wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2021 – 05:09 pm BST

PDB ID	:	7O49
Title	:	Crystal structure of Penicillin-Binding Protein 1 (PBP1) from Staphylococcus aureus
Authors	:	Martinez Caballero, S.; Hermoso, J.A.
Deposited on	:	2021-04-05
Resolution	:	3.03 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 (i) symbol.

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

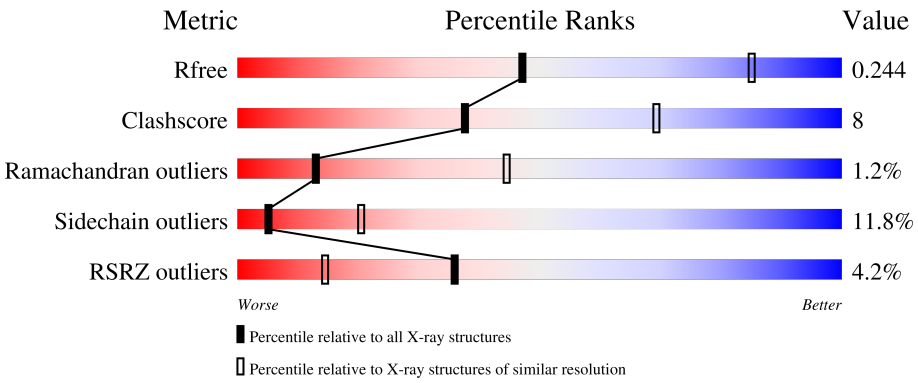
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	650	2% 62% 17% • 20%
1	B	650	% 62% 17% • 19%
1	C	650	% 62% 16% • 20%
1	D	650	6% 59% 16% • 23%
1	E	650	% 60% 18% • 20%

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Mol	Chain	Length	Quality of chain
1	F	650	3% 61% 17% • 19%
1	G	650	% 62% 17% • 20%
1	H	650	4% 55% 16% • 28%
1	I	650	% 64% 14% • 20%
1	J	650	4% 60% 18% • 20%
1	K	650	7% 59% 16% • 21%
1	L	650	8% 57% 16% • 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	C	802	-	-	X	-
4	CL	E	802	-	-	X	-
4	CL	K	801	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 48707 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 Penicillin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	4105	2609	706	774	16	0	0	0
1	B	527	4156	2639	716	785	16	0	0	0
1	C	520	4098	2604	705	773	16	0	0	0
1	D	502	3958	2514	677	751	16	0	0	0
1	E	523	4120	2617	709	778	16	0	0	0
1	F	528	4165	2645	718	786	16	0	0	0
1	G	520	4098	2604	705	773	16	0	0	0
1	H	471	3703	2355	631	702	15	0	0	0
1	I	518	4083	2595	702	770	16	0	0	0
1	J	518	4080	2592	701	771	16	0	0	0
1	K	511	4029	2562	690	761	16	0	0	0
1	L	494	3894	2479	662	737	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	initiating methionine	UNP A0A0H2WVW5
B	64	MET	-	initiating methionine	UNP A0A0H2WVW5
C	64	MET	-	initiating methionine	UNP A0A0H2WVW5
D	64	MET	-	initiating methionine	UNP A0A0H2WVW5
E	64	MET	-	initiating methionine	UNP A0A0H2WVW5

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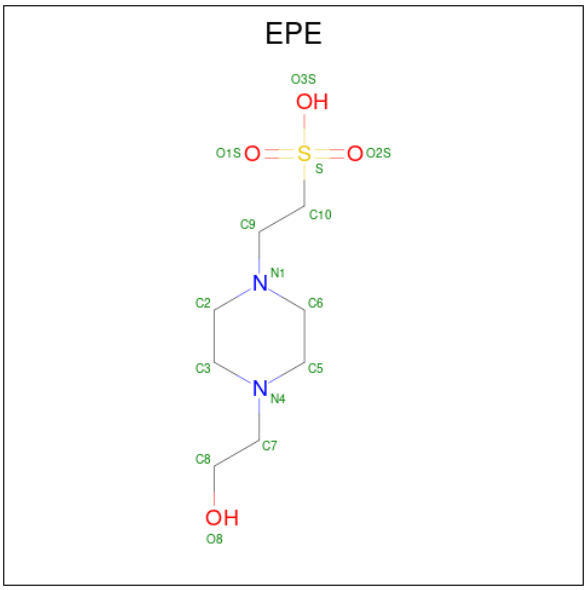
Chain	Residue	Modelled	Actual	Comment	Reference
F	64	MET	-	initiating methionine	UNP A0A0H2WVW5
G	64	MET	-	initiating methionine	UNP A0A0H2WVW5
H	64	MET	-	initiating methionine	UNP A0A0H2WVW5
I	64	MET	-	initiating methionine	UNP A0A0H2WVW5
J	64	MET	-	initiating methionine	UNP A0A0H2WVW5
K	64	MET	-	initiating methionine	UNP A0A0H2WVW5
L	64	MET	-	initiating methionine	UNP A0A0H2WVW5

