



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 04:20 PM EDT

PDB ID : 9BJ6 / pdb_00009bj6
Title : Crystal structure of the HEPN family member AbiV, an RNase in a two-component antiphage system in *Lactococcus lactis*
Authors : Picard, M.-E.; Moineau, S.; Shi, R.
Deposited on : 2024-04-25
Resolution : 2.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

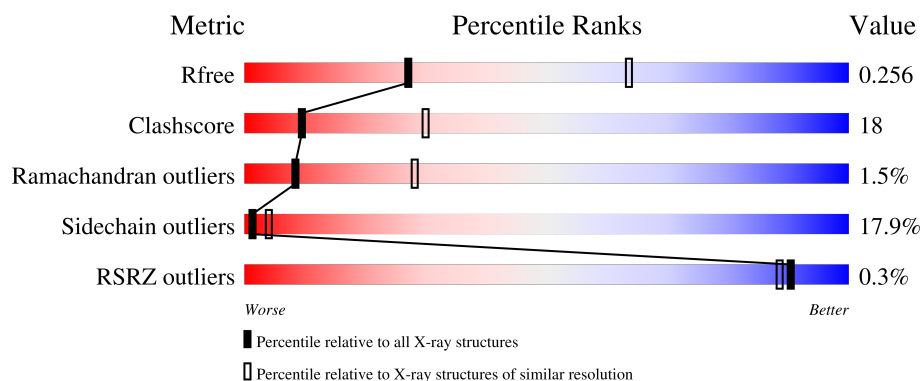
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	
1	B	207	
1	C	207	
1	D	207	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5383 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 AbiV family abortive infection protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1502	949	245	302	6			
1	B	164	Total	C	N	O	S	0	0	0
			1290	821	200	264	5			
1	C	167	Total	C	N	O	S	0	0	0
			1312	833	203	271	5			
1	D	158	Total	C	N	O	S	0	0	0
			1246	792	192	257	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	-	expression tag	UNP Q9AGY3
A	203	HIS	-	expression tag	UNP Q9AGY3
A	204	HIS	-	expression tag	UNP Q9AGY3
A	205	HIS	-	expression tag	UNP Q9AGY3
A	206	HIS	-	expression tag	UNP Q9AGY3
A	207	HIS	-	expression tag	UNP Q9AGY3
B	202	HIS	-	expression tag	UNP Q9AGY3
B	203	HIS	-	expression tag	UNP Q9AGY3
B	204	HIS	-	expression tag	UNP Q9AGY3
B	205	HIS	-	expression tag	UNP Q9AGY3
B	206	HIS	-	expression tag	UNP Q9AGY3
B	207	HIS	-	expression tag	UNP Q9AGY3
C	202	HIS	-	expression tag	UNP Q9AGY3
C	203	HIS	-	expression tag	UNP Q9AGY3
C	204	HIS	-	expression tag	UNP Q9AGY3
C	205	HIS	-	expression tag	UNP Q9AGY3
C	206	HIS	-	expression tag	UNP Q9AGY3
C	207	HIS	-	expression tag	UNP Q9AGY3
D	202	HIS	-	expression tag	UNP Q9AGY3
D	203	HIS	-	expression tag	UNP Q9AGY3
D	204	HIS	-	expression tag	UNP Q9AGY3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	205	HIS	-	expression tag	UNP Q9AGY3
D	206	HIS	-	expression tag	UNP Q9AGY3
D	207	HIS	-	expression tag	UNP Q9AGY3

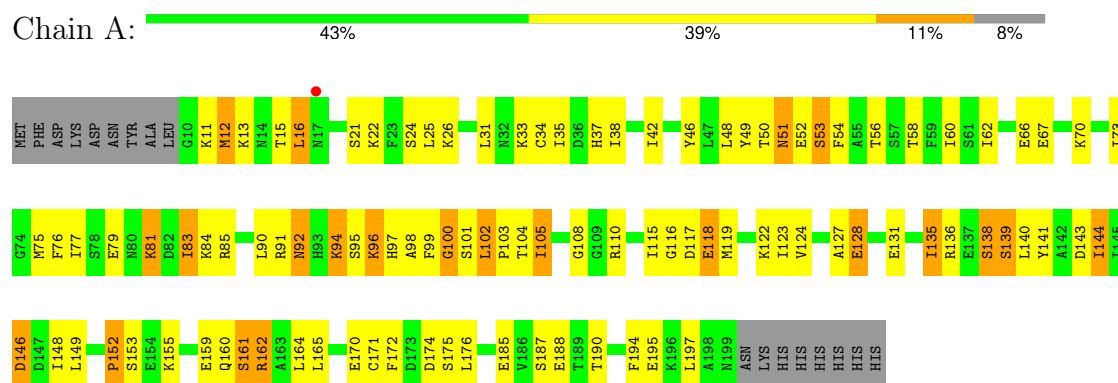
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	9	Total O 9 9	0	0
2	C	6	Total O 6 6	0	0
2	D	13	Total O 13 13	0	0

3 Residue-property plots [i](#)

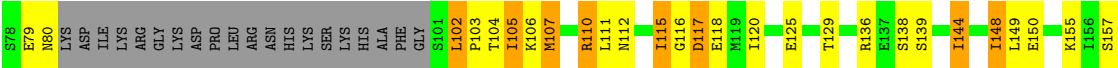
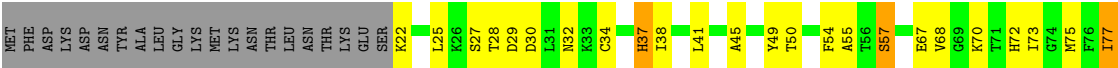
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: AbiV family abortive infection protein





● Molecule 1: AbiV family abortive infection protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.17Å 144.96Å 55.56Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	72.48 – 2.92 72.48 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.48-2.92) 99.1 (72.48-2.92)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.254 0.214 , 0.256	Depositor DCC
