



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:48 am BST

PDB ID : 5L6M
Title : Structure of *Caulobacter crescentus* VapBC1 (VapB1deltaC:VapC1 form)
Authors : Bendtsen, K.L.; Xu, K.; Luckmann, M.; Brodersen, D.E.
Deposited on : 2016-05-30
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

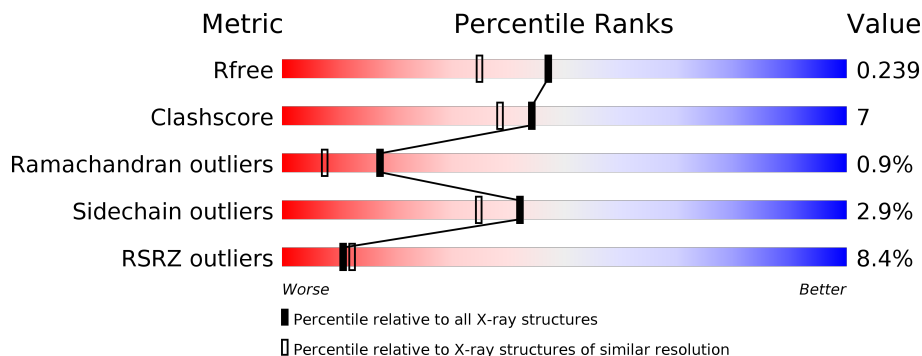
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



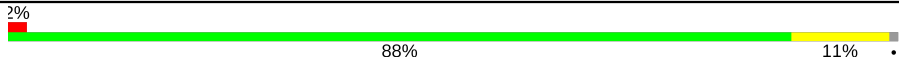
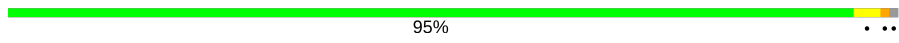

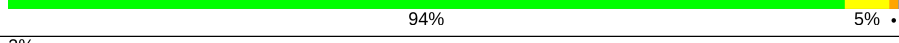


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	78	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 76% 8% • 15%</p>
1	D	78	<div style="display: flex; align-items: center;"> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">81% 10% 9%</p>
1	E	78	<div style="display: flex; align-items: center;"> <div style="width: 18%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">18% 63% 17% • • 15%</p>
1	H	78	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">15% 79% 9% • 10%</p>
1	I	78	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 76% 10% • 13%</p>
1	L	78	<div style="display: flex; align-items: center;"> <div style="width: 26%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">26% 54% 31% • • 10%</p>

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Mol	Chain	Length	Quality of chain
2	B	128	
2	C	128	
2	F	128	
2	G	128	
2	J	128	
2	K	128	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9654 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 VapB family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	66	Total 492	C 305	N 89	O 97	S 1	0	0	0
1	D	71	Total 539	C 333	N 97	O 108	S 1	0	0	0
1	E	66	Total 496	C 307	N 93	O 95	S 1	0	0	0
1	H	70	Total 533	C 329	N 98	O 105	S 1	0	0	0
1	I	68	Total 517	C 320	N 97	O 99	S 1	0	0	0
1	L	70	Total 528	C 326	N 96	O 105	S 1	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q9AC34
A	-4	HIS	-	expression tag	UNP Q9AC34
A	-3	HIS	-	expression tag	UNP Q9AC34
A	-2	HIS	-	expression tag	UNP Q9AC34
A	-1	HIS	-	expression tag	UNP Q9AC34
A	0	HIS	-	expression tag	UNP Q9AC34
A	1	HIS	-	expression tag	UNP Q9AC34
D	-5	MET	-	initiating methionine	UNP Q9AC34
D	-4	HIS	-	expression tag	UNP Q9AC34
D	-3	HIS	-	expression tag	UNP Q9AC34
D	-2	HIS	-	expression tag	UNP Q9AC34
D	-1	HIS	-	expression tag	UNP Q9AC34
D	0	HIS	-	expression tag	UNP Q9AC34
D	1	HIS	-	expression tag	UNP Q9AC34
E	-5	MET	-	initiating methionine	UNP Q9AC34
E	-4	HIS	-	expression tag	UNP Q9AC34
E	-3	HIS	-	expression tag	UNP Q9AC34