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	15	8	2	4	1	0	0
2	B	1	15	8	2	4	1	0	0
2	C	1	15	8	2	4	1	0	0
2	D	1	15	8	2	4	1	0	0
2	E	1	15	8	2	4	1	0	0
2	F	1	15	8	2	4	1	0	0
2	G	1	15	8	2	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	H	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
2	I	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
2	J	1	15	8	2	4	1	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	1	1	1	0	0
			Total	Cd		
3	B	1	1	1	0	0
			Total	Cd		
3	C	1	1	1	0	0
			Total	Cd		
3	D	1	1	1	0	0
			Total	Cd		
3	E	1	1	1	0	0
			Total	Cd		
3	F	1	1	1	0	0
			Total	Cd		
3	G	1	1	1	0	0
			Total	Cd		
3	H	1	1	1	0	0
			Total	Cd		
3	I	1	1	1	0	0
			Total	Cd		
3	J	1	1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	C	1	1	1	0	0
			Total	Cl		
4	D	1	1	1	0	0
			Total	Cl		
4	E	1	1	1	0	0
			Total	Cl		
4	F	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0

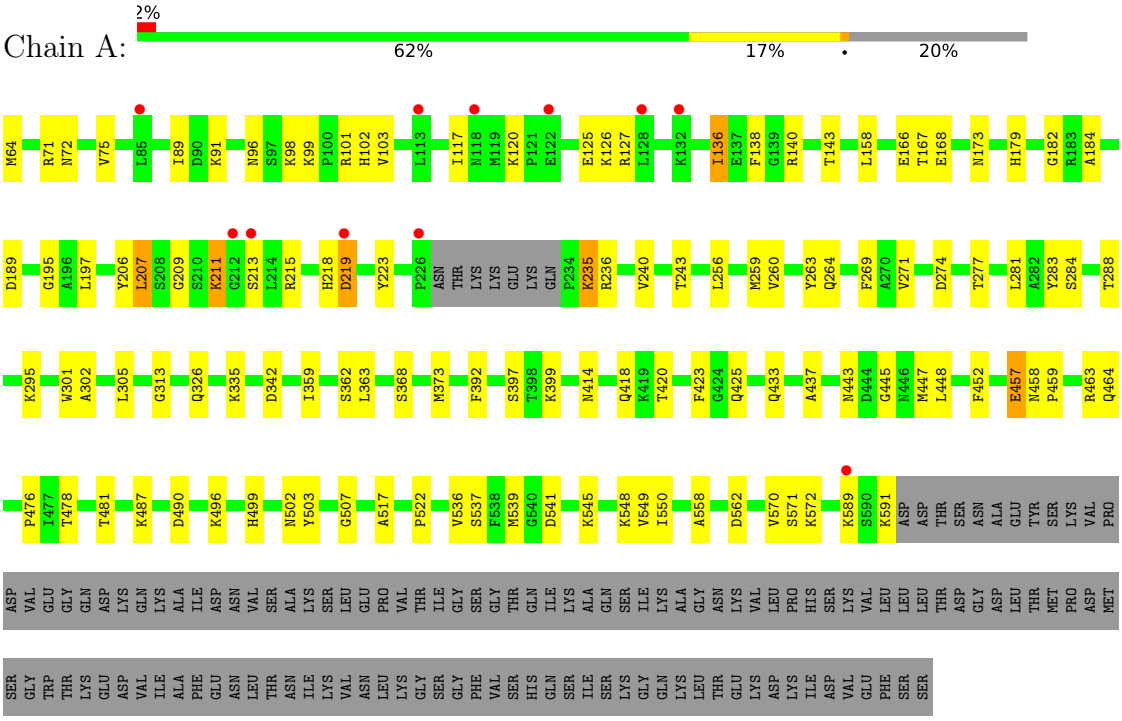
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	3	Total O 3 3	0	0
5	C	6	Total O 6 6	0	0
5	D	3	Total O 3 3	0	0
5	E	7	Total O 7 7	0	0
5	F	8	Total O 8 8	0	0
5	G	5	Total O 5 5	0	0
5	H	3	Total O 3 3	0	0
5	I	4	Total O 4 4	0	0
5	J	4	Total O 4 4	0	0
5	K	3	Total O 3 3	0	0
5	L	1	Total O 1 1	0	0

