



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

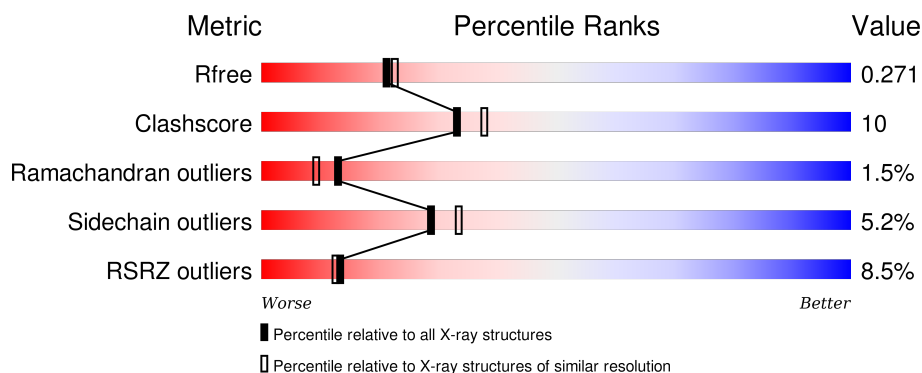
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>15%</div> <div>71%</div> <div>18%</div> <div>7%</div> </div>
1	B	218	<div> <div>3%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
2	C	92	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>6%</div> </div>
2	D	92	<div> <div>5%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div>

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

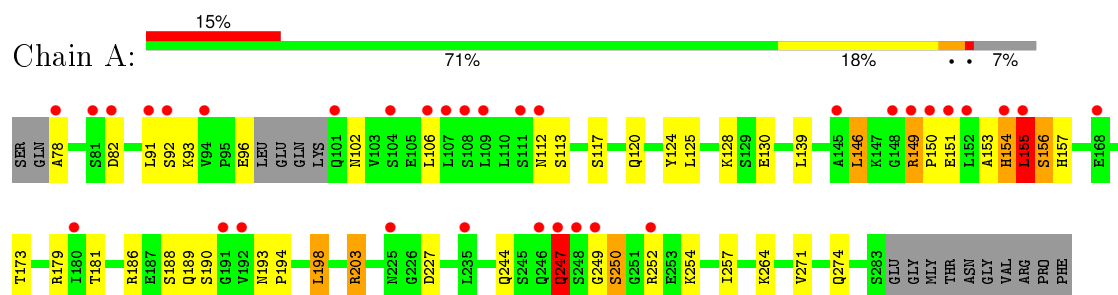
- Molecule 3 is water.

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		

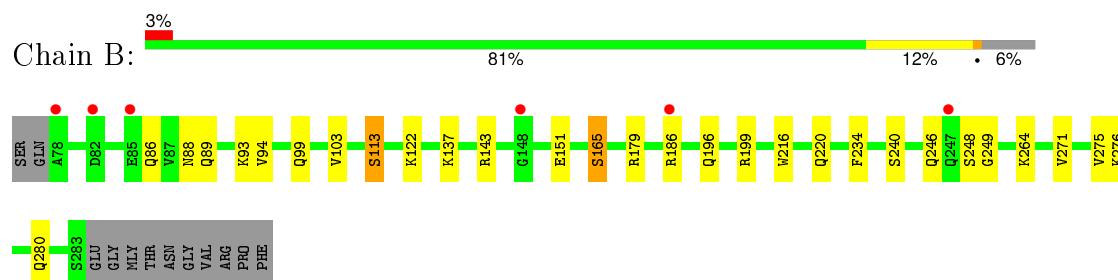
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

