



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 07:15 am GMT

PDB ID : 2CB4
Title : Crystal structure of the catalytic domain of the mosquitocidal toxin from *Bacillus sphaericus*, mutant E197Q
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.
Deposited on : 2005-12-29
Resolution : 2.50 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
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

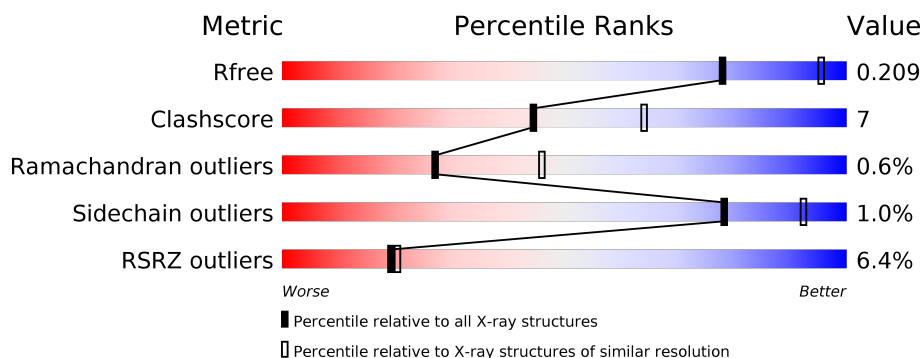
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	291	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	291	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div></div> <div>11%</div> </div> </div>
1	C	291	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	291	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	291	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div></div> <div>11%</div> </div> </div>
1	F	291	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div></div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	291	<p>3% 76% 12% 11%</p>
1	H	291	<p>6% 73% 15% 11%</p>
1	I	291	<p>6% 73% 16% 11%</p>
1	J	291	<p>3% 74% 14% 11%</p>
1	K	291	<p>5% 76% 13% 11%</p>
1	L	291	<p>8% 75% 13% 11%</p>
1	M	291	<p>6% 76% 13% 11%</p>
1	N	291	<p>10% 75% 13% 11%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30680 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	B	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	C	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	D	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	E	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	F	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	G	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	H	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	I	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	J	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	K	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	L	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	M	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			
1	N	258	Total	C	N	O	Se	0	0	0
			2095	1315	374	401	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLN	GLU	engineered mutation	UNP Q03988

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Chain	Residue	Modelled	Actual	Comment	Reference
B	197	GLN	GLU	engineered mutation	UNP Q03988
C	197	GLN	GLU	engineered mutation	UNP Q03988
D	197	GLN	GLU	engineered mutation	UNP Q03988
E	197	GLN	GLU	engineered mutation	UNP Q03988
F	197	GLN	GLU	engineered mutation	UNP Q03988
G	197	GLN	GLU	engineered mutation	UNP Q03988
H	197	GLN	GLU	engineered mutation	UNP Q03988
I	197	GLN	GLU	engineered mutation	UNP Q03988
J	197	GLN	GLU	engineered mutation	UNP Q03988
K	197	GLN	GLU	engineered mutation	UNP Q03988
L	197	GLN	GLU	engineered mutation	UNP Q03988
M	197	GLN	GLU	engineered mutation	UNP Q03988
N	197	GLN	GLU	engineered mutation	UNP Q03988

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	108	Total O 108 108	0	0
2	C	120	Total O 120 120	0	0
2	D	114	Total O 114 114	0	0
2	E	82	Total O 82 82	0	0
2	F	81	Total O 81 81	0	0
2	G	96	Total O 96 96	0	0
2	H	86	Total O 86 86	0	0
2	I	109	Total O 109 109	0	0
2	J	112	Total O 112 112	0	0
2	K	80	Total O 80 80	0	0
2	L	92	Total O 92 92	0	0
2	M	93	Total O 93 93	0	0