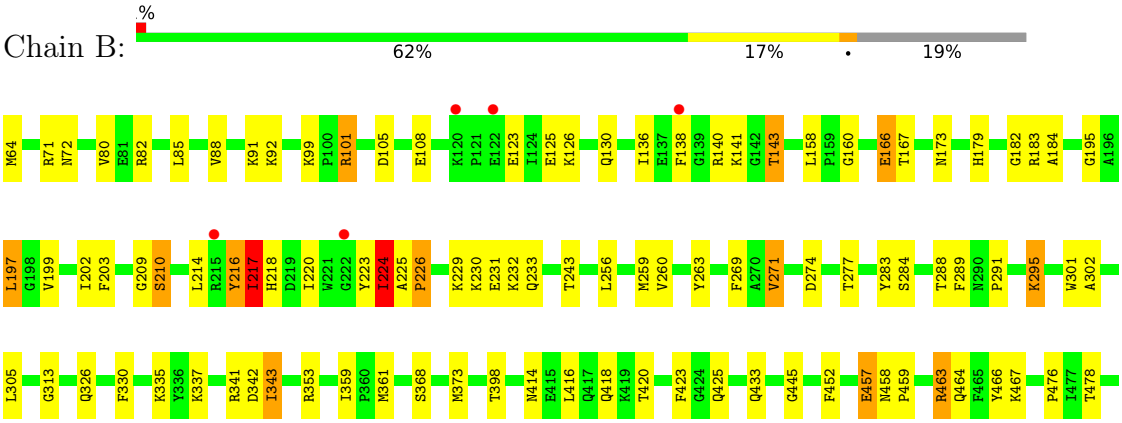
3 Residue-property plots (i)

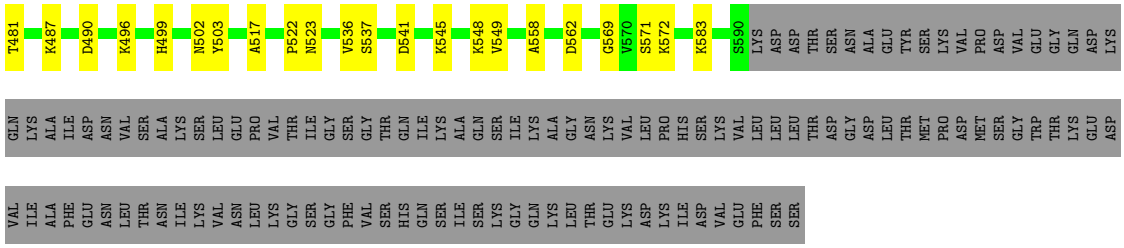
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Penicillin-binding protein 1



