



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:08 am BST

PDB ID : 1XL3  
Title : Complex structure of Y.pestis virulence Factors YopN and TyeA  
Authors : Schubot, F.D.; Jackson, M.W.; Penrose, K.J.; Cherry, S.; Tropea, J.E.; Plano, G.V.; Waugh, D.S.  
Deposited on : 2004-09-30  
Resolution : 2.20 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.

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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 : 2.11  
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) : 2.11

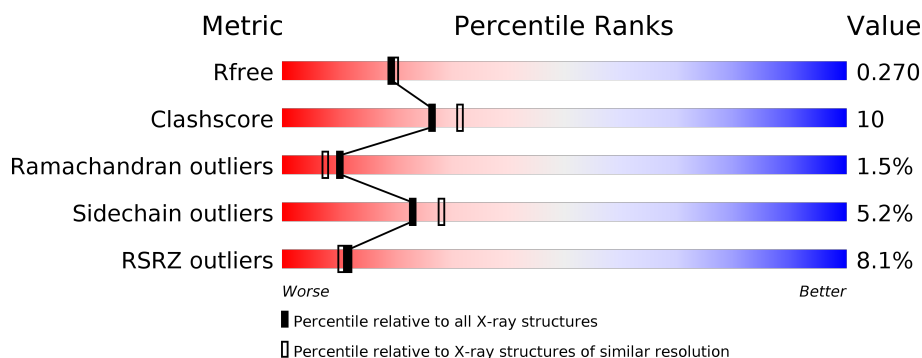
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	218	<div> <div>14%</div> <div> <div>71%</div> <div>18%</div> <div>7%</div> </div> </div>
1	B	218	<div> <div>3%</div> <div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
2	C	92	<div> <div>3%</div> <div> <div>74%</div> <div>21%</div> <div>5%</div> </div> </div>
2	D	92	<div> <div>5%</div> <div> <div>66%</div> <div>25%</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	147	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4878 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 Secretion control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1604	1018	270	312	4			
1	B	206	Total	C	N	O	S	0	0	0
			1640	1040	276	320	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	122	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	128	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	137	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	147	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	221	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	237	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	254	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	264	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	266	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	276	MLY	LYS	MODIFIED RESIDUE	GB 3822072
A	286	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	93	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	122	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	128	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	137	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	147	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	221	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	237	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	254	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	264	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	266	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	276	MLY	LYS	MODIFIED RESIDUE	GB 3822072
B	286	MLY	LYS	MODIFIED RESIDUE	GB 3822072

- Molecule 2 is a protein called protein type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	91	Total	C	N	O	S	0	0	0
			751	479	122	145	5			
2	D	85	Total	C	N	O	S	0	0	0
			703	450	116	132	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	MLY	LYS	MODIFIED RESIDUE	UNP P16161
C	41	MLY	LYS	MODIFIED RESIDUE	UNP P16161
C	49	MLY	LYS	MODIFIED RESIDUE	UNP P16161
D	18	MLY	LYS	MODIFIED RESIDUE	UNP P16161
D	41	MLY	LYS	MODIFIED RESIDUE	UNP P16161
D	49	MLY	LYS	MODIFIED RESIDUE	UNP P16161

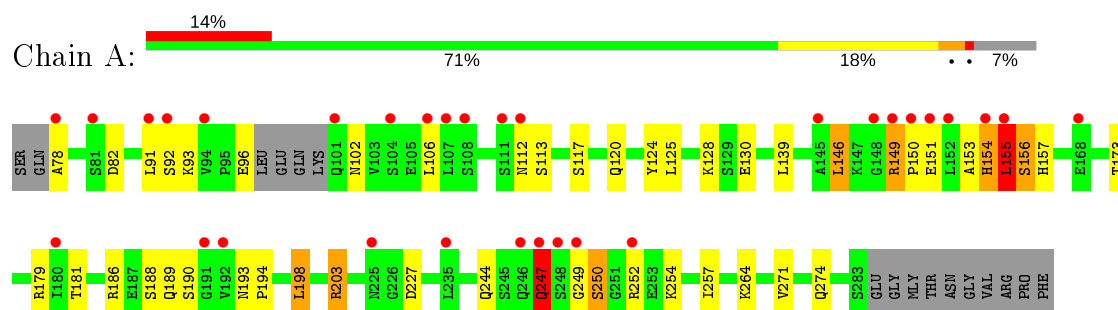
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	61	Total	O	0	0
			61	61		
3	C	35	Total	O	0	0
			35	35		
3	D	31	Total	O	0	0
			31	31		