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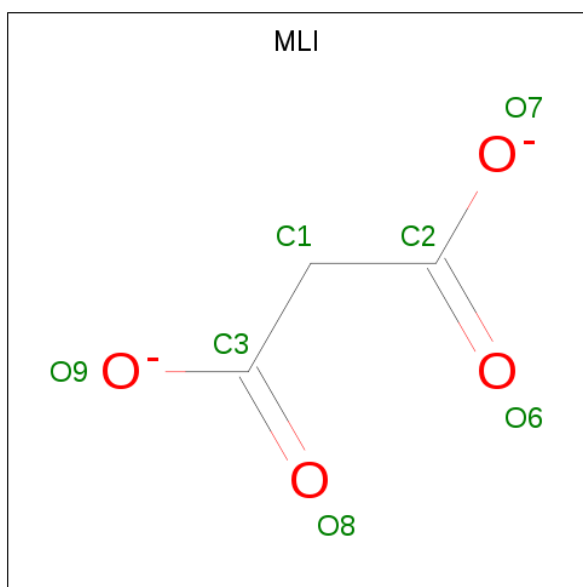
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	expression tag	UNP Q9AC34
E	-1	HIS	-	expression tag	UNP Q9AC34
E	0	HIS	-	expression tag	UNP Q9AC34
E	1	HIS	-	expression tag	UNP Q9AC34
H	-5	MET	-	initiating methionine	UNP Q9AC34
H	-4	HIS	-	expression tag	UNP Q9AC34
H	-3	HIS	-	expression tag	UNP Q9AC34
H	-2	HIS	-	expression tag	UNP Q9AC34
H	-1	HIS	-	expression tag	UNP Q9AC34
H	0	HIS	-	expression tag	UNP Q9AC34
H	1	HIS	-	expression tag	UNP Q9AC34
I	-5	MET	-	initiating methionine	UNP Q9AC34
I	-4	HIS	-	expression tag	UNP Q9AC34
I	-3	HIS	-	expression tag	UNP Q9AC34
I	-2	HIS	-	expression tag	UNP Q9AC34
I	-1	HIS	-	expression tag	UNP Q9AC34
I	0	HIS	-	expression tag	UNP Q9AC34
I	1	HIS	-	expression tag	UNP Q9AC34
L	-5	MET	-	initiating methionine	UNP Q9AC34
L	-4	HIS	-	expression tag	UNP Q9AC34
L	-3	HIS	-	expression tag	UNP Q9AC34
L	-2	HIS	-	expression tag	UNP Q9AC34
L	-1	HIS	-	expression tag	UNP Q9AC34
L	0	HIS	-	expression tag	UNP Q9AC34
L	1	HIS	-	expression tag	UNP Q9AC34

- Molecule 2 is a protein called Ribonuclease VapC.

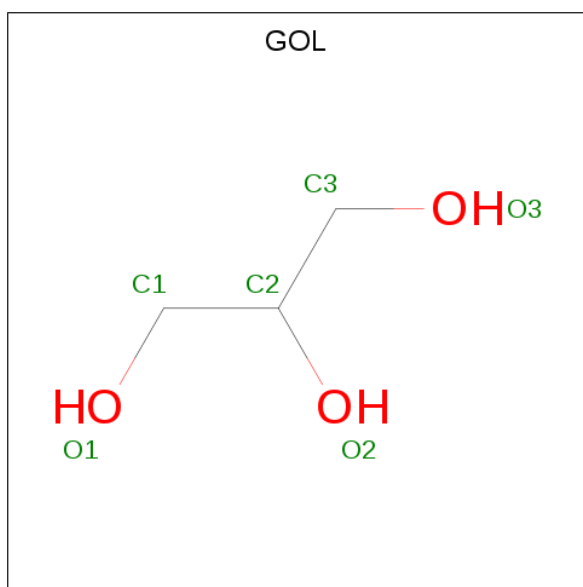
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	127	986	621	181	182	2	0	0	0
2	C	127	986	621	181	182	2	0	0	0
2	F	127	986	621	181	182	2	0	0	0
2	G	127	986	621	181	182	2	0	0	0
2	J	127	986	621	181	182	2	0	0	0
2	K	127	986	621	181	182	2	0	0	0