R_{free} test set	889 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.086 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5383	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.19	2/1501 (0.1%)	1.68	13/2019 (0.6%)
1	B	1.14	0/1286	1.60	9/1735 (0.5%)
1	C	1.15	3/1307 (0.2%)	1.71	6/1762 (0.3%)
1	D	1.19	3/1240 (0.2%)	1.60	3/1674 (0.2%)
All	All	1.17	8/5334 (0.1%)	1.65	31/7190 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	HIS	CD2-NE2	8.91	1.47	1.37
1	D	37	HIS	CG-ND1	7.66	1.46	1.38
1	A	95	SER	C-O	6.16	1.31	1.23
1	C	149	LEU	C-O	5.75	1.30	1.24
1	C	99	PHE	C-O	5.75	1.31	1.24
1	A	176	LEU	C-O	5.52	1.31	1.23
1	C	150	GLU	C-O	5.40	1.30	1.24
1	D	37	HIS	ND1-CE1	5.39	1.38	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ASP	CA-CB-CG	7.55	120.16	112.60
1	C	149	LEU	O-C-N	7.01	131.64	123.02
1	A	116	GLY	CA-C-O	-6.52	117.73	122.23
1	B	108	GLY	CA-C-N	6.30	126.97	120.60
1	B	108	GLY	C-N-CA	6.30	126.97	120.60
1	A	108	GLY	CA-C-N	6.16	125.95	120.10
1	A	108	GLY	C-N-CA	6.16	125.95	120.10
1	A	174	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	169	ILE	N-CA-C	-5.94	104.95	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	GLY	CA-C-O	-5.84	116.51	122.59
1	A	51	ASN	N-CA-C	-5.70	106.22	112.72
1	A	46	TYR	CA-C-N	5.58	128.02	120.38
1	A	46	TYR	C-N-CA	5.58	128.02	120.38
1	A	188	GLU	CA-C-N	5.55	127.66	120.44
1	A	188	GLU	C-N-CA	5.55	127.66	120.44
1	D	29	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	195	GLU	CA-C-N	5.43	127.55	120.28
1	B	195	GLU	C-N-CA	5.43	127.55	120.28
1	C	50	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	195	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	59	PHE	CA-C-N	5.33	127.76	120.46
1	B	59	PHE	C-N-CA	5.33	127.76	120.46
1	B	183	SER	CA-C-O	-5.31	114.89	120.63
1	B	171	CYS	CB-CA-C	-5.22	102.12	110.79
1	D	174	ASP	CA-C-O	-5.19	114.92	120.42
1	C	20	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	73	ILE	CA-C-N	5.16	126.64	120.13
1	A	73	ILE	C-N-CA	5.16	126.64	120.13
1	C	52	GLU	CA-C-O	-5.08	115.65	121.54
1	D	37	HIS	O-C-N	5.08	127.51	122.08
1	A	146	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1502	0	1511	73	0
1	B	1290	0	1281	49	0
1	C	1312	0	1298	40	0
1	D	1246	0	1238	37	0
2	A	5	0	0	0	0
2	B	9	0	0	0	0
2	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	13	0	0	0	0
All	All	5383	0	5328	188	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 18.