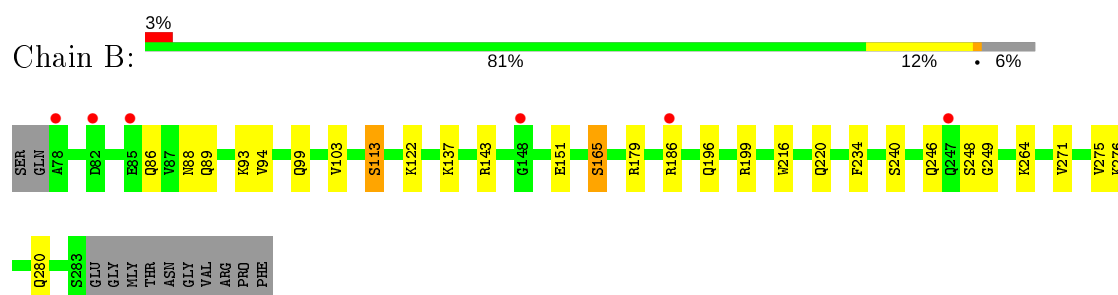
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

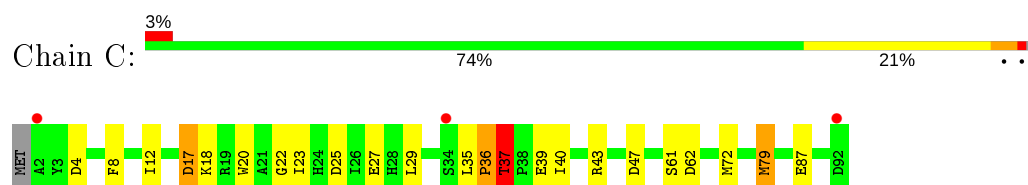
- Molecule 1: Secretion control protein



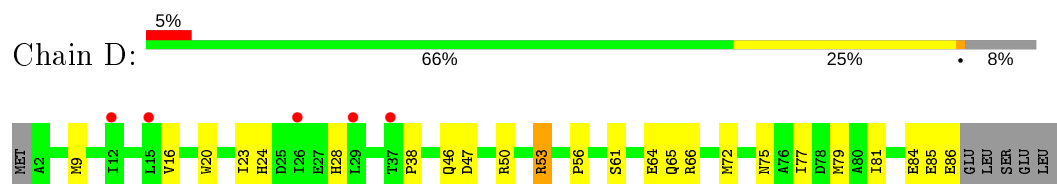
- Molecule 1: Secretion control protein



- Molecule 2: protein type A



- Molecule 2: protein type A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.17Å 170.72Å 55.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.51 – 2.20 24.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.1 (84.51-2.20) 94.1 (24.97-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.250 0.212 , 0.270	Depositor DCC
$R_{free}$ test set	1949 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.82	0/1508	0.87	2/2045 (0.1%)
1	B	0.95	0/1545	0.83	1/2096 (0.0%)
2	C	0.97	1/732 (0.1%)	0.87	2/990 (0.2%)
2	D	0.95	1/684 (0.1%)	0.89	1/925 (0.1%)
All	All	0.91	2/4469 (0.0%)	0.86	6/6056 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	16	VAL	CB-CG1	-5.76	1.40	1.52
2	C	20	TRP	CB-CG	-5.31	1.40	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	227	ASP	CB-CG-OD1	6.31	123.98	118.30
2	D	66	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	203	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	C	17	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	143	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	C	47	ASP	CB-CG-OD1	5.17	122.95	118.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	HIS	Peptide
1	A	155	LEU	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	1604	0	1606	38	0
1	B	1640	0	1645	21	0
2	C	751	0	725	25	0
2	D	703	0	682	23	0
3	A	53	0	0	5	0
3	B	61	0	0	3	0
3	C	35	0	0	5	0
3	D	31	0	0	2	0
All	All	4878	0	4658	96	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 10.