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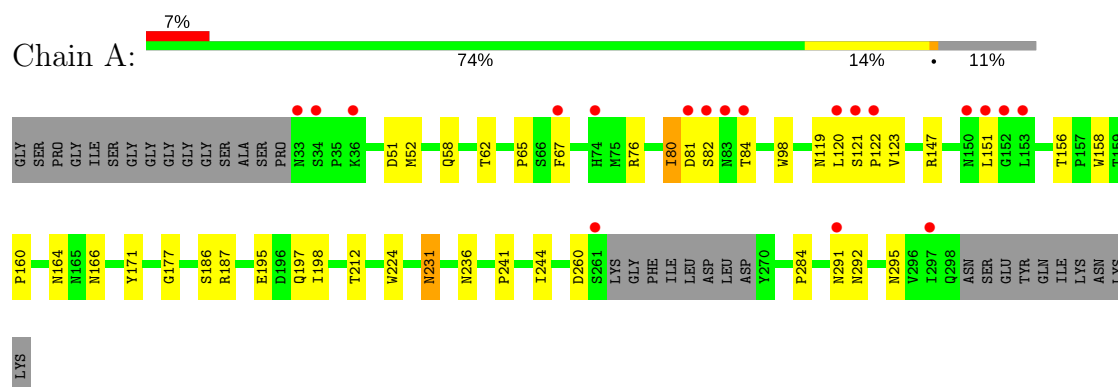
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	84	Total	O	0	0
			84	84		

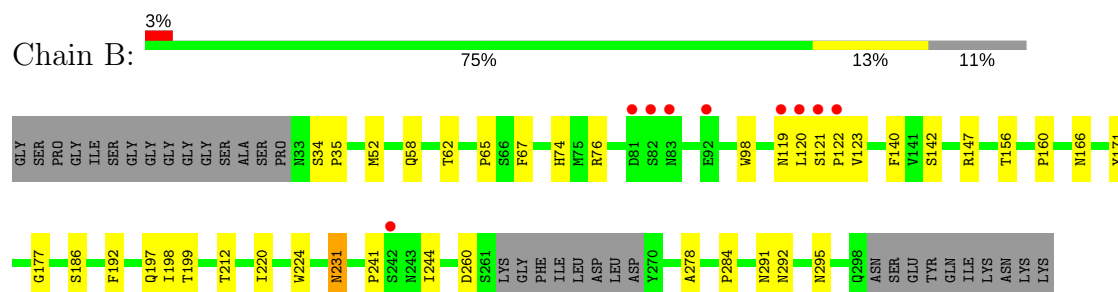
3 Residue-property plots [i](#)

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.