All (188) 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:B:75:MET:HE1	1:B:179:TYR:CE1	1.68	1.28
1:B:75:MET:HE1	1:B:179:TYR:CD1	1.88	1.07
1:C:75:MET:HE1	1:C:179:TYR:CE2	2.00	0.95
1:C:171:CYS:O	1:C:175:SER:HB2	1.69	0.91
1:A:160:GLN:O	1:A:164:LEU:HD12	1.69	0.91
1:B:75:MET:HE1	1:B:179:TYR:HE1	1.22	0.87
1:D:125:GLU:O	1:D:129:THR:HG23	1.79	0.83
1:B:75:MET:CE	1:B:179:TYR:CE1	2.59	0.80
1:B:75:MET:CE	1:B:179:TYR:HE1	1.93	0.80
1:C:120:ILE:O	1:C:124:VAL:HG23	1.82	0.80
1:A:92:ASN:OD1	1:A:94:LYS:HB3	1.83	0.78
1:C:69:GLY:HA2	1:C:101:SER:HB3	1.65	0.78
1:A:110:ARG:HD2	1:A:194:PHE:CZ	2.18	0.77
1:C:75:MET:HE1	1:C:179:TYR:CD2	2.20	0.76
1:D:105:ILE:HD12	1:D:105:ILE:H	1.51	0.75
1:C:55:ALA:O	1:C:139:SER:HB2	1.87	0.75
1:A:165:LEU:HD23	1:A:197:LEU:HD11	1.69	0.75
1:D:110:ARG:NH2	1:D:170:GLU:OE2	2.22	0.73
1:B:37:HIS:NE2	1:B:67:GLU:OE2	2.21	0.73
1:C:46:TYR:O	1:C:50:THR:HG23	1.92	0.70
1:D:34:CYS:O	1:D:37:HIS:HB3	1.91	0.70
1:C:140:LEU:HD23	1:C:141:TYR:CE2	2.27	0.70
1:D:150:GLU:OE1	1:D:155:LYS:HE2	1.92	0.69
1:B:115:ILE:HG13	1:B:119:MET:HB3	1.74	0.69
1:C:23:PHE:CD2	1:D:144:ILE:HD12	2.29	0.68
1:A:91:ARG:NH2	1:B:143:ASP:OD2	2.27	0.67
1:A:34:CYS:O	1:A:37:HIS:HB3	1.94	0.67
1:B:55:ALA:O	1:B:139:SER:HB2	1.94	0.67
1:C:106:LYS:O	1:C:112:ASN:ND2	2.28	0.65
1:A:160:GLN:O	1:A:164:LEU:CD1	2.44	0.65
1:D:75:MET:HE1	1:D:179:TYR:CE2	2.31	0.65
1:B:105:ILE:HG23	1:B:112:ASN:OD1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:OG1	1:A:161:SER:HB2	1.96	0.64
1:D:115:ILE:HD11	1:D:120:ILE:HG12	1.79	0.64
1:A:25:LEU:HB2	1:A:75:MET:HA	1.79	0.64
1:A:103:PRO:HD3	1:A:171:CYS:SG	2.38	0.64
1:A:164:LEU:HD12	1:A:164:LEU:H	1.63	0.63
1:C:39:SER:OG	1:C:43:MLY:HH22	1.99	0.63
1:A:16:LEU:H	1:A:16:LEU:HD12	1.63	0.63
1:B:67:GLU:OE1	1:B:70:LYS:HE2	1.99	0.63
1:A:102:LEU:H	1:A:102:LEU:HD13	1.65	0.62
1:D:136:ARG:O	1:D:139:SER:OG	2.17	0.61
1:A:49:TYR:HD2	1:A:161:SER:HG	1.48	0.61
1:A:123:ILE:O	1:A:127:ALA:N	2.34	0.59
1:A:131:GLU:O	1:A:135:ILE:HG13	2.02	0.59
1:A:26:LYS:NZ	1:A:79:GLU:OE2	2.36	0.59
1:A:144:ILE:HG21	1:B:22:LYS:O	2.03	0.58
1:D:165:LEU:HD23	1:D:197:LEU:HD11	1.85	0.58