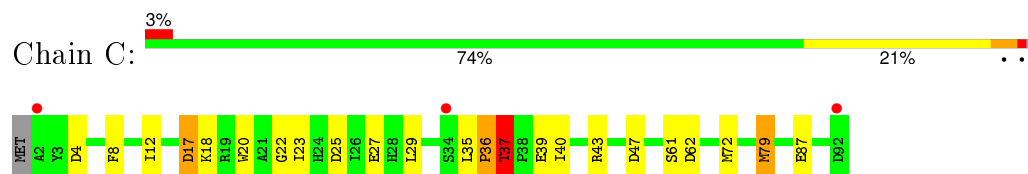
• Molecule 1: Secretion control protein



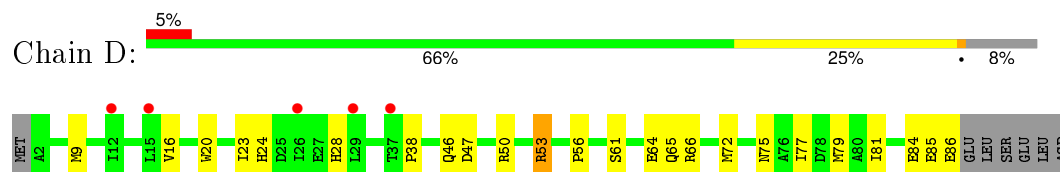
• Molecule 1: Secretion control protein



• Molecule 2: protein type A



• Molecule 2: protein type A



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.250 0.213 , 0.271	Depositor DCC
R_{free} test set	1949 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 38190 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4878	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	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
2:C:22:GLY:HA2	2:C:72:MET:HE2	1.78	0.64
1:A:146:LEU:CD2	1:A:156:SER:HB2	2.28	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
2:C:36:PRO:O	2:C:37:THR:HB	2.03	0.58
1:A:188:SER:HA	1:A:193:ASN:O	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:B:196:GLN:NE2	1:B:199:ARG:HE	2.07	0.53
1:A:128:MLY:HE2	3:A:303:HOH:O	2.09	0.53
1:A:264:MLY:HH11	2:C:17:ASP:HA	1.92	0.52
2:C:37:THR:HG22	2:C:40:ILE:H	1.74	0.52
1:B:216:TRP:O	1:B:220:GLN:HG2	2.09	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:D:20:TRP:H	2:D:65:GLN:NE2	2.07	0.50
2:C:87:GLU:HB3	3:C:125:HOH:O	2.10	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
2:C:18:MLY:HH12	2:D:28:HIS:HB3	1.94	0.49
1:A:112:ASN:O	1:A:113:SER:OG	2.29	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
2:C:23:ILE:N	2:C:72:MET:CE	2.78	0.47
1:A:264:MLY:CH1	2:C:17:ASP:OD2	2.63	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:B:196:GLN:HE21	1:B:199:ARG:HH21	1.62	0.46
1:A:264:MLY:HH23	2:C:61:SER:N	2.29	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:254:MLY:HH23	2:D:64:GLU:OE2	2.21	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

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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%)	6	3
1	B	193/218 (88%)	187 (97%)	5 (3%)	1 (0%)	34	35
2	C	86/92 (94%)	81 (94%)	3 (4%)	2 (2%)	8	4
2	D	80/92 (87%)	80 (100%)	0	0	100	100
All	All	546/620 (88%)	520 (95%)	18 (3%)	8 (2%)	13	9

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%)	20	21
1	B	169/178 (95%)	163 (96%)	6 (4%)	42	52
2	C	78/79 (99%)	73 (94%)	5 (6%)	22	24
2	D	72/79 (91%)	69 (96%)	3 (4%)	36	44
All	All	484/514 (94%)	459 (95%)	25 (5%)	29	33

