W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 07:21 AM EDT

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)

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

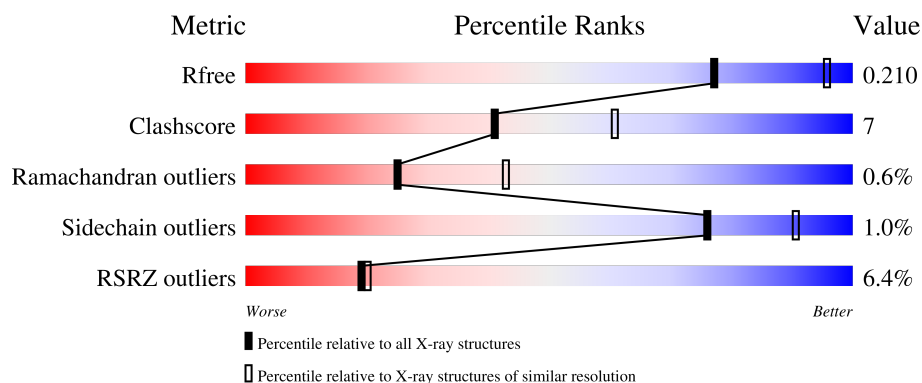|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
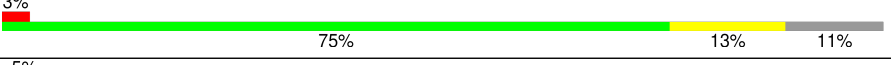*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.210
Clashscore		7
Ramachandran outliers		0.6%
Sidechain outliers		1.0%
RSRZ outliers		6.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	7% / 74% 14% • 11%
1	B	291	3% / 75% 13% 11%
1	C	291	5% / 74% 14% • 11%
1	D	291	4% / 75% 13% • 11%
1	E	291	5% / 77% 12% 11%

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

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

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

3 Residue-property plots ⓘ

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: MOSQUITOCIDAL TOXIN
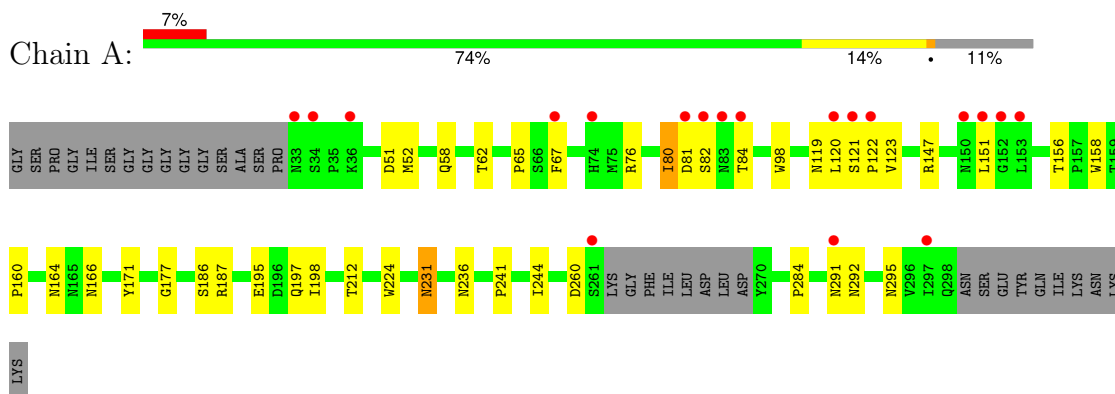
Chain A:

- Molecule 1: MOSQUITOCIDAL TOXIN
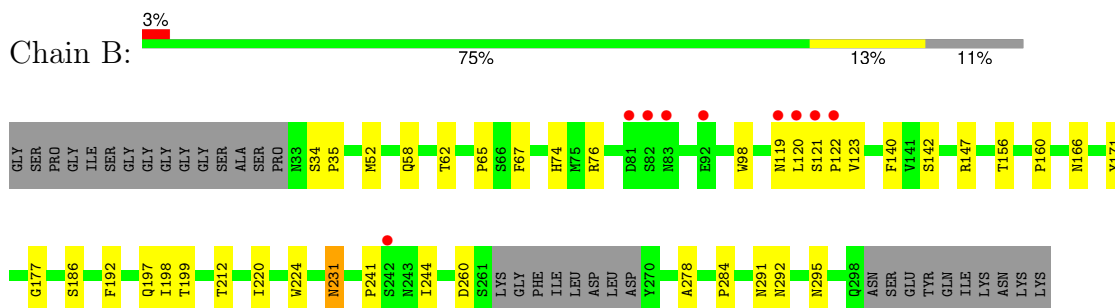
Chain B:
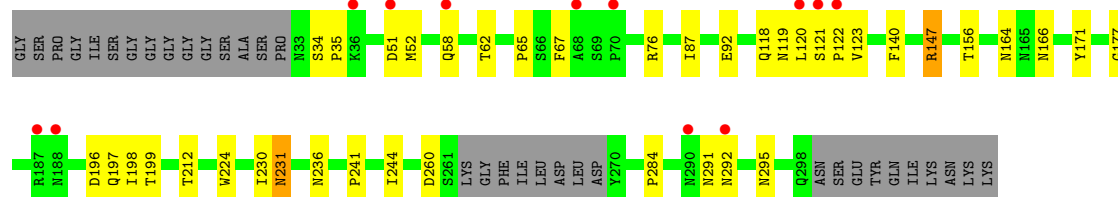
- Molecule 1: MOSQUITOCIDAL TOXIN
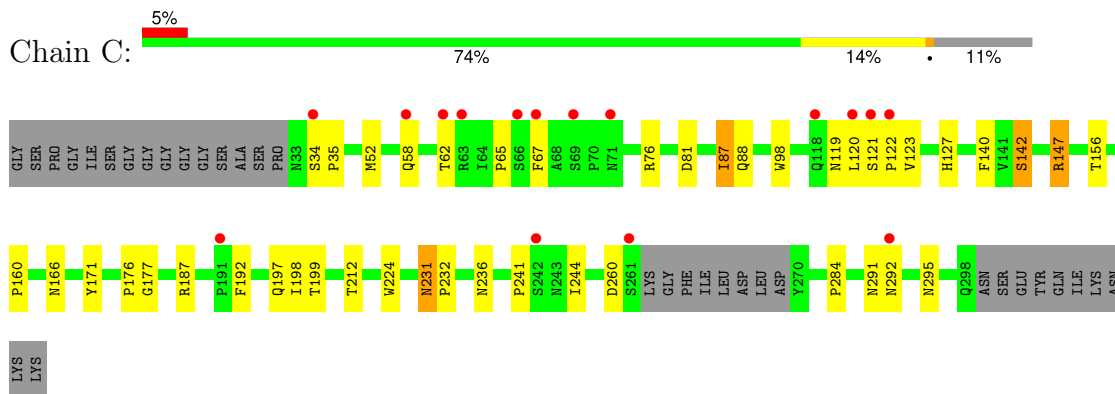
Chain C:

- Molecule 1: MOSQUITOCIDAL TOXIN

Chain D:
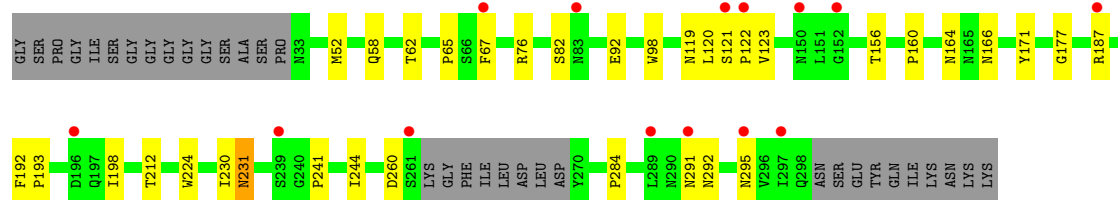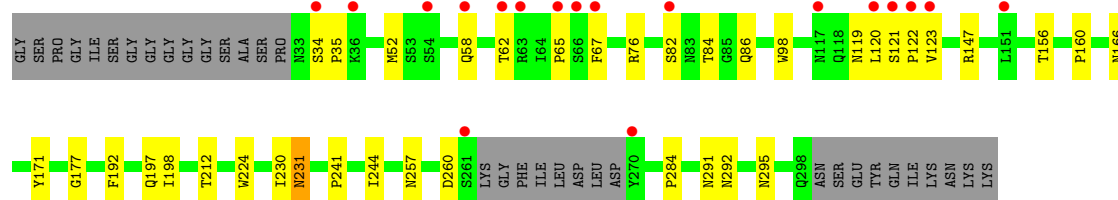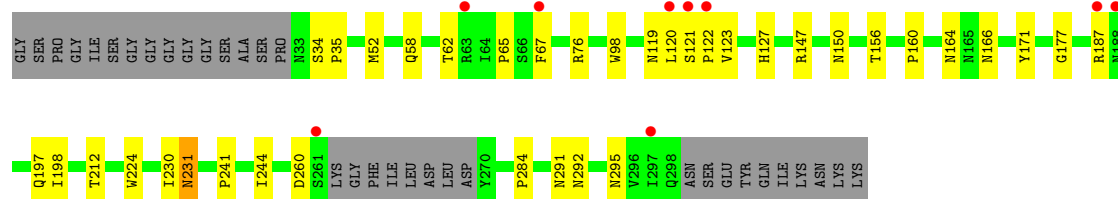

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain E:

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain F:

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain G:

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain H:

T156 P157 W158 T159 P160 N164 N165 N166 Y171 G177 R187 N188 H189 N190 P191 E195 I198 T199 T212 W224 N231 S239 G240 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 L288 L289 N290 N291 N292 N295

Q298 ASN SER GLU TYR GLN ILE LYS ASN LYS LYS

• **Molecule 1: MOSQUITOCIDAL TOXIN**

Chain I:

6%

73%   16%   11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 S34 P35 K36 D51 M52 Q58 S61 T62 R63 I64 P65 S66 F67 A68 R76 T84 G85 Q86 E92 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158 T159

P160 N164 N165 N166 Y171 G177 F185 S186 R187 N188 H189 N190 E195 D196 Q197 I198 T212 W224 N231 P241 S242 N243 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N290 N291 N292 N295 V296 I297 Q298 ASN SER GLU TYR GLN

ILE LYS ASN LYS

• **Molecule 1: MOSQUITOCIDAL TOXIN**

Chain J:

3%

74%   14%   11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 S34 D51 M52 Q58 T62 R63 I64 P65 S66 F67 R76 N83 I87 E92 W98 N119 L120 S121 P122 V123 H127 Y131 F140 V141 S142 R147 T156 P160

N166 Y171 P176 G177 R187 Q197 I198 T199 T212 W224 N231 P232 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N285 N286 N291 N292 N295 Q298 ASN SER GLU TYR GLN ILE LYS ASN LYS LYS

• **Molecule 1: MOSQUITOCIDAL TOXIN**

Chain K:

5%

76%   13%   11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 S34 P35 K36 D51 M52 Q58 T62 P65 S66 F67 R76 I80 D81 S82 N83 T84 G85 Q86 I87 Q88 W98 N119 L120 S121 P122 V123 H127 R147 N150 T156 P157 W158

T159 P160 N166 Y171 G177 R187 N188 E195 D196 Q197 I198 T212 W224 N231 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N291 N292 N295 Q298 ASN SER GLU TYR GLN ILE LYS ASN LYS LYS

• **Molecule 1: MOSQUITOCIDAL TOXIN**

Chain L:

8%

75%   13% • 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 S34 P35 K36 D51 M52 Q58 T62 P65 S66 F67 R76 D81 S82 N83 T84 G85 Q86 I87 H93 W98 N119 L120 S121 P122 V123 H127 F140 T143 R147 Y148 N149

N150 L151 G152 L153 E154 I155 T156 P160 N164 N165 N166 Y171 G177 R187 Q197 I198 T199 T212 W224 N231 N236 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N290 N291 N292 N295 Q298 ASN SER GLU
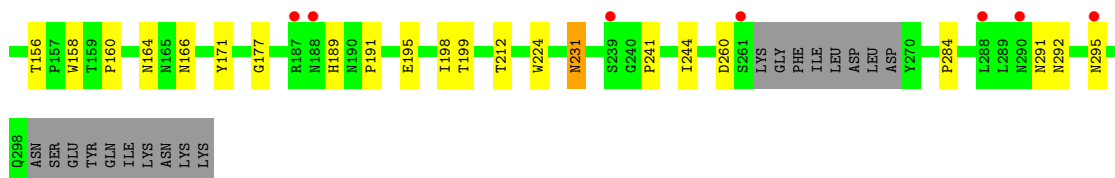
TYR GLN ILE LYS ASN LYS LYS

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain M:

6%

76%   13%   11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 S34 P35 K36 D51 M52 Q58 T62 R63 I64 P65 S66 F67 A68 R76 T79 I80 I87 W98 N119 L120 S121 P122 V123 R147 L151 T156 P160 N164 N165 N166

Y171 P176 G177 S186 R187 N188 H189 I198 T212 W224 N231 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N291 N292 N295 V296 I297 Q298 ASN SER GLU TYR GLN ILE LYS ASN LYS LYS

• Molecule 1: MOSQUITOCIDAL TOXIN

Chain N:

10%

75%   13% • 11%

GLY SER PRO GLY ILE SER GLY GLY GLY GLY SER ALA SER PRO N33 K36 M52 S53 S54 L55 L56 Y57 Q58 T62 P65 S66 F67 A68 S69 P70 N71 R76 I80 D81 S82 N83 T84 G85 Q86 W98 Q118 N119 L120 S121 P122 V123 F140 R147 Y148

N149 N150 L151 G152 L153 T156 P160 N166 Y171 P176 G177 A183 S184 F185 S186 R187 E195 D196 Q197 I198 T199 T212 W224 N231 S239 G240 P241 I244 D260 S261 LYS GLY PHE ILE LEU ASP LEU ASP Y270 P284 N291 N292 N295

Q298 ASN SER GLU TYR GLN ILE LYS ASN LYS LYS

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
$<I/\sigma(I)>$ [1]	5.57 (at 2.51Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.174 , 0.194 0.193 , 0.210	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]	$<|L|> = 0.48$, $<L^2> = 0.30$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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 ⓘ

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 (i)

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%)	19	35
1	B	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	34	54
1	C	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	34	54
1	D	254/291 (87%)	239 (94%)	14 (6%)	1 (0%)	34	54
1	E	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	19	35
1	F	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	34	54
1	G	254/291 (87%)	241 (95%)	11 (4%)	2 (1%)	19	35
1	H	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	34	54
1	I	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	19	35
1	J	254/291 (87%)	240 (94%)	12 (5%)	2 (1%)	19	35
1	K	254/291 (87%)	240 (94%)	11 (4%)	3 (1%)	13	24
1	L	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	34	54

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	254/291 (87%)	241 (95%)	12 (5%)	1 (0%)	34	54
1	N	254/291 (87%)	240 (94%)	13 (5%)	1 (0%)	34	54
All	All	3556/4074 (87%)	3363 (95%)	172 (5%)	21 (1%)	25	43

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%)	60	82
1	B	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	C	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	D	238/257 (93%)	235 (99%)	3 (1%)	69	87
1	E	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	F	238/257 (93%)	235 (99%)	3 (1%)	69	87
1	G	238/257 (93%)	237 (100%)	1 (0%)	91	97
1	H	238/257 (93%)	235 (99%)	3 (1%)	69	87
1	I	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	J	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	K	238/257 (93%)	237 (100%)	1 (0%)	91	97
1	L	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	M	238/257 (93%)	236 (99%)	2 (1%)	81	93
1	N	238/257 (93%)	235 (99%)	3 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3332/3598 (93%)	3300 (99%)	32 (1%)	76 90

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

Mol	Chain	Res	Type
1	M	231	ASN
1	N	82	SER
1	E	231	ASN
1	E	82	SER
1	N	186	SER

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

Mol	Chain	Res	Type
1	J	295	ASN
1	M	217	ASN
1	K	164	ASN
1	L	164	ASN
1	N	164	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	33	21, 34, 72, 104	0
1	E	253/291 (86%)	0.10	14 (5%)	25	26	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%)	17	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%)	17	18	21, 35, 72, 105	0
1	N	253/291 (86%)	0.34	29 (11%)	4	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.