1:D:54:PHE:CZ	1:D:158:MLY:HD3	2.38	0.58
1:D:38:ILE:HD13	1:D:68:VAL:HG22	1.84	0.58
1:A:124:VAL:HA	1:A:127:ALA:HB3	1.86	0.57
1:A:49:TYR:CZ	1:A:162:ARG:HB2	2.38	0.57
1:A:110:ARG:HD2	1:A:194:PHE:CE2	2.39	0.57
1:B:75:MET:HE1	1:B:179:TYR:HD1	1.62	0.57
1:C:105:ILE:HG22	1:C:112:ASN:HD21	1.70	0.57
1:C:26:LYS:NZ	1:C:79:GLU:OE2	2.29	0.57
1:C:75:MET:CE	1:C:179:TYR:CE2	2.82	0.57
1:A:110:ARG:NE	1:A:170:GLU:OE2	2.35	0.56
1:B:31:LEU:HD22	1:B:75:MET:SD	2.45	0.56
1:A:49:TYR:HD2	1:A:161:SER:OG	1.89	0.56
1:C:112:ASN:OD1	1:C:117:ASP:OD1	2.24	0.56
1:C:24:SER:CB	1:C:79:GLU:HG3	2.36	0.56
1:B:70:LYS:O	1:B:73:ILE:HG22	2.06	0.55
1:C:117:ASP:O	1:C:121:ASP:OD1	2.23	0.55
1:B:58:THR:HG23	1:B:164:LEU:HD12	1.89	0.55
1:A:141:TYR:O	1:A:152:PRO:HG3	2.06	0.55
1:C:24:SER:HB3	1:C:79:GLU:HG3	1.88	0.55
1:B:178:GLY:HA2	1:B:184:PHE:CE1	2.43	0.54
1:A:11:LYS:HD3	1:A:102:LEU:CD1	2.38	0.54
1:D:72:HIS:CD2	1:D:175:SER:O	2.60	0.54
1:A:105:ILE:HD13	1:A:105:ILE:O	2.08	0.54
1:C:170:GLU:OE2	1:C:170:GLU:HA	2.08	0.54
1:D:116:GLY:O	1:D:118:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:O	1:A:101:SER:N	2.41	0.53
1:A:119:MET:O	1:A:122:LYS:HB3	2.07	0.53
1:C:150:GLU:CD	1:C:155:LYS:HE2	2.34	0.53
1:A:81:LYS:HE3	1:B:147:ASP:OD1	2.09	0.53
1:C:172:PHE:CE1	1:C:190:THR:HG21	2.44	0.52
1:A:11:LYS:CD	1:A:102:LEU:HD11	2.40	0.52
1:B:37:HIS:CD2	1:B:67:GLU:OE2	2.62	0.52
1:A:102:LEU:HD13	1:A:102:LEU:N	2.26	0.51
1:D:67:GLU:OE1	1:D:70:LYS:HE2	2.11	0.51
1:D:37:HIS:CD2	1:D:67:GLU:OE2	2.63	0.51
1:D:159:GLU:HG3	1:D:160:GLN:N	2.27	0.50
1:B:194:PHE:CD1	1:B:194:PHE:C	2.90	0.49
1:A:194:PHE:C	1:A:194:PHE:CD1	2.90	0.49
1:A:141:TYR:O	1:A:152:PRO:CG	2.61	0.49
1:A:171:CYS:O	1:A:175:SER:HB2	2.11	0.49
1:C:36:ASP:O	1:C:39:SER:HB3	2.13	0.49
1:D:75:MET:HE1	1:D:179:TYR:CZ	2.47	0.49
1:A:33:LYS:HD2	1:B:149:LEU:HD23	1.95	0.48
1:A:67:GLU:OE2	1:B:141:TYR:HA	2.13	0.48
1:D:199:ASN:C	1:D:199:ASN:HD22	2.21	0.48
1:A:84:LYS:HG2	1:A:85:ARG:H	1.77	0.48
1:D:25:LEU:HD22	1:D:30:ASP:HB3	1.95	0.48
1:A:12:MET:HB2	1:A:100:GLY:O	2.13	0.48
1:A:11:LYS:HE3	1:A:128:GLU:OE1	2.14	0.48
1:C:112:ASN:O	1:C:116:GLY:N	2.46	0.48
1:D:144:ILE:HA	1:D:148:ILE:O	2.14	0.48