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		
3	G	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	J	1	6	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	78	Total	O	0	0
			78	78		
5	C	66	Total	O	0	0
			66	66		
5	D	50	Total	O	0	0
			50	50		
5	E	26	Total	O	0	0
			26	26		
5	F	65	Total	O	0	0
			65	65		
5	G	75	Total	O	0	0
			75	75		
5	H	36	Total	O	0	0
			36	36		
5	I	42	Total	O	0	0
			42	42		
5	J	46	Total	O	0	0
			46	46		
5	K	43	Total	O	0	0
			43	43		
5	L	19	Total	O	0	0
			19	19		

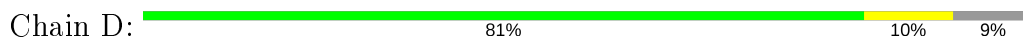
3 Residue-property plots [i](#)

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.

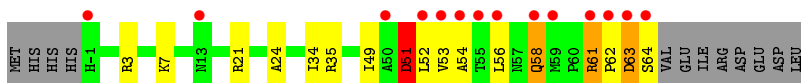
- Molecule 1: VapB family protein



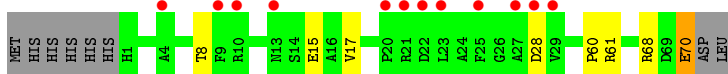
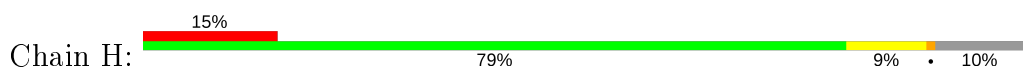
- Molecule 1: VapB family protein



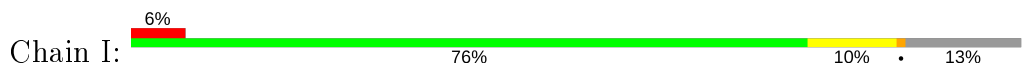
- Molecule 1: VapB family protein



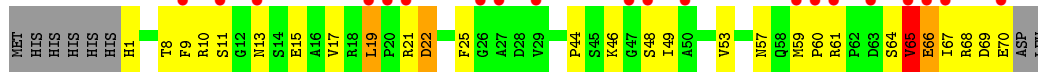
- Molecule 1: VapB family protein



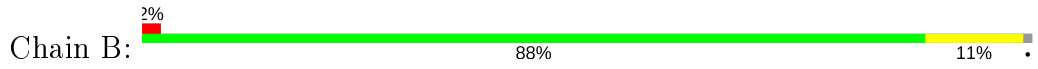
- Molecule 1: VapB family protein



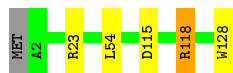
- Molecule 1: VapB family protein



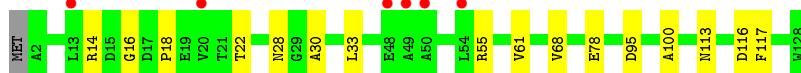
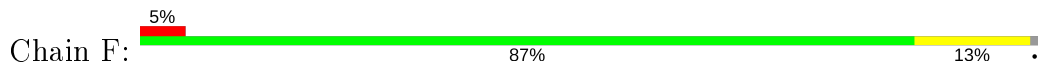
• Molecule 2: Ribonuclease VapC