All (96) 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)
2:D:72:MET:HE3	2:D:75:ASN:HD22	1.32	0.94
1:A:117:SER:H	1:A:120:GLN:HE21	1.25	0.84
1:A:154:HIS:CE1	1:A:157:HIS:HB2	2.21	0.75
1:B:88:ASN:OD1	1:B:137:MLY:HH13	1.86	0.74
1:B:196:GLN:NE2	1:B:199:ARG:HH21	1.86	0.74
2:D:20:TRP:H	2:D:65:GLN:HE22	1.36	0.73
1:A:117:SER:H	1:A:120:GLN:NE2	1.90	0.69
2:D:47:ASP:OD1	2:D:50:ARG:NH1	2.26	0.69
1:A:130:GLU:HG3	3:A:318:HOH:O	1.93	0.68
2:C:37:THR:HG23	2:C:39:GLU:OE2	1.95	0.66
2:C:72:MET:CE	3:C:104:HOH:O	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD11	1:A:156:SER:CB	2.27	0.65
1:A:146:LEU:HD11	1:A:156:SER:HB3	1.79	0.65
1:A:146:LEU:CD2	1:A:156:SER:HB2	2.28	0.64
2:C:22:GLY:HA2	2:C:72:MET:HE2	1.78	0.64
2:C:27:GLU:OE2	2:C:79:MET:SD	2.56	0.64
1:A:194:PRO:O	1:A:198:LEU:HD22	2.00	0.61
2:C:17:ASP:OD1	2:D:24:HIS:HE1	1.84	0.61
1:A:146:LEU:HD21	1:A:156:SER:HB2	1.85	0.59
1:A:173:THR:HG23	1:A:203:ARG:HD2	1.84	0.59
2:D:46:GLN:O	2:D:50:ARG:HG3	2.03	0.58
2:C:35:LEU:HD22	2:C:40:ILE:HG22	1.85	0.58
1:A:188:SER:HA	1:A:193:ASN:O	2.03	0.58
2:C:36:PRO:O	2:C:37:THR:HB	2.03	0.58
2:D:85:GLU:O	2:D:86:GLU:HB2	2.04	0.57
1:B:86:GLN:O	1:B:89:GLN:HG2	2.04	0.57
1:B:246:GLN:HE21	1:B:248:SER:HB2	1.70	0.57
2:C:18:MLY:NZ	2:C:25:ASP:OD2	2.38	0.56
1:B:113:SER:O	1:B:113:SER:OG	2.14	0.56
2:C:72:MET:HE2	3:C:104:HOH:O	2.04	0.55
1:B:151:GLU:O	3:B:353:HOH:O	2.17	0.55
1:A:146:LEU:CD1	1:A:156:SER:HB2	2.36	0.55
2:D:72:MET:CE	2:D:75:ASN:HD22	2.14	0.55
1:B:151:GLU:C	3:B:353:HOH:O	2.45	0.55
2:C:37:THR:HG22	2:C:40:ILE:HB	1.88	0.54
1:B:246:GLN:HE21	1:B:248:SER:CB	2.20	0.54
1:A:188:SER:O	3:A:346:HOH:O	2.18	0.54
2:C:23:ILE:N	2:C:72:MET:HE3	2.23	0.53
1:B:196:GLN:HE22	1:B:199:ARG:HE	1.55	0.53
2:D:23:ILE:HB	2:D:72:MET:HE1	1.90	0.53
2:D:72:MET:HE3	2:D:72:MET:HA	1.91	0.53
1:A:128:MLY:HE2	3:A:303:HOH:O	2.09	0.53
1:B:196:GLN:NE2	1:B:199:ARG:HE	2.07	0.53
1:A:264:MLY:HH11	2:C:17:ASP:HA	1.92	0.52
1:B:216:TRP:O	1:B:220:GLN:HG2	2.09	0.52
2:C:37:THR:HG22	2:C:40:ILE:H	1.74	0.52
1:A:146:LEU:HD21	1:A:156:SER:CB	2.39	0.52
1:A:264:MLY:HH11	2:C:17:ASP:OD2	2.10	0.51
1:A:91:LEU:HD11	1:A:181:THR:HG21	1.92	0.51
2:D:23:ILE:HB	2:D:72:MET:CE	2.41	0.50
2:C:87:GLU:HB3	3:C:125:HOH:O	2.10	0.50
2:D:20:TRP:H	2:D:65:GLN:NE2	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:ASP:OD1	2:D:24:HIS:CE1	2.65	0.49
2:D:72:MET:CE	2:D:72:MET:HA	2.42	0.49
1:A:112:ASN:O	1:A:113:SER:OG	2.29	0.49
2:C:18:MLY:HH12	2:D:28:HIS:HB3	1.94	0.49
1:B:276:MLY:O	1:B:280:GLN:HG3	2.13	0.49
1:A:146:LEU:HD11	1:A:156:SER:HB2	1.94	0.47
2:D:77:ILE:O	2:D:81:ILE:HG12	2.15	0.47
1:A:102:ASN:O	1:A:106:LEU:HG	2.15	0.47
1:A:154:HIS:O	1:A:155:LEU:HD12	2.15	0.47
1:B:196:GLN:HE22	1:B:199:ARG:HH21	1.59	0.47
1:A:264:MLY:CH1	2:C:17:ASP:OD2	2.63	0.47
2:C:23:ILE:N	2:C:72:MET:CE	2.78	0.47
2:C:72:MET:HE1	3:C:120:HOH:O	2.14	0.47
3:A:295:HOH:O	2:D:24:HIS:HD2	1.96	0.47
2:D:53:ARG:HD3	3:D:118:HOH:O	2.15	0.46
1:A:264:MLY:HH23	2:C:61:SER:N	2.29	0.46
1:B:196:GLN:HE21	1:B:199:ARG:HH21	1.62	0.46
2:C:8:PHE:CZ	2:C:12:ILE:HD11	2.50	0.46
1:B:93:MLY:HH12	1:B:93:MLY:HD2	1.79	0.45
2:C:72:MET:HE1	3:C:104:HOH:O	2.13	0.45
2:D:23:ILE:HA	2:D:72:MET:HE2	1.98	0.45
1:A:250:SER:O	1:A:254:MLY:HG2	2.17	0.44
2:C:36:PRO:O	2:C:37:THR:CB	2.65	0.44
1:B:271:VAL:HG11	2:D:56:PRO:HD3	2.00	0.44
1:B:264:MLY:HH11	3:D:117:HOH:O	2.16	0.44
1:A:257:ILE:CD1	2:D:20:TRP:CD1	3.01	0.43
1:A:92:SER:OG	1:A:93:MLY:HH23	2.18	0.43
1:B:275:VAL:HG11	2:D:9:MET:HG2	2.01	0.43
1:A:151:GLU:C	1:A:153:ALA:N	2.72	0.42
1:A:78:ALA:HB3	3:A:322:HOH:O	2.18	0.42
2:D:38:PRO:HB2	2:D:84:GLU:HG3	2.01	0.42
1:B:122:MLY:HH12	1:B:165:SER:OG	2.20	0.42
1:A:149:ARG:N	1:A:150:PRO:HD3	2.34	0.42
1:A:106:LEU:HD22	1:A:124:TYR:HE2	1.85	0.42
1:A:125:LEU:HD11	1:A:139:LEU:HD21	2.01	0.42
1:A:247:GLN:OE1	1:A:252:ARG:HG3	2.19	0.41
1:A:149:ARG:N	1:A:150:PRO:CD	2.83	0.41
1:A:154:HIS:NE2	1:A:157:HIS:HB2	2.36	0.41
1:A:186:ARG:O	1:A:189:GLN:HB2	2.21	0.41
2:C:29:LEU:HD23	2:C:29:LEU:HA	1.92	0.41
1:A:254:MLY:HH23	2:D:64:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HD3	3:B:327:HOH:O	2.21	0.41
1:B:99:GLN:O	1:B:103:VAL:HG23	2.21	0.40
1:A:247:GLN:CD	1:A:252:ARG:HD2	2.42	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	187/218 (86%)	172 (92%)	10 (5%)	5 (3%)	5	2
1	B	193/218 (88%)	187 (97%)	5 (3%)	1 (0%)	29	31
2	C	86/92 (94%)	81 (94%)	3 (4%)	2 (2%)	6	3
2	D	80/92 (87%)	80 (100%)	0	0	100	100
All	All	546/620 (88%)	520 (95%)	18 (3%)	8 (2%)	10	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	37	THR
1	A	155	LEU
1	A	190	SER
1	A	247	GLN
1	B	249	GLY
1	A	249	GLY
2	C	36	PRO
1	A	149	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/178 (93%)	154 (93%)	11 (7%)	16	18
1	B	169/178 (95%)	163 (96%)	6 (4%)	35	45
2	C	78/79 (99%)	73 (94%)	5 (6%)	17	20
2	D	72/79 (91%)	69 (96%)	3 (4%)	30	38
All	All	484/514 (94%)	459 (95%)	25 (5%)	23	28