1:C:172:PHE:HE1	1:C:190:THR:HG21	1.79	0.48
1:D:77:ILE:HD12	1:D:77:ILE:HA	1.77	0.48
1:D:45:ALA:O	1:D:57:SER:OG	2.27	0.47
1:A:12:MET:CE	1:A:101:SER:HB2	2.43	0.47
1:C:69:GLY:CA	1:C:101:SER:HB3	2.41	0.47
1:D:106:LYS:O	1:D:112:ASN:ND2	2.47	0.47
1:C:38:ILE:O	1:C:39:SER:C	2.58	0.47
1:D:107:MET:HE2	1:D:107:MET:HB3	1.67	0.47
1:B:103:PRO:HD3	1:B:171:CYS:SG	2.55	0.47
1:B:125:GLU:O	1:B:129:THR:HG23	2.15	0.47
1:C:144:ILE:HG22	1:C:144:ILE:O	2.15	0.47
1:C:194:PHE:C	1:C:194:PHE:CD1	2.93	0.47
1:D:105:ILE:HD12	1:D:105:ILE:N	2.27	0.47
1:A:138:SER:O	1:A:152:PRO:HA	2.15	0.47
1:A:124:VAL:O	1:A:128:GLU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ARG:NH2	1:C:170:GLU:OE2	2.45	0.46
1:A:49:TYR:CE2	1:A:162:ARG:HB2	2.50	0.46
1:A:11:LYS:HD3	1:A:102:LEU:HD11	1.98	0.46
1:B:55:ALA:HB1	1:B:152:PRO:HB3	1.97	0.46
1:A:96:LYS:HE3	1:A:97:HIS:CE1	2.51	0.45
1:A:172:PHE:CE1	1:A:190:THR:HG21	2.51	0.45
1:B:42:ILE:HG12	1:B:64:ILE:HD13	1.97	0.45
1:A:16:LEU:HB3	1:A:77:ILE:HA	1.98	0.45
1:A:136:ARG:O	1:A:139:SER:OG	2.29	0.45
1:A:110:ARG:HD2	1:A:194:PHE:CE1	2.50	0.45
1:B:48:LEU:HD13	1:B:56:THR:HG22	1.98	0.45
1:A:38:ILE:O	1:A:42:ILE:HG13	2.16	0.45
1:A:141:TYR:O	1:A:152:PRO:HD3	2.17	0.45
1:C:178:GLY:HA2	1:C:184:PHE:CZ	2.52	0.45
1:D:25:LEU:CD2	1:D:30:ASP:HB3	2.47	0.45
1:D:55:ALA:O	1:D:139:SER:HB2	2.17	0.45
1:B:173:ASP:HA	1:B:177:VAL:HG23	1.99	0.45
1:B:178:GLY:HA2	1:B:184:PHE:CZ	2.52	0.45
1:A:66:GLU:OE1	1:A:136:ARG:NH1	2.50	0.44
1:A:96:LYS:HD2	1:A:128:GLU:O	2.17	0.44
1:A:37:HIS:CE1	1:B:140:LEU:O	2.70	0.44
1:B:75:MET:CE	1:B:179:TYR:CD1	2.79	0.44
1:C:145:ILE:O	1:C:145:ILE:HG22	2.17	0.44
1:A:62:ILE:HB	1:A:136:ARG:HG3	1.98	0.44
1:A:140:LEU:HD23	1:A:141:TYR:CZ	2.53	0.44
1:B:73:ILE:CG2	1:B:74:GLY:N	2.80	0.44
1:B:136:ARG:O	1:B:139:SER:OG	2.36	0.44
1:B:35:ILE:HD13	1:B:183:SER:HB3	1.99	0.44
1:C:39:SER:O	1:C:43:MLY:HG2	2.18	0.44
1:D:32:ASN:OD1	1:D:182:HIS:HB3	2.18	0.43
1:D:166:LEU:HD21	1:D:197:LEU:HB2	2.00	0.43
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.86	0.43
1:B:116:GLY:O	1:B:120:ILE:HG13	2.17	0.43
1:C:73:ILE:HD13	1:C:73:ILE:N	2.33	0.43