• Molecule 2: Ribonuclease VapC



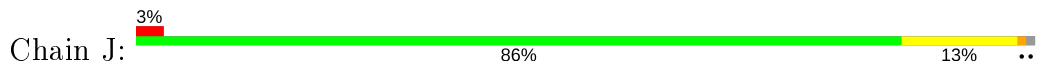
• Molecule 2: Ribonuclease VapC



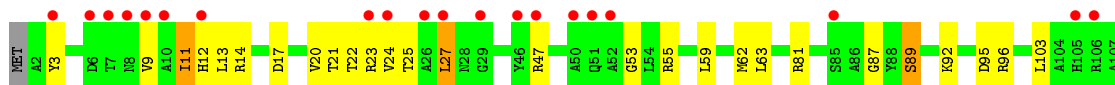
• Molecule 2: Ribonuclease VapC



• Molecule 2: Ribonuclease VapC



• Molecule 2: Ribonuclease VapC



T108	F109	V110	T111	F112	N113	A114	D115	D116	F117	R118	D119	I120	F121	G122	L123	S124	L125	L126	A127	W128
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.40Å 63.60Å 184.70Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	46.60 – 1.90 47.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.60-1.90) 98.8 (47.08-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.196 , 0.240 0.196 , 0.239	Depositor DCC
R_{free} test set	4165 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9654	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/498	0.55	0/675
1	D	0.44	0/545	0.60	1/738 (0.1%)
1	E	0.40	0/504	0.68	1/683 (0.1%)
1	H	0.32	0/540	0.56	0/731
1	I	0.37	0/526	0.60	0/713
1	L	0.34	0/534	0.62	0/723
2	B	0.42	0/1000	0.60	0/1356
2	C	0.46	0/1000	0.60	0/1356
2	F	0.36	0/1000	0.53	0/1356
2	G	0.43	0/1000	0.57	0/1356
2	J	0.39	0/1000	0.56	0/1356
2	K	0.39	0/1000	0.63	0/1356
All	All	0.40	0/9147	0.59	2/12399 (0.0%)

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	L	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ASP	N-CA-C	8.28	133.37	111.00
1	D	60	PRO	C-N-CA	-5.03	109.13	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	65	VAL	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	492	0	497	8	0
1	D	539	0	544	6	0
1	E	496	0	499	14	0
1	H	533	0	539	7	0
1	I	517	0	519	9	0
1	L	528	0	534	16	0
2	B	986	0	1001	11	0
2	C	986	0	1001	3	0
2	F	986	0	1001	9	0
2	G	986	0	1001	8	0
2	J	986	0	1001	9	0
2	K	986	0	1001	33	0
3	A	7	0	2	1	0
3	C	7	0	2	0	0
3	G	7	0	2	1	0
4	B	6	0	8	0	0
4	J	6	0	8	0	0
5	A	54	0	0	5	1
5	B	78	0	0	3	2
5	C	66	0	0	0	1
5	D	50	0	0	3	0
5	E	26	0	0	4	2
5	F	65	0	0	0	1
5	G	75	0	0	4	0
5	H	36	0	0	4	1
5	I	42	0	0	4	1
5	J	46	0	0	0	0
5	K	43	0	0	8	0
5	L	19	0	0	3	0
All	All	9654	0	9160	120	5

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 7.

The worst 5 of 120 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:K:12:HIS:HB3	2:K:20:VAL:HG11	1.54	0.88
1:E:52:LEU:HD12	2:F:61:VAL:HG13	1.55	0.87
1:L:59:MET:O	5:L:101:HOH:O	1.97	0.80
1:H:61:ARG:NH2	5:H:103:HOH:O	2.18	0.77
1:H:70:GLU:OE2	5:H:101:HOH:O	2.03	0.77

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:123:HOH:O	5:H:123:HOH:O[2_456]	1.94	0.26
5:B:332:HOH:O	5:I:117:HOH:O[1_565]	2.13	0.07
5:E:125:HOH:O	5:F:262:HOH:O[4_456]	2.13	0.07
5:C:341:HOH:O	5:E:108:HOH:O[4_456]	2.15	0.05
5:A:245:HOH:O	5:B:359:HOH:O[3_445]	2.18	0.02

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	64/78 (82%)	61 (95%)	2 (3%)	1 (2%)	9 2
1	D	69/78 (88%)	69 (100%)	0	0	100 100
1	E	64/78 (82%)	54 (84%)	8 (12%)	2 (3%)	4 0
1	H	68/78 (87%)	66 (97%)	2 (3%)	0	100 100
1	I	66/78 (85%)	63 (96%)	3 (4%)	0	100 100
1	L	68/78 (87%)	62 (91%)	2 (3%)	4 (6%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
2	C	125/128 (98%)	125 (100%)	0	0	100	100
2	F	125/128 (98%)	122 (98%)	1 (1%)	2 (2%)	9	2
2	G	125/128 (98%)	124 (99%)	1 (1%)	0	100	100
2	J	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
2	K	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	19	9
All	All	1149/1236 (93%)	1109 (96%)	30 (3%)	10 (1%)	17	7