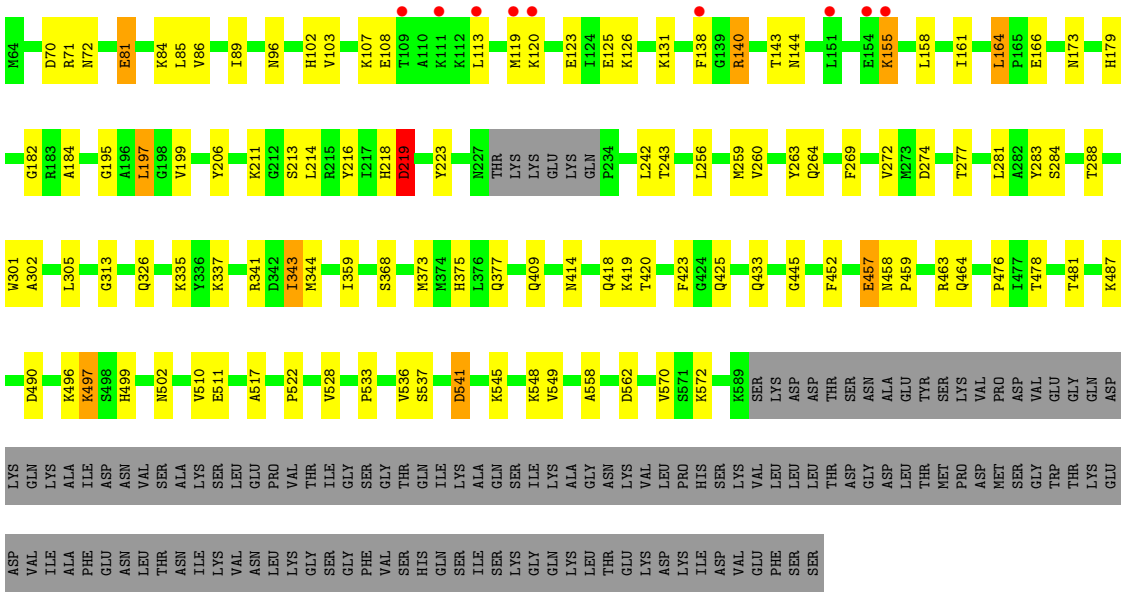
• Molecule 1: Penicillin-binding protein 1





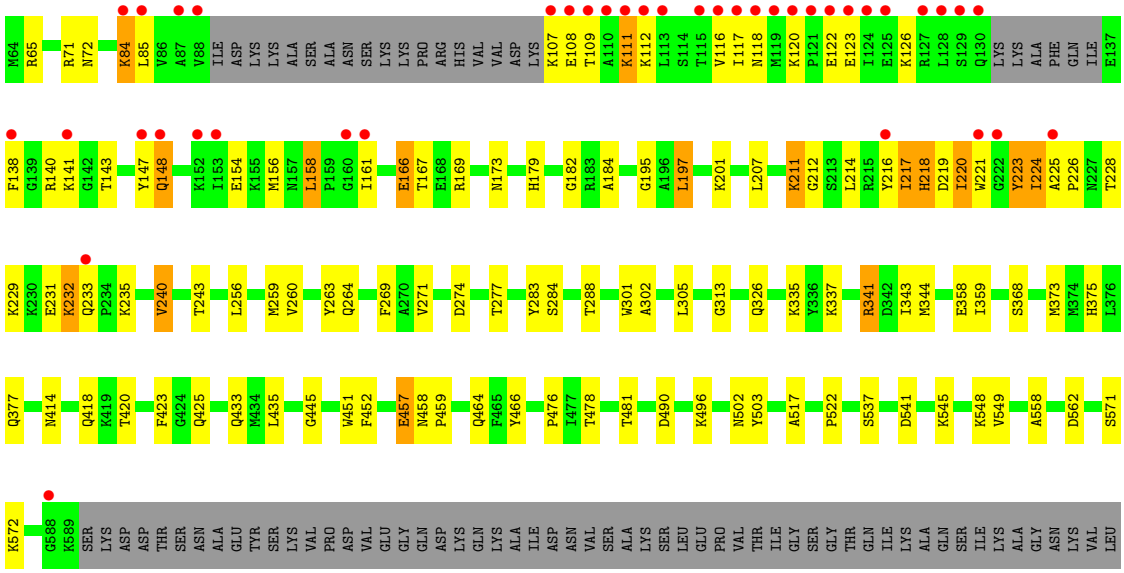
- Molecule 1: Penicillin-binding protein 1