1:D:49:TYR:N	1:D:57:SER:OG	2.51	0.43
1:D:110:ARG:HG2	1:D:194:PHE:CE1	2.53	0.43
1:D:111:LEU:HD22	1:D:170:GLU:HG2	2.00	0.43
1:A:21:SER:OG	1:A:22:LYS:N	2.51	0.43
1:A:96:LYS:HG2	1:A:97:HIS:ND1	2.34	0.43
1:C:136:ARG:HH11	1:C:136:ARG:HB3	1.83	0.43
1:A:53:SER:OG	1:B:44:ASP:OD1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:O	1:A:35:ILE:HD12	2.19	0.43
1:A:52:GLU:HA	1:A:54:PHE:CZ	2.54	0.43
1:A:144:ILE:CG2	1:B:22:LYS:O	2.66	0.42
1:B:73:ILE:HD12	1:B:77:ILE:HD12	2.01	0.42
1:B:60:ILE:O	1:B:64:ILE:N	2.45	0.42
1:B:115:ILE:HD11	1:B:120:ILE:HG12	2.01	0.42
1:C:136:ARG:HH11	1:C:136:ARG:CG	2.32	0.42
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.91	0.42
1:C:21:SER:OG	1:C:23:PHE:N	2.52	0.42
1:D:193:LEU:O	1:D:197:LEU:HG	2.19	0.42
1:B:144:ILE:HA	1:B:148:ILE:O	2.19	0.42
1:B:20:GLU:HG2	1:B:78:SER:C	2.44	0.42
1:D:41:LEU:HD23	1:D:41:LEU:HA	1.88	0.42
1:D:102:LEU:HB2	1:D:103:PRO:CD	2.50	0.42
1:A:171:CYS:O	1:A:175:SER:CB	2.68	0.42
1:B:120:ILE:O	1:B:124:VAL:HG23	2.19	0.42
1:C:33:LYS:HD2	1:D:149:LEU:HD23	2.01	0.42
1:A:102:LEU:HB2	1:A:103:PRO:HD2	2.02	0.42
1:A:140:LEU:HB3	1:A:141:TYR:CD2	2.55	0.41
1:A:11:LYS:HD3	1:A:102:LEU:HD12	2.02	0.41
1:B:166:LEU:HD21	1:B:197:LEU:HB3	2.03	0.41
1:C:135:ILE:O	1:C:138:SER:HB2	2.20	0.41
1:A:11:LYS:O	1:A:12:MET:HB3	2.21	0.41
1:A:16:LEU:CD2	1:A:76:PHE:HB2	2.50	0.41
1:B:177:VAL:HA	1:B:183:SER:HB2	2.03	0.41
1:B:102:LEU:O	1:B:103:PRO:C	2.61	0.41
1:A:37:HIS:HE1	1:B:140:LEU:O	2.04	0.41
1:B:162:ARG:O	1:B:163:ALA:C	2.64	0.41
1:A:48:LEU:O	1:A:51:ASN:N	2.48	0.40
1:A:31:LEU:O	1:A:31:LEU:HG	2.21	0.40
1:A:70:LYS:HA	1:A:90:LEU:HD22	2.02	0.40
1:C:24:SER:HB2	1:C:79:GLU:HG3	2.01	0.40
1:C:62:ILE:HG21	1:C:136:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/207 (90%)	159 (86%)	23 (12%)	4 (2%)	5	20
1	B	158/207 (76%)	146 (92%)	12 (8%)	0	100	100
1	C	161/207 (78%)	141 (88%)	16 (10%)	4 (2%)	4	17
1	D	152/207 (73%)	136 (90%)	14 (9%)	2 (1%)	10	31
All	All	657/828 (79%)	582 (89%)	65 (10%)	10 (2%)	8	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ALA
1	A	100	GLY
1	A	118	GLU
1	D	110	ARG
1	D	117	ASP
1	C	100	GLY
1	C	102	LEU
1	C	175	SER
1	C	116	GLY