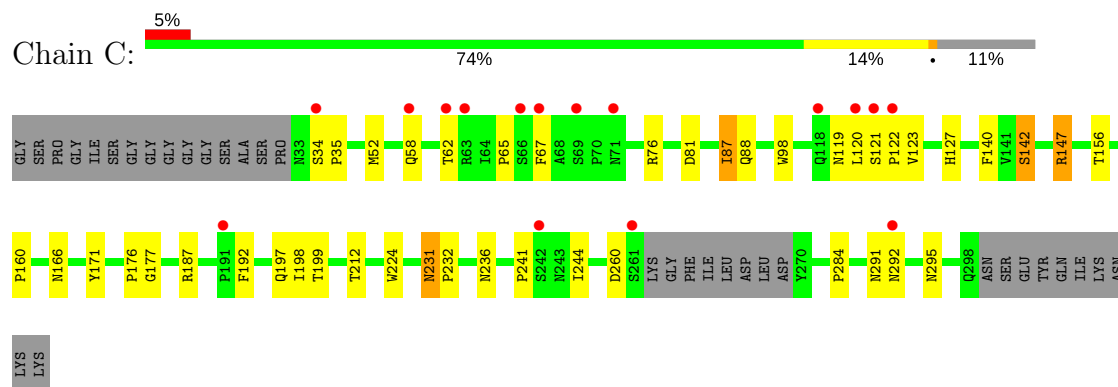
• Molecule 1: MOSQUITOCIDAL TOXIN



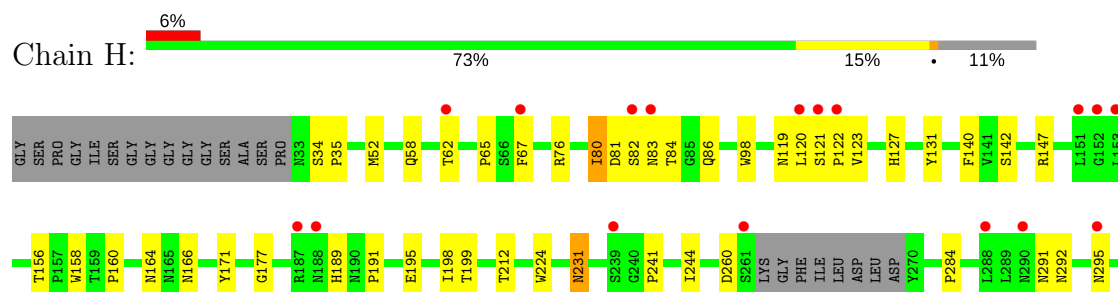
• Molecule 1: MOSQUITOCIDAL TOXIN



• Molecule 1: MOSQUITOCIDAL TOXIN



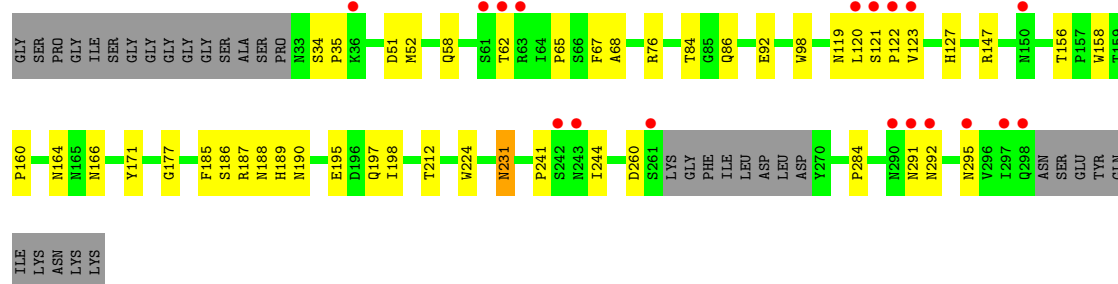
• Molecule 1: MOSQUITOCIDAL TOXIN




N298
ASN
SER
GLY
TYR
GLN
ILE
LYS
ASN
LYS

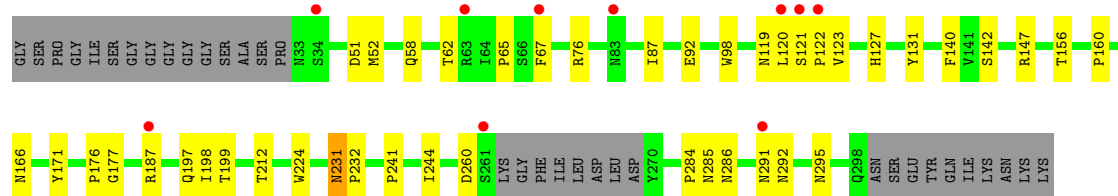
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain I: 




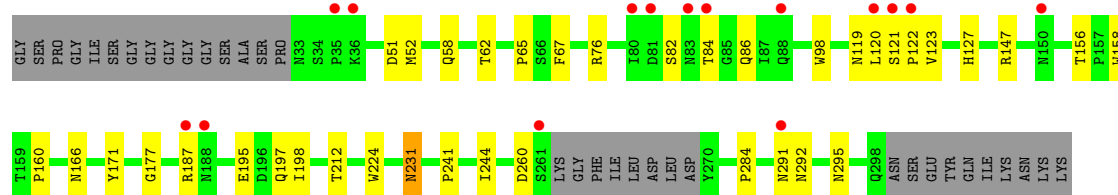
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain J: 




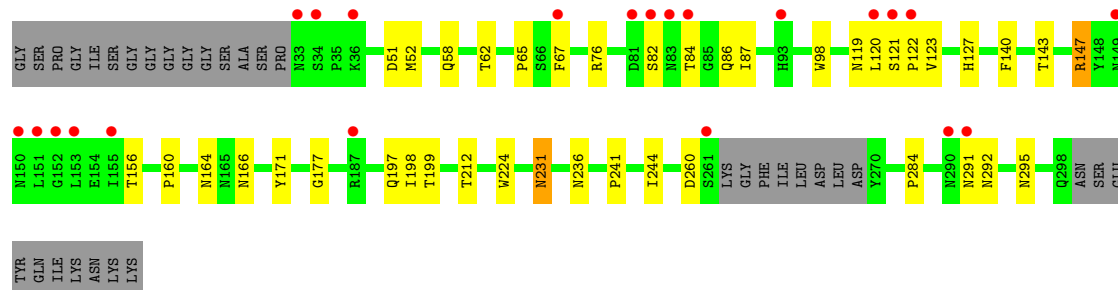
• Molecule 1: MOSQUITOCIDAL TOXIN

Chain K: 