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	A	122	1	9,10,11	0.73	0	9,11,13	0.93	1 (11%)
1	MLY	A	128	1	9,10,11	0.60	0	9,11,13	1.08	1 (11%)
1	MLY	A	137	1	9,10,11	0.60	0	9,11,13	1.19	1 (11%)
1	MLY	A	147	1	9,10,11	0.71	0	9,11,13	1.07	1 (11%)
1	MLY	A	221	1	9,10,11	0.76	0	9,11,13	0.67	0
1	MLY	A	237	1	9,10,11	0.59	0	9,11,13	0.94	0
1	MLY	A	254	1	9,10,11	1.23	1 (11%)	9,11,13	1.01	1 (11%)
1	MLY	A	264	1	9,10,11	0.79	0	9,11,13	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	266	1	9,10,11	0.49	0	9,11,13	1.15	1 (11%)
1	MLY	A	276	1	9,10,11	0.86	0	9,11,13	1.19	1 (11%)
1	MLY	A	93	1	9,10,11	0.57	0	9,11,13	0.92	1 (11%)
1	MLY	B	122	1	9,10,11	0.65	0	9,11,13	1.04	1 (11%)
1	MLY	B	128	1	9,10,11	1.06	1 (11%)	9,11,13	1.02	1 (11%)
1	MLY	B	137	1	9,10,11	0.64	0	9,11,13	1.15	1 (11%)
1	MLY	B	147	1	9,10,11	0.69	0	9,11,13	1.05	0
1	MLY	B	221	1	9,10,11	0.81	0	9,11,13	0.83	0
1	MLY	B	237	1	9,10,11	0.67	0	9,11,13	0.85	1 (11%)
1	MLY	B	254	1	9,10,11	0.86	0	9,11,13	0.98	0
1	MLY	B	264	1	9,10,11	1.00	1 (11%)	9,11,13	1.15	0
1	MLY	B	266	1	9,10,11	0.67	0	9,11,13	0.74	0
1	MLY	B	276	1	9,10,11	1.07	0	9,11,13	1.20	1 (11%)
1	MLY	B	93	1	9,10,11	0.74	0	9,11,13	1.03	1 (11%)
2	MLY	C	18	2	9,10,11	0.53	0	9,11,13	0.98	0
2	MLY	C	41	2	9,10,11	0.80	0	9,11,13	1.17	0
2	MLY	C	49	2	9,10,11	0.77	0	9,11,13	1.03	0
2	MLY	D	18	2	9,10,11	0.68	0	9,11,13	1.66	4 (44%)
2	MLY	D	41	2	9,10,11	0.98	0	9,11,13	1.28	1 (11%)
2	MLY	D	49	2	9,10,11	0.91	1 (11%)	9,11,13	1.20	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	122	1	-	0/7/9/11	0/0/0/0
1	MLY	A	128	1	-	0/7/9/11	0/0/0/0
1	MLY	A	137	1	-	0/7/9/11	0/0/0/0
1	MLY	A	147	1	-	0/7/9/11	0/0/0/0
1	MLY	A	221	1	-	0/7/9/11	0/0/0/0
1	MLY	A	237	1	-	0/7/9/11	0/0/0/0
1	MLY	A	254	1	-	0/7/9/11	0/0/0/0
1	MLY	A	264	1	-	0/7/9/11	0/0/0/0
1	MLY	A	266	1	-	0/7/9/11	0/0/0/0
1	MLY	A	276	1	-	0/7/9/11	0/0/0/0
1	MLY	A	93	1	-	0/7/9/11	0/0/0/0
1	MLY	B	122	1	-	0/7/9/11	0/0/0/0
1	MLY	B	128	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	137	1	-	0/7/9/11	0/0/0/0
1	MLY	B	147	1	-	0/7/9/11	0/0/0/0
1	MLY	B	221	1	-	0/7/9/11	0/0/0/0
1	MLY	B	237	1	-	0/7/9/11	0/0/0/0
1	MLY	B	254	1	-	0/7/9/11	0/0/0/0
1	MLY	B	264	1	-	0/7/9/11	0/0/0/0
1	MLY	B	266	1	-	0/7/9/11	0/0/0/0
1	MLY	B	276	1	-	0/7/9/11	0/0/0/0
1	MLY	B	93	1	-	0/7/9/11	0/0/0/0
2	MLY	C	18	2	-	0/7/9/11	0/0/0/0
2	MLY	C	41	2	-	0/7/9/11	0/0/0/0
2	MLY	C	49	2	-	0/7/9/11	0/0/0/0
2	MLY	D	18	2	-	0/7/9/11	0/0/0/0
2	MLY	D	41	2	-	0/7/9/11	0/0/0/0
2	MLY	D	49	2	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	MLY	CB-CA	-2.88	1.51	1.53
2	D	49	MLY	CB-CA	-2.36	1.51	1.53
1	B	264	MLY	CB-CA	-2.04	1.51	1.53
1	B	128	MLY	CB-CA	2.58	1.56	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	MLY	O-C-CA	-3.08	117.46	125.49
1	A	128	MLY	O-C-CA	-2.56	118.83	125.49
2	D	41	MLY	O-C-CA	-2.53	118.89	125.49
1	B	276	MLY	O-C-CA	-2.51	118.94	125.49
2	D	18	MLY	CB-CA-N	-2.43	103.61	110.52
2	D	18	MLY	CD-CE-NZ	-2.35	107.86	113.92
2	D	18	MLY	CG-CD-CE	-2.34	102.23	113.27
1	B	137	MLY	O-C-CA	-2.34	119.40	125.49
1	B	93	MLY	O-C-CA	-2.33	119.41	125.49
1	B	122	MLY	O-C-CA	-2.24	119.65	125.49
2	D	49	MLY	O-C-CA	-2.18	119.81	125.49