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	96	GLU
1	A	146	LEU
1	A	156	SER
1	A	179	ARG
1	A	198	LEU
1	A	244	GLN
1	A	247	GLN
1	A	250	SER
1	A	271	VAL
1	A	274	GLN
1	B	94	VAL
1	B	113	SER
1	B	165	SER
1	B	179	ARG
1	B	234	PHE
1	B	240	SER
2	C	4	ASP
2	C	37	THR
2	C	43	ARG
2	C	62	ASP
2	C	79	MET
2	D	53	ARG
2	D	61	SER
2	D	79	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	157	HIS
1	A	196	GLN
1	A	280	GLN
1	B	196	GLN
1	B	246	GLN
2	C	31	ASN
2	C	71	GLN
2	C	74	GLN
2	D	24	HIS
2	D	65	GLN
2	D	68	ASN
2	D	75	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	264	1	9,10,11	0.90	0	6,11,13	1.11	0
1	MLY	A	221	1	9,10,11	0.72	0	6,11,13	0.31	0
1	MLY	A	266	1	9,10,11	0.52	0	6,11,13	0.62	0
2	MLY	D	49	2	9,10,11	0.72	0	6,11,13	1.04	0
1	MLY	B	128	1	9,10,11	0.93	0	6,11,13	0.89	0
1	MLY	A	264	1	9,10,11	0.74	0	6,11,13	0.85	0
2	MLY	C	18	2	9,10,11	0.59	0	6,11,13	0.58	0
1	MLY	B	266	1	9,10,11	0.70	0	6,11,13	0.62	0
1	MLY	B	93	1	9,10,11	0.78	0	6,11,13	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	221	1	9,10,11	0.85	0	6,11,13	0.54	0
2	MLY	C	41	2	9,10,11	0.71	0	6,11,13	1.08	0
1	MLY	A	254	1	9,10,11	1.06	0	6,11,13	0.82	0
1	MLY	B	137	1	9,10,11	0.62	0	6,11,13	1.04	0
1	MLY	A	122	1	9,10,11	0.77	0	6,11,13	0.75	0
2	MLY	C	49	2	9,10,11	0.72	0	6,11,13	0.98	0
1	MLY	B	237	1	9,10,11	0.70	0	6,11,13	0.39	0
1	MLY	B	122	1	9,10,11	0.65	0	6,11,13	0.87	0
1	MLY	A	137	1	9,10,11	0.63	0	6,11,13	0.86	0
1	MLY	B	276	1	9,10,11	1.02	0	6,11,13	1.04	0
1	MLY	A	128	1	9,10,11	0.61	0	6,11,13	0.64	0
1	MLY	A	147	1	9,10,11	0.75	0	6,11,13	0.81	0
1	MLY	A	276	1	9,10,11	0.89	0	6,11,13	1.20	0
1	MLY	B	147	1	9,10,11	0.67	0	6,11,13	0.87	0
1	MLY	A	237	1	9,10,11	0.63	0	6,11,13	0.74	0
2	MLY	D	41	2	9,10,11	1.03	0	6,11,13	1.00	0
1	MLY	B	254	1	9,10,11	0.90	0	6,11,13	0.87	0
1	MLY	A	93	1	9,10,11	0.58	0	6,11,13	0.58	0
2	MLY	D	18	2	9,10,11	0.62	0	6,11,13	1.47	2 (33%)