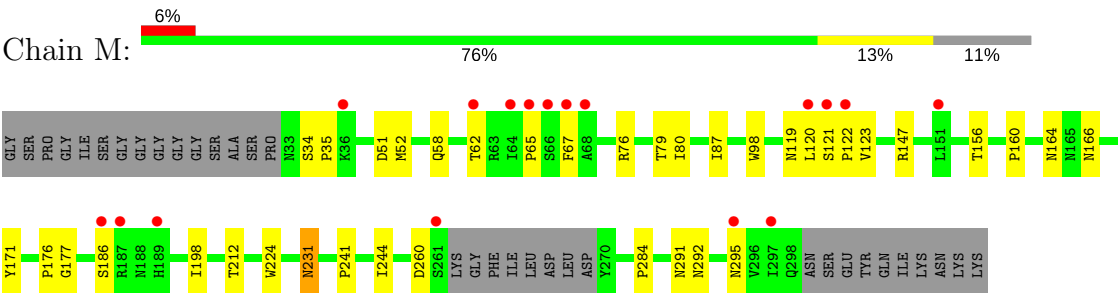


• Molecule 1: MOSQUITOCIDAL TOXIN

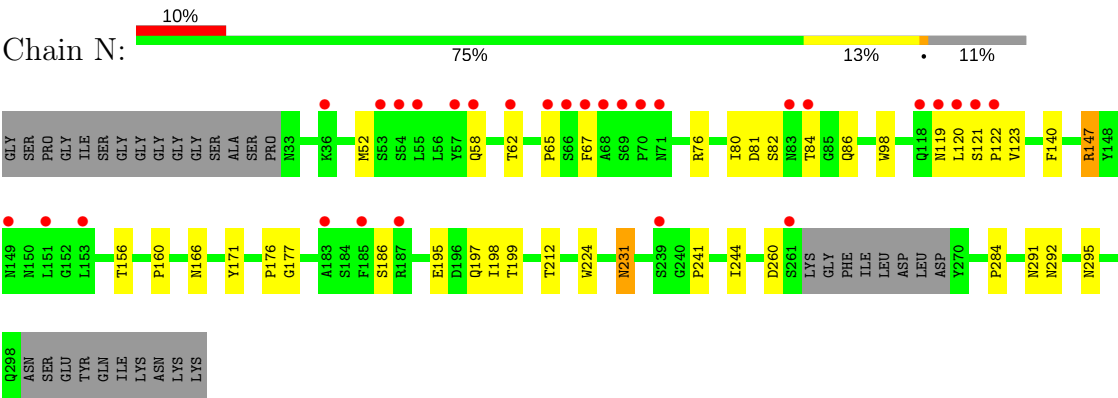
Chain L: 



● Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 143.27Å 135.81Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 99.9 (49.73-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.51Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.174 , 0.194 0.192 , 0.209	Depositor DCC
R_{free} test set	8035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30680	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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)

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	0.70	0/2149	0.82	2/2928 (0.1%)
1	B	0.71	0/2149	0.80	1/2928 (0.0%)
1	C	0.73	0/2149	0.84	3/2928 (0.1%)
1	D	0.69	0/2149	0.80	1/2928 (0.0%)
1	E	0.71	1/2149 (0.0%)	0.81	0/2928
1	F	0.69	1/2149 (0.0%)	0.83	1/2928 (0.0%)
1	G	0.72	0/2149	0.82	1/2928 (0.0%)
1	H	0.69	0/2149	0.81	1/2928 (0.0%)
1	I	0.70	0/2149	0.82	1/2928 (0.0%)
1	J	0.72	0/2149	0.83	1/2928 (0.0%)
1	K	0.69	0/2149	0.81	1/2928 (0.0%)
1	L	0.68	0/2149	0.81	1/2928 (0.0%)
1	M	0.70	0/2149	0.81	1/2928 (0.0%)
1	N	0.69	0/2149	0.81	1/2928 (0.0%)
All	All	0.70	2/30086 (0.0%)	0.82	16/40992 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	192	PHE	CE1-CZ	5.21	1.47	1.37
1	E	92	GLU	CG-CD	5.19	1.59	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ILE	CG1-CB-CG2	-8.96	91.68	111.40
1	C	192	PHE	C-N-CD	-5.92	107.57	120.60
1	A	147	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	147	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	L	147	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	2095	0	1976	31	1
1	B	2095	0	1976	27	0
1	C	2095	0	1976	36	0
1	D	2095	0	1976	32	0
1	E	2095	0	1976	26	0
1	F	2095	0	1976	26	0
1	G	2095	0	1976	27	1
1	H	2095	0	1976	33	0
1	I	2095	0	1976	33	0
1	J	2095	0	1976	29	1
1	K	2095	0	1976	27	0
1	L	2095	0	1976	30	0
1	M	2095	0	1976	31	0
1	N	2095	0	1976	28	1
2	A	93	0	0	3	0
2	B	108	0	0	3	0
2	C	120	0	0	4	0
2	D	114	0	0	6	0
2	E	82	0	0	2	0
2	F	81	0	0	3	0
2	G	96	0	0	3	0
2	H	86	0	0	1	0
2	I	109	0	0	2	0
2	J	112	0	0	3	0
2	K	80	0	0	1	0
2	L	92	0	0	2	0
2	M	93	0	0	2	0
2	N	84	0	0	1	0
All	All	30680	0	27664	404	2