1	A	254	MLY	O-C-CA	-2.18	119.81	125.49
2	D	18	MLY	O-C-CA	-2.14	119.92	125.49
1	A	93	MLY	O-C-CA	-2.13	119.94	125.49
1	A	147	MLY	O-C-CA	-2.10	120.02	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	MLY	O-C-CA	-2.09	120.06	125.49
1	B	237	MLY	O-C-CA	-2.07	120.10	125.49
1	A	137	MLY	CB-CA-N	-2.04	104.72	110.52
1	A	276	MLY	O-C-CA	-2.03	120.21	125.49
1	B	128	MLY	O-C-CA	-2.01	120.25	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	128	MLY	1	0
1	A	254	MLY	2	0
1	A	264	MLY	4	0
1	A	93	MLY	1	0
1	B	122	MLY	1	0
1	B	137	MLY	1	0
1	B	264	MLY	1	0
1	B	276	MLY	1	0
1	B	93	MLY	1	0
2	C	18	MLY	2	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, 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	191/218 (87%)	0.75	33 (17%) 2 2	29, 44, 81, 90	0
1	B	195/218 (89%)	0.12	6 (3%) 52 51	27, 37, 53, 63	0
2	C	88/92 (95%)	0.42	3 (3%) 49 47	32, 43, 53, 56	0
2	D	82/92 (89%)	0.37	5 (6%) 25 24	31, 39, 46, 56	0
All	All	556/620 (89%)	0.42	47 (8%) 13 12	27, 41, 67, 90	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	7.8
1	B	247	GLN	6.6
1	A	247	GLN	5.9
1	A	148	GLY	5.9
1	B	148	GLY	5.9
1	A	150	PRO	5.1
1	A	106	LEU	4.6
1	A	191	GLY	4.6
1	A	192	VAL	4.4
2	C	2	ALA	4.0
2	C	34	SER	3.8
1	A	91	LEU	3.7
1	A	248	SER	3.5
1	A	249	GLY	3.4
2	C	92	ASP	3.3
1	A	101	GLN	3.3
1	B	78	ALA	3.2
1	A	107	LEU	3.2
1	A	149	ARG	3.2
2	D	29	LEU	3.1
1	A	180	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	151	GLU	3.0
1	A	104	SER	2.9
1	A	92	SER	2.9
1	A	246	GLN	2.8
1	A	78	ALA	2.8
1	A	154	HIS	2.8
2	D	26	ILE	2.7
2	D	15	LEU	2.7
1	A	155	LEU	2.6
1	A	112	ASN	2.6
1	A	94	VAL	2.5
1	A	252	ARG	2.5
1	A	81	SER	2.4
2	D	37	THR	2.3
1	B	186	ARG	2.3
1	A	108	SER	2.3
1	B	82	ASP	2.3
1	A	111	SER	2.2
2	D	12	ILE	2.2
1	A	235	LEU	2.2
1	A	225	ASN	2.2
1	A	145	ALA	2.2
1	A	168	GLU	2.1
1	A	82	ASP	2.1
1	B	85	GLU	2.1
1	A	109	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MLY	B	264	11/12	0.95	0.13	-	31,33,49,49	0
1	MLY	A	221	11/12	0.95	0.17	-	42,44,60,62	0
1	MLY	A	266	11/12	0.94	0.14	-	35,39,40,46	0
2	MLY	D	49	11/12	0.89	0.17	-	36,37,41,44	0
1	MLY	B	128	11/12	0.93	0.12	-	36,37,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLY	A	264	11/12	0.95	0.15	-	36,37,62,63	0
2	MLY	C	18	11/12	0.94	0.22	-	32,33,40,46	0
1	MLY	B	266	11/12	0.95	0.15	-	34,37,59,61	0
1	MLY	B	93	11/12	0.91	0.35	-	53,55,73,74	0
1	MLY	B	221	11/12	0.90	0.29	-	38,41,72,73	0
2	MLY	C	41	11/12	0.93	0.13	-	47,49,59,61	0
1	MLY	A	254	11/12	0.90	0.20	-	39,40,64,65	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
2	MLY	C	49	11/12	0.90	0.19	-	41,42,59,61	0
1	MLY	B	237	11/12	0.93	0.14	-	32,33,54,54	0
1	MLY	B	122	11/12	0.95	0.15	-	29,32,46,46	0
1	MLY	A	137	11/12	0.90	0.22	-	38,42,61,62	0
1	MLY	B	276	11/12	0.86	0.19	-	31,32,48,49	0
1	MLY	A	128	11/12	0.93	0.12	-	33,34,44,45	0
1	MLY	A	147	11/12	0.79	0.53	-	72,74,76,77	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	A	237	11/12	0.93	0.16	-	37,38,51,52	0
2	MLY	D	41	11/12	0.89	0.19	-	38,41,57,59	0
1	MLY	B	254	11/12	0.87	0.20	-	36,40,64,64	0
1	MLY	A	93	11/12	0.81	0.31	-	80,81,84,84	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.