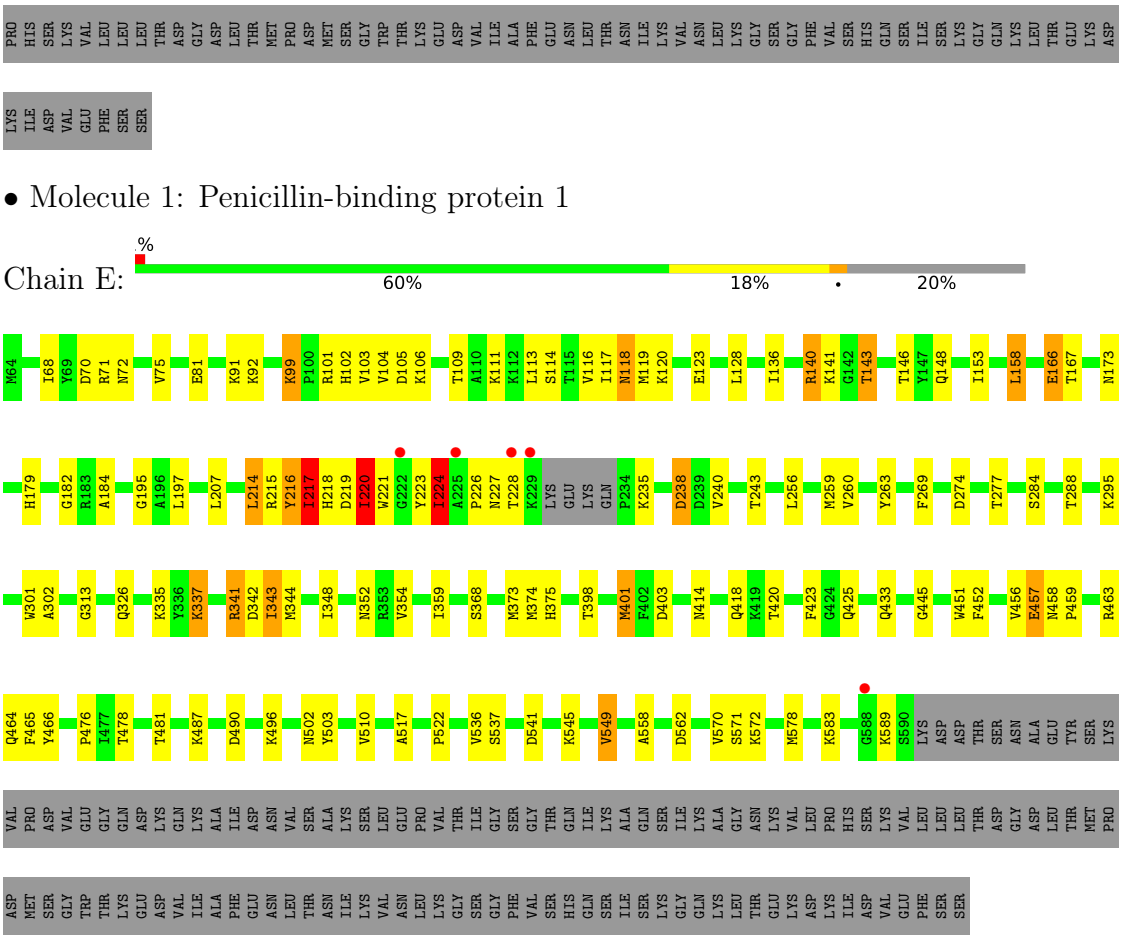
Chain C:



- Molecule 1: Penicillin-binding protein 1

Chain D:



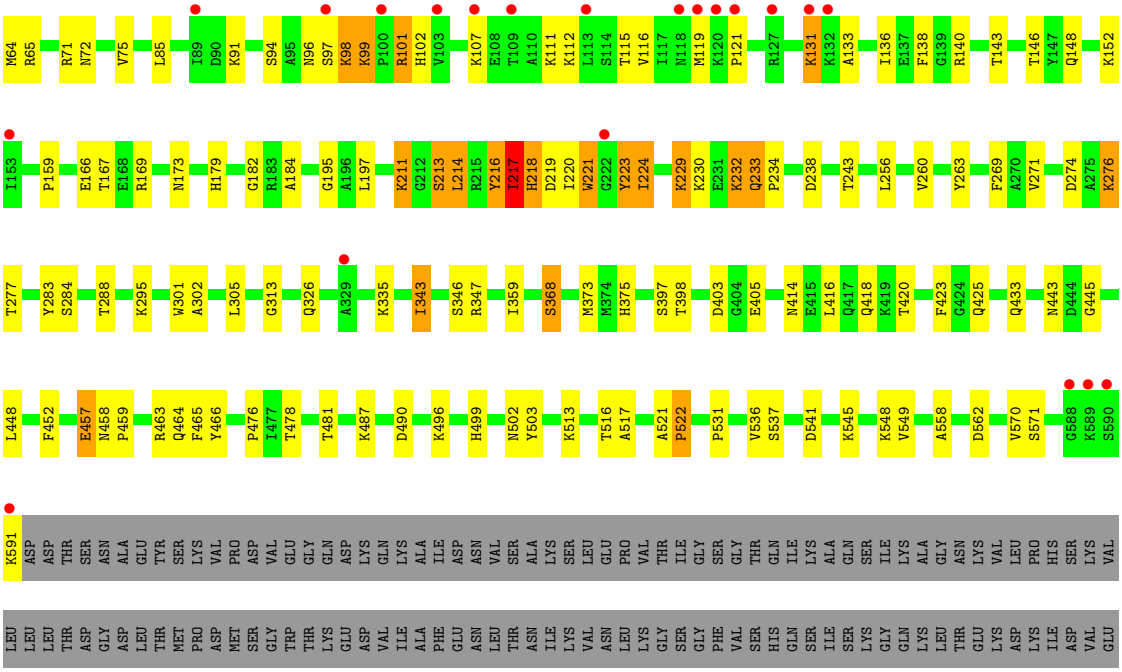


• Molecule 1: Penicillin-binding protein 1

Chain E:

• Molecule 1: Penicillin-binding protein 1

Chain F:



PHE SER SER

• Molecule 1: Penicillin-binding protein 1

Chain G: % 62% 17% • 20%

M64 R65 D70 R71 N72 K91 N96 V103 V104 D105 K106 K107 E108 T109 T115 V116 I117 N118 M119 K120 E123 I124 E125 K126 K132 F138 G139 R140 K141 G142 T143 Q148 K152 I153 E154 K155 I161 E166 T167 E168 R169 N173 H179 L180 I181 G182

R183 A184 G195 A196 L197 G198 V199 Y206 K211 G212 S213 L214 R215 D219 I220 W221 G222 Y223 N227 THR LYS LYS GLU LYS GLN P234 D238 L242 T243 I244 L256 M259 V260 Y263 Q264 F269 A270 V271 D274 T277 Y283 S284 T288 L305

G313 Q326 F330 K335 H340 R341 M344 R347 N352 R353 V354 I359 P360 M361 S368 M373 G381 K399 N414 Q418 K419 T420 F423 G424 Q425 Q433 G445 K449 F452 E457 N458 P459 Q464 A473 P476 I477

T478 T481 D490 K496 K497 S498 H499 N502 A517 P522 V536 S537 F538 M539 G540 D541 K545 V549 I550 V551 A558 D562 V570 S571 K572 A573 F574 M578 T581 L582 K583 Y584 L585 K589 SER LYS ASP ASP THR SER ASN ALA GLU TYR SER

LYS VAL PRO ASP VAL GLU GLY GLN ASP LYS GLN LYS ALA ILE ASP ASN VAL SER ALA LYS SER LEU GLU PRO VAL THR ILE GLY SER GLY THR GLN ILE LYS ALA GLN SER ILE LYS ALA GLY ASN LYS VAL LEU PRO HIS SER LYS VAL LEU LEU LEU THR ASP GLY ASP LEU THR MET

PRO ASP MET SER GLY TRP THR LYS GLU ASP VAL ILE ALA PHE GLU ASN LEU THR ASN ILE LYS VAL ASN LEU LYS GLY SER GLY PHE VAL SER HIS GLN SER ILE SER LYS GLY GLN LYS LEU THR GLU LYS ASP LYS ILE ASP VAL GLU PHE SER SER

• Molecule 1: Penicillin-binding protein 1

Chain H: 4% 55% 16% • 28%

M64 R65 D70 R71 N72 V80 K84 L85 V86 A87 V88 ILE ASP LYS LYS ALA SER ALA ASN SER LYS LYS PRO ARG HIS VAL VAL ASP LYS LYS GLU THR ALA LYS LYS LEU SER THR VAL ILE ASN MET LYS PRO GLU GLU ILE GLU LYS ARG LEU SER GLN LYS LYS ALA PHE

GLN ILE E137 F138 G139 R140 K141 G142 T143 N144 L145 T146 Y147 Q148 D149 K150 L151 K152 I153 E154 K155 M156 N157 G160 I161 S162 L163 L164 P165 E166 R169 F170 N173 H179 G182 R183 A184 G195 A196 L197 S205 K211 L214 R215 Y216 I217 H218 D219 I220 W221 G222