1	A	83	ILE

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	169/185 (91%)	133 (79%)	36 (21%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	145/185 (78%)	125 (86%)	20 (14%)	3	8
1	C	147/185 (80%)	118 (80%)	29 (20%)	1	3
1	D	141/185 (76%)	118 (84%)	23 (16%)	2	5
All	All	602/740 (81%)	494 (82%)	108 (18%)	1	4

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	13	LYS
1	A	15	THR
1	A	16	LEU
1	A	24	SER
1	A	50	THR
1	A	53	SER
1	A	56	THR
1	A	60	ILE
1	A	81	LYS
1	A	83	ILE
1	A	92	ASN
1	A	94	LYS
1	A	96	LYS
1	A	102	LEU
1	A	104	THR
1	A	105	ILE
1	A	115	ILE
1	A	117	ASP
1	A	118	GLU
1	A	128	GLU
1	A	135	ILE
1	A	138	SER
1	A	139	SER
1	A	143	ASP
1	A	144	ILE
1	A	146	ASP
1	A	148	ILE
1	A	149	LEU
1	A	152	PRO
1	A	153	SER
1	A	159	GLU
1	A	161	SER

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	185	GLU
1	A	187	SER
1	B	28	THR
1	B	39	SER
1	B	53	SER
1	B	60	ILE
1	B	70	LYS
1	B	73	ILE
1	B	77	ILE
1	B	97	HIS
1	B	102	LEU
1	B	115	ILE
1	B	117	ASP
1	B	118	GLU
1	B	120	ILE
1	B	122	LYS
1	B	136	ARG
1	B	147	ASP
1	B	153	SER
1	B	160	GLN
1	B	189	THR
1	B	197	LEU
1	C	19	LYS
1	C	21	SER
1	C	22	LYS
1	C	24	SER
1	C	27	SER
1	C	71	THR
1	C	73	ILE
1	C	78	SER
1	C	82	ASP
1	C	102	LEU
1	C	105	ILE
1	C	110	ARG
1	C	118	GLU
1	C	119	MET
1	C	129	THR
1	C	133	ILE
1	C	136	ARG
1	C	144	ILE
1	C	145	ILE

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Mol	Chain	Res	Type
1	C	148	ILE
1	C	151	VAL
1	C	152	PRO
1	C	155	LYS
1	C	174	ASP
1	C	175	SER
1	C	183	SER
1	C	190	THR
1	C	195	GLU
1	C	197	LEU
1	D	22	LYS
1	D	27	SER
1	D	28	THR
1	D	50	THR
1	D	57	SER
1	D	73	ILE
1	D	77	ILE
1	D	79	GLU
1	D	80	ASN
1	D	102	LEU
1	D	104	THR
1	D	105	ILE
1	D	107	MET
1	D	115	ILE
1	D	117	ASP
1	D	138	SER
1	D	144	ILE
1	D	148	ILE
1	D	157	SER
1	D	161	SER
1	D	162	ARG
1	D	175	SER
1	D	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	51	ASN
1	C	112	ASN
1	D	37	HIS
1	D	72	HIS

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Mol	Chain	Res	Type
1	D	80	ASN
1	D	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	158	1	9,10,11	0.62	0	6,11,13	0.42	0
1	MLY	C	158	1	9,10,11	0.65	0	6,11,13	0.90	0
1	MLY	B	158	1	9,10,11	0.58	0	6,11,13	0.39	0