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	264	1	-	3/8/9/11	-
1	MLY	A	221	1	-	3/8/9/11	-
1	MLY	A	266	1	-	0/8/9/11	-
2	MLY	D	49	2	-	0/8/9/11	-
1	MLY	B	128	1	-	2/8/9/11	-
1	MLY	A	264	1	-	4/8/9/11	-
2	MLY	C	18	2	-	0/8/9/11	-
1	MLY	B	266	1	-	2/8/9/11	-
1	MLY	B	93	1	-	2/8/9/11	-
1	MLY	B	221	1	-	0/8/9/11	-
2	MLY	C	41	2	-	3/8/9/11	-
1	MLY	A	254	1	-	2/8/9/11	-
1	MLY	B	137	1	-	3/8/9/11	-
1	MLY	A	122	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	C	49	2	-	1/8/9/11	-
1	MLY	B	237	1	-	1/8/9/11	-
1	MLY	B	122	1	-	1/8/9/11	-
1	MLY	A	137	1	-	5/8/9/11	-
1	MLY	B	276	1	-	0/8/9/11	-
1	MLY	A	128	1	-	3/8/9/11	-
1	MLY	A	147	1	-	0/8/9/11	-
1	MLY	A	276	1	-	2/8/9/11	-
1	MLY	B	147	1	-	1/8/9/11	-
1	MLY	A	237	1	-	2/8/9/11	-
2	MLY	D	41	2	-	4/8/9/11	-
1	MLY	B	254	1	-	2/8/9/11	-
1	MLY	A	93	1	-	2/8/9/11	-
2	MLY	D	18	2	-	5/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	MLY	CG-CD-CE	-2.38	102.23	113.21
2	D	18	MLY	CD-CE-NZ	-2.19	107.86	113.79

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	MLY	N-CA-CB-CG
1	A	264	MLY	C-CA-CB-CG
1	A	137	MLY	C-CA-CB-CG
1	A	128	MLY	C-CA-CB-CG
2	D	18	MLY	C-CA-CB-CG
1	B	266	MLY	CD-CE-NZ-CH2
2	C	41	MLY	CD-CE-NZ-CH2
2	D	41	MLY	CD-CE-NZ-CH2
1	B	254	MLY	CD-CE-NZ-CH2
2	C	49	MLY	CG-CD-CE-NZ
1	B	93	MLY	CG-CD-CE-NZ
2	C	41	MLY	CG-CD-CE-NZ
1	A	122	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	128	MLY	CG-CD-CE-NZ
1	B	137	MLY	CG-CD-CE-NZ
1	B	266	MLY	CD-CE-NZ-CH1
2	C	41	MLY	CD-CE-NZ-CH1
1	B	137	MLY	CD-CE-NZ-CH2
2	D	41	MLY	CD-CE-NZ-CH1
1	B	254	MLY	CD-CE-NZ-CH1
1	B	264	MLY	CG-CD-CE-NZ
1	A	264	MLY	CD-CE-NZ-CH1
1	B	122	MLY	CD-CE-NZ-CH2
1	B	147	MLY	CD-CE-NZ-CH1
1	A	137	MLY	CA-CB-CG-CD
1	A	254	MLY	CG-CD-CE-NZ
1	A	93	MLY	CE-CD-CG-CB
1	A	254	MLY	CE-CD-CG-CB
1	A	93	MLY	CA-CB-CG-CD
1	A	264	MLY	CE-CD-CG-CB
1	A	122	MLY	CE-CD-CG-CB
1	A	237	MLY	CG-CD-CE-NZ
1	A	221	MLY	CA-CB-CG-CD
2	D	41	MLY	CE-CD-CG-CB
1	A	221	MLY	C-CA-CB-CG
1	B	128	MLY	CD-CE-NZ-CH2
1	A	137	MLY	CD-CE-NZ-CH1
1	A	237	MLY	CE-CD-CG-CB
1	A	276	MLY	CE-CD-CG-CB
1	B	93	MLY	CD-CE-NZ-CH1
1	A	264	MLY	CD-CE-NZ-CH2
1	B	137	MLY	CD-CE-NZ-CH1
1	B	128	MLY	CA-CB-CG-CD
2	D	18	MLY	CE-CD-CG-CB
1	B	237	MLY	CE-CD-CG-CB
1	A	122	MLY	CA-CB-CG-CD
2	D	18	MLY	CD-CE-NZ-CH1
2	D	18	MLY	N-CA-CB-CG
1	A	122	MLY	C-CA-CB-CG
2	D	41	MLY	C-CA-CB-CG
2	D	18	MLY	CD-CE-NZ-CH2
1	A	128	MLY	CA-CB-CG-CD
1	A	276	MLY	CD-CE-NZ-CH1
1	A	137	MLY	CG-CD-CE-NZ
1	B	264	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	137	MLY	CE-CD-CG-CB
1	B	264	MLY	CA-CB-CG-CD