Y223 P226 ASN THR LYS LYS GLU LYS GLN PRO K235 T243 L256 M259 V260 Y263 Q264 F269 D274 T277 L281 A282 Y283 S284 T288 W301 A302 L305 G313 Q326 K335 R341 D342 I343 M344 G345 S346 R347 R353 I359 S368

M373 M374 H375 L376 Q377 K386 K396 I410 N414 Q418 K419 T420 F423 G424 Q425 Q433 G445 K449 P450 W451 F452 E457 N458 P459 R463 Q464 Q469 A473 P476 I477 T478 T481 K487 D490 K496 H499 N502 Y503

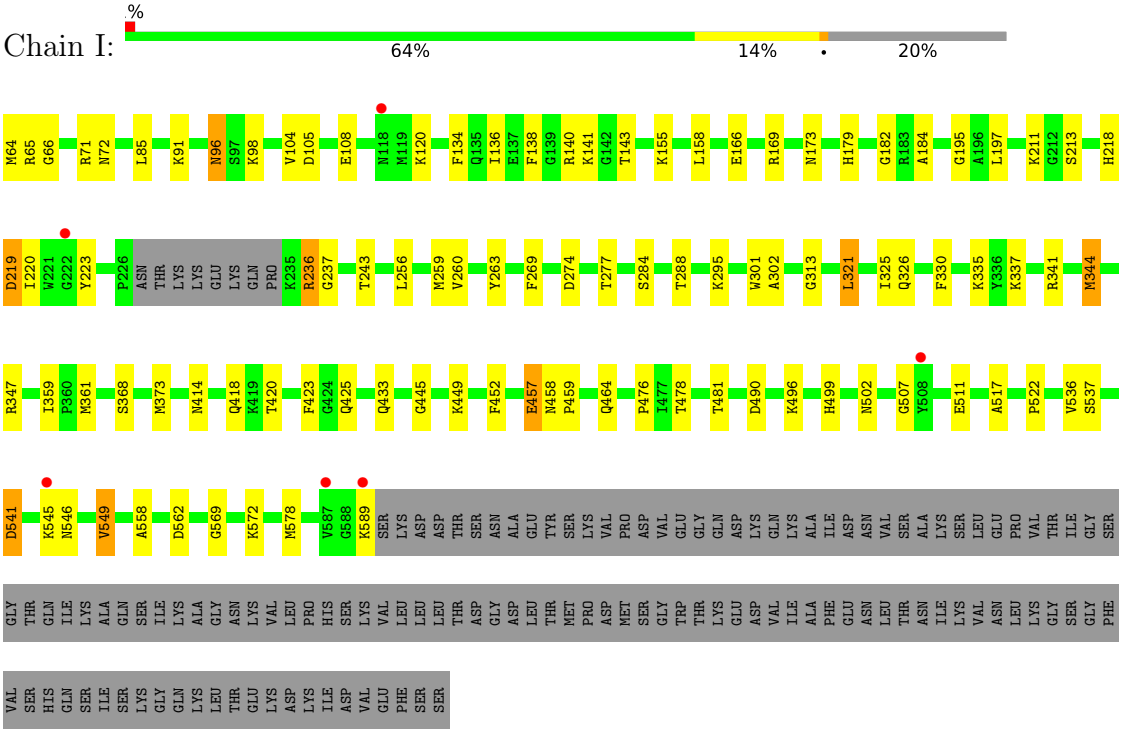
D506 A517 P522 V536 S537 D541 K545 K548 V549 A558 D562 Y566 V570 S571 K572 K589 S590 LYS ASP ASP THR SER ASN ALA GLU TYR SER LYS VAL PRO ASP VAL GLU GLY GLN ASP LYS GLN LYS ALA ILE ASP ASN VAL SER ALA LYS SER LEU

GLU PRO VAL THR ILE GLY SER GLY THR GLN ILE LYS ALA GLN SER ILE ILE LYS ALA GLY ASN LYS VAL LEU PRO HIS SER LYS VAL LEU LEU LEU THR ASP GLY ASP LEU THR MET PRO ASP MET SER GLY TRP THR LYS GLU ASP VAL ILE ALA PHE GLU ASN LEU THR ASN ILE LYS VAL

ASN LEU LYS GLY SER GLY PHE VAL SER HIS GLN SER ILE SER LYS GLY GