	0
1	MLY	A	453	9/12	0.82	0.24	34,34,34,35	0
1	MLY	B	280	11/12	0.83	0.24	20,22,26,26	0
1	MLY	A	422	11/12	0.84	0.20	28,29,39,39	0
1	MLY	A	584	11/12	0.84	0.23	28,28,30,30	0
1	MLY	B	82	11/12	0.84	0.26	18,19,32,33	0
1	MLY	B	235	11/12	0.84	0.27	41,42,47,47	0
1	MLY	B	604	11/12	0.84	0.19	18,19,34,34	0
1	MLY	A	604	11/12	0.85	0.24	21,22,33,33	0
1	MLY	A	592	9/12	0.85	0.33	28,29,29,30	0
1	MLY	B	221	9/12	0.85	0.28	32,34,35,35	0
1	MLY	A	221	11/12	0.86	0.41	28,30,37,37	0
1	MLY	A	280	11/12	0.86	0.22	26,28,34,34	0
1	MLY	A	576	11/12	0.86	0.18	29,31,39,39	0
1	MLY	A	362	11/12	0.87	0.21	21,22,34,35	0
1	MLY	B	469	11/12	0.87	0.31	43,43,43,43	0
1	MLY	A	406	11/12	0.87	0.22	25,26,32,33	0
1	MLY	B	422	9/12	0.87	0.18	31,32,34,34	0
1	MLY	A	179	11/12	0.88	0.18	16,16,28,28	0
1	MLY	B	362	11/12	0.88	0.17	15,16,27,27	0
1	MLY	A	600	11/12	0.88	0.18	24,24,30,30	0
1	MLY	A	279	11/12	0.88	0.18	24,25,31,31	0
1	MLY	A	532	11/12	0.89	0.21	25,26,27,27	0
1	MLY	A	396	11/12	0.89	0.17	22,23,31,32	0
1	MLY	A	688	11/12	0.89	0.15	22,23,35,36	0
1	MLY	A	72	11/12	0.89	0.17	17,18,27,28	0
1	MLY	A	181	11/12	0.89	0.15	16,16,23,24	0
1	MLY	A	220	11/12	0.89	0.14	24,26,31,31	0
1	MLY	B	584	11/12	0.89	0.18	21,21,30,30	0
1	MLY	B	600	11/12	0.89	0.19	19,20,32,34	0
1	MLY	A	82	9/12	0.89	0.19	16,17,22,23	0
1	MLY	B	576	11/12	0.90	0.15	24,25,35,35	0
1	MLY	B	532	11/12	0.90	0.15	21,22,30,30	0
1	MLY	A	570	11/12	0.90	0.26	27,27,33,33	0
1	MLY	B	570	11/12	0.90	0.17	19,21,28,29	0
1	MLY	B	674	11/12	0.90	0.20	17,19,32,32	0
1	MLY	B	25	11/12	0.91	0.16	14,14,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	B	396	11/12	0.91	0.24	20,20,29,29	0
1	MLY	A	158	11/12	0.91	0.13	12,13,25,25	0
1	MLY	B	579	9/12	0.91	0.16	23,24,29,29	0
1	MLY	A	6	11/12	0.91	0.16	14,15,29,30	0
1	MLY	B	592	11/12	0.91	0.15	20,21,30,30	0
1	MLY	B	6	11/12	0.91	0.17	20,22,30,31	0
1	MLY	B	279	9/12	0.91	0.13	18,20,22,24	0
1	MLY	B	19	11/12	0.91	0.16	12,13,25,25	0
1	MLY	A	651	11/12	0.92	0.12	15,16,20,22	0
1	MLY	B	179	11/12	0.92	0.18	16,17,27,28	0
1	MLY	A	19	11/12	0.92	0.15	11,13,24,25	0
1	MLY	A	732	11/12	0.92	0.15	17,18,28,28	0
1	MLY	A	56	11/12	0.92	0.13	18,19,30,31	0
1	MLY	B	527	11/12	0.92	0.19	22,23,31,31	0
1	MLY	A	527	11/12	0.92	0.17	25,26,34,34	0
1	MLY	A	245	11/12	0.92	0.13	15,18,32,32	0
1	MLY	A	65	11/12	0.93	0.11	15,15,21,22	0
1	MLY	B	72	11/12	0.93	0.14	16,17,22,22	0
1	MLY	B	220	11/12	0.93	0.16	27,29,30,30	0
1	MLY	B	708	11/12	0.93	0.13	17,18,25,25	0
1	MLY	A	25	11/12	0.94	0.10	11,13,26,27	0
1	MLY	A	659	11/12	0.94	0.15	16,17,24,25	0
1	MLY	B	56	9/12	0.94	0.11	19,20,24,26	0
1	MLY	A	674	11/12	0.94	0.21	20,20,33,34	0
1	MLY	B	651	11/12	0.94	0.10	17,17,19,20	0
1	MLY	B	18	11/12	0.94	0.13	13,13,16,17	0
1	MLY	B	688	11/12	0.94	0.10	19,20,30,30	0
1	MLY	B	158	11/12	0.94	0.17	14,15,27,28	0
1	MLY	B	65	11/12	0.95	0.08	14,15,21,22	0
1	MLY	A	21	11/12	0.95	0.11	12,12,21,22	0
1	MLY	B	245	11/12	0.95	0.10	14,15,26,26	0
1	MLY	B	181	11/12	0.95	0.15	16,16,20,20	0
1	MLY	A	708	11/12	0.95	0.12	18,19,27,27	0
1	MLY	B	659	11/12	0.96	0.14	15,16,22,23	0
1	OCS	A	717	9/10	0.96	0.12	24,25,27,29	0
1	MLY	B	21	11/12	0.96	0.11	11,12,16,17	0
1	MLY	A	18	11/12	0.96	0.09	12,13,14,15	0
1	MLY	B	732	11/12	0.96	0.15	16,17,24,25	0
1	OCS	B	717	9/10	0.98	0.13	21,21,23,23	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	A	753	1/1	0.99	0.12	16,16,16,16	0
2	ZN	B	753	1/1	1.00	0.13	17,17,17,17	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.