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 404 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:F:241:PRO:HB2	1:F:244:ILE:HD12	1.48	0.96
1:C:241:PRO:HB2	1:C:244:ILE:HD12	1.48	0.96
1:J:241:PRO:HB2	1:J:244:ILE:HD12	1.48	0.96
1:L:241:PRO:HB2	1:L:244:ILE:HD12	1.48	0.96
1:B:241:PRO:HB2	1:B:244:ILE:HD12	1.48	0.96

All (2) 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)
1:G:150:ASN:N	1:J:286:ASN:ND2[2_557]	2.14	0.06
1:A:151:LEU:CD2	1:N:62:THR:CG2[2_556]	2.17	0.03

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	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	B	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	C	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	36	57
1	D	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	36	57
1	E	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	F	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	36	57
1	G	254/291 (87%)	241 (95%)	11 (4%)	2 (1%)	21	37
1	H	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	I	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	J	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	21	37
1	K	254/291 (87%)	240 (94%)	11 (4%)	3 (1%)	14	26
1	L	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	36	57
1	N	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	36	57
All	All	3556/4074 (87%)	3363 (95%)	172 (5%)	21 (1%)	27	46

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	187	ARG
1	I	187	ARG
1	K	187	ARG
1	J	187	ARG
1	A	187	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	238/257 (93%)	234 (98%)	4 (2%)	63	85
1	B	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	C	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	D	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	E	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	F	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	G	238/257 (93%)	237 (100%)	1 (0%)	92	98
1	H	238/257 (93%)	235 (99%)	3 (1%)	71	89
1	I	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	J	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	K	238/257 (93%)	237 (100%)	1 (0%)	92	98
1	L	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	M	238/257 (93%)	236 (99%)	2 (1%)	83	94
1	N	238/257 (93%)	235 (99%)	3 (1%)	71	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3332/3598 (93%)	3300 (99%)	32 (1%)	78 92

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	197	GLN
1	H	80	ILE
1	N	82	SER
1	G	231	ASN
1	H	82	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	295	ASN
1	H	217	ASN
1	M	295	ASN
1	G	127	HIS
1	G	231	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	253/291 (86%)	0.23	19 (7%)	14 14	22, 36, 76, 105	0
1	B	253/291 (86%)	0.12	9 (3%)	42 46	21, 35, 72, 96	0
1	C	253/291 (86%)	0.29	16 (6%)	20 21	17, 34, 72, 98	0
1	D	253/291 (86%)	0.20	12 (4%)	31 34	21, 34, 72, 104	0
1	E	253/291 (86%)	0.10	14 (5%)	25 27	21, 35, 74, 106	0
1	F	253/291 (86%)	0.16	18 (7%)	16 16	21, 36, 76, 98	0
1	G	253/291 (86%)	-0.03	9 (3%)	42 46	20, 34, 67, 96	0
1	H	253/291 (86%)	0.08	17 (6%)	18 18	21, 36, 76, 104	0
1	I	253/291 (86%)	0.25	18 (7%)	16 16	21, 35, 72, 108	0
1	J	253/291 (86%)	0.06	10 (3%)	38 41	21, 34, 73, 97	0
1	K	253/291 (86%)	0.14	15 (5%)	22 23	21, 36, 73, 108	0
1	L	253/291 (86%)	0.33	22 (8%)	10 10	21, 36, 75, 101	0
1	M	253/291 (86%)	0.26	17 (6%)	18 18	21, 35, 72, 105	0
1	N	253/291 (86%)	0.34	29 (11%)	5 4	22, 36, 77, 110	0
All	All	3542/4074 (86%)	0.18	225 (6%)	19 20	17, 35, 75, 110	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	PRO	8.8
1	I	122	PRO	8.6
1	N	120	LEU	7.9
1	L	122	PRO	7.8
1	B	83	ASN	7.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.