1	MLY	D	43	1	9,10,11	0.85	0	6,11,13	0.55	0
1	MLY	C	43	1	9,10,11	0.68	0	6,11,13	0.55	0
1	MLY	B	43	1	9,10,11	0.61	0	6,11,13	0.56	0
1	MLY	D	158	1	9,10,11	0.59	0	6,11,13	0.48	0
1	MLY	A	43	1	9,10,11	0.74	0	6,11,13	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	158	1	-	3/8/9/11	-
1	MLY	C	158	1	-	3/8/9/11	-
1	MLY	B	158	1	-	4/8/9/11	-
1	MLY	D	43	1	-	2/8/9/11	-
1	MLY	C	43	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	43	1	-	3/8/9/11	-
1	MLY	D	158	1	-	2/8/9/11	-
1	MLY	A	43	1	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	158	MLY	O-C-CA-CB
1	D	158	MLY	C-CA-CB-CG
1	A	43	MLY	CG-CD-CE-NZ
1	C	43	MLY	CG-CD-CE-NZ
1	B	43	MLY	CD-CE-NZ-CH1
1	C	158	MLY	CD-CE-NZ-CH2
1	D	158	MLY	CD-CE-NZ-CH2
1	D	43	MLY	CG-CD-CE-NZ
1	A	158	MLY	CD-CE-NZ-CH2
1	C	158	MLY	CG-CD-CE-NZ
1	B	43	MLY	CE-CD-CG-CB
1	B	158	MLY	CG-CD-CE-NZ
1	D	43	MLY	CE-CD-CG-CB
1	A	158	MLY	C-CA-CB-CG
1	B	158	MLY	C-CA-CB-CG
1	C	158	MLY	C-CA-CB-CG
1	A	43	MLY	CD-CE-NZ-CH1
1	B	43	MLY	CD-CE-NZ-CH2
1	A	158	MLY	CG-CD-CE-NZ
1	A	43	MLY	CE-CD-CG-CB
1	B	158	MLY	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	43	MLY	2	0
1	D	158	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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, 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	188/207 (90%)	-0.01	1 (0%) 87 84	51, 84, 137, 155	0
1	B	162/207 (78%)	-0.28	0 100 100	39, 61, 113, 143	0
1	C	165/207 (79%)	-0.25	1 (0%) 85 83	44, 70, 107, 138	0
1	D	156/207 (75%)	-0.34	0 100 100	40, 60, 97, 128	0
All	All	671/828 (81%)	-0.21	2 (0%) 90 88	39, 69, 123, 155	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	ASN	2.7
1	C	99	PHE	2.3

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLY	C	158	11/12	0.89	0.12	56,60,69,79	0
1	MLY	D	43	11/12	0.90	0.14	43,49,55,56	0
1	MLY	B	43	11/12	0.91	0.13	49,55,67,70	0
1	MLY	D	158	11/12	0.91	0.12	50,52,60,61	0
1	MLY	C	43	11/12	0.92	0.09	47,50,53,55	0
1	MLY	A	43	11/12	0.92	0.11	50,51,54,59	0
1	MLY	A	158	11/12	0.93	0.12	73,76,79,80	0
1	MLY	B	158	11/12	0.95	0.09	50,53,60,61	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.