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	58	GLN
1	E	63	ASP
2	F	14	ARG
1	L	61	ARG
2	K	115	ASP

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	53/66 (80%)	52 (98%)	1 (2%)	57	53
1	D	59/66 (89%)	59 (100%)	0	100	100
1	E	53/66 (80%)	47 (89%)	6 (11%)	6	2
1	H	58/66 (88%)	56 (97%)	2 (3%)	37	28
1	I	56/66 (85%)	55 (98%)	1 (2%)	59	55
1	L	57/66 (86%)	50 (88%)	7 (12%)	4	1
2	B	101/102 (99%)	101 (100%)	0	100	100
2	C	101/102 (99%)	100 (99%)	1 (1%)	76	76
2	F	101/102 (99%)	101 (100%)	0	100	100
2	G	101/102 (99%)	100 (99%)	1 (1%)	76	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	101/102 (99%)	97 (96%)	4 (4%)	31	22
2	K	101/102 (99%)	97 (96%)	4 (4%)	31	22
All	All	942/1008 (94%)	915 (97%)	27 (3%)	42	35

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	85	SER
2	J	116	ASP
1	L	65	VAL
2	J	89	SER
1	E	51	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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
3	MLI	C	201	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	101	-	0,6,6	0.00	-	0,7,7	0.00	-
4	GOL	J	201	-	5,5,5	0.40	0	5,5,5	0.57	0
3	MLI	G	201	-	0,6,6	0.00	-	0,7,7	0.00	-
4	GOL	B	201	-	5,5,5	0.44	0	5,5,5	0.57	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
3	MLI	C	201	-	-	0/0/4/4	-
3	MLI	A	101	-	-	0/0/4/4	-
4	GOL	J	201	-	-	4/4/4/4	-
3	MLI	G	201	-	-	0/0/4/4	-
4	GOL	B	201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	201	GOL	O1-C1-C2-C3
4	B	201	GOL	O1-C1-C2-C3
4	B	201	GOL	C1-C2-C3-O3
4	J	201	GOL	O1-C1-C2-O2
4	B	201	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	MLI	1	0
3	G	201	MLI	1	0

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	66/78 (84%)	0.06	3 (4%) 33 36	27, 40, 70, 88	0
1	D	71/78 (91%)	-0.10	0 100 100	22, 39, 58, 67	0
1	E	66/78 (84%)	1.03	14 (21%) 0 0	34, 65, 95, 114	0
1	H	70/78 (89%)	0.80	12 (17%) 1 1	28, 61, 91, 108	0
1	I	68/78 (87%)	0.40	5 (7%) 14 16	29, 49, 82, 84	0
1	L	70/78 (89%)	1.47	20 (28%) 0 0	22, 69, 105, 120	0
2	B	127/128 (99%)	-0.19	2 (1%) 72 74	18, 33, 62, 89	0
2	C	127/128 (99%)	-0.24	0 100 100	19, 31, 56, 70	0
2	F	127/128 (99%)	0.21	6 (4%) 31 34	23, 46, 82, 98	0
2	G	127/128 (99%)	-0.12	0 100 100	18, 36, 59, 73	0
2	J	127/128 (99%)	0.15	4 (3%) 49 51	21, 44, 72, 92	0
2	K	127/128 (99%)	1.24	32 (25%) 0 0	29, 69, 93, 112	0
All	All	1173/1236 (94%)	0.33	98 (8%) 11 12	18, 45, 88, 120	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	65	VAL	8.3
1	E	53	VAL	7.4
1	E	52	LEU	6.4
1	L	61	ARG	6.0
1	H	13	ASN	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	201	6/6	0.94	0.15	35,45,54,59	0
4	GOL	J	201	6/6	0.95	0.10	30,32,41,54	0
3	MLI	G	201	7/7	0.96	0.10	27,28,31,32	0
3	MLI	A	101	7/7	0.97	0.10	29,34,36,37	0
3	MLI	C	201	7/7	0.97	0.17	34,38,42,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.