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	264	MLY	1	0
1	A	264	MLY	4	0
2	C	18	MLY	2	0
1	B	93	MLY	1	0
1	A	254	MLY	2	0
1	B	137	MLY	1	0
1	B	122	MLY	1	0
1	B	276	MLY	1	0
1	A	128	MLY	1	0
1	A	93	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	191/218 (87%)	0.68	31 (16%) 1 1	29, 44, 81, 90	0
1	B	195/218 (89%)	0.07	6 (3%) 49 47	27, 37, 53, 63	0
2	C	88/92 (95%)	0.36	3 (3%) 45 43	32, 43, 53, 56	0
2	D	82/92 (89%)	0.31	5 (6%) 21 20	31, 39, 46, 56	0
All	All	556/620 (89%)	0.36	45 (8%) 12 10	27, 41, 67, 90	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	7.5
1	B	247	GLN	6.5
1	A	247	GLN	5.8
1	B	148	GLY	5.7
1	A	148	GLY	5.7
1	A	150	PRO	4.9
1	A	106	LEU	4.5
1	A	191	GLY	4.4
1	A	192	VAL	4.2
2	C	2	ALA	3.9
2	C	34	SER	3.6
1	A	91	LEU	3.6
1	A	248	SER	3.4
1	A	249	GLY	3.2
1	A	101	GLN	3.2
2	C	92	ASP	3.2
1	A	107	LEU	3.1
1	A	149	ARG	3.1
1	B	78	ALA	3.1
2	D	29	LEU	2.9
1	A	151	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	2.8
1	A	104	SER	2.8
1	A	92	SER	2.8
1	A	246	GLN	2.7
1	A	78	ALA	2.7
1	A	154	HIS	2.7
2	D	26	ILE	2.6
2	D	15	LEU	2.6
1	A	155	LEU	2.5
1	A	112	ASN	2.4
1	A	252	ARG	2.4
1	A	94	VAL	2.3
1	A	81	SER	2.3
2	D	37	THR	2.2
1	B	186	ARG	2.2
1	B	82	ASP	2.2
1	A	108	SER	2.2
1	A	235	LEU	2.1
2	D	12	ILE	2.1
1	A	111	SER	2.1
1	A	225	ASN	2.1
1	A	168	GLU	2.0
1	B	85	GLU	2.0
1	A	145	ALA	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	147	11/12	0.78	0.53	72,74,76,77	0
1	MLY	A	93	11/12	0.81	0.31	80,81,84,84	0
1	MLY	A	276	11/12	0.84	0.17	42,44,65,65	0
1	MLY	B	147	11/12	0.86	0.19	45,48,61,61	0
1	MLY	B	276	11/12	0.86	0.19	31,32,48,49	0
1	MLY	B	254	11/12	0.87	0.20	36,40,64,64	0
2	MLY	D	49	11/12	0.89	0.17	36,37,41,44	0
1	MLY	B	221	11/12	0.89	0.29	38,41,72,73	0
1	MLY	A	254	11/12	0.90	0.20	39,40,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLY	D	41	11/12	0.90	0.19	38,41,57,59	0
2	MLY	C	49	11/12	0.90	0.19	41,42,59,61	0
1	MLY	A	137	11/12	0.90	0.22	38,42,61,62	0
1	MLY	B	93	11/12	0.91	0.35	53,55,73,74	0
2	MLY	C	41	11/12	0.93	0.13	47,49,59,61	0
1	MLY	A	237	11/12	0.93	0.16	37,38,51,52	0
1	MLY	A	128	11/12	0.93	0.12	33,34,44,45	0
1	MLY	B	237	11/12	0.93	0.14	32,33,54,54	0
1	MLY	B	128	11/12	0.93	0.12	36,37,41,41	0
1	MLY	A	266	11/12	0.94	0.14	35,39,40,46	0
2	MLY	C	18	11/12	0.94	0.22	32,33,40,46	0
1	MLY	B	137	11/12	0.94	0.15	31,33,49,51	0
1	MLY	A	122	11/12	0.94	0.12	31,33,50,51	0
1	MLY	B	264	11/12	0.95	0.13	31,33,49,49	0
1	MLY	A	264	11/12	0.95	0.15	36,37,62,63	0
1	MLY	A	221	11/12	0.95	0.17	42,44,60,62	0
1	MLY	B	266	11/12	0.95	0.15	34,37,59,61	0
1	MLY	B	122	11/12	0.95	0.15	29,32,46,46	0
2	MLY	D	18	11/12	0.96	0.15	36,37,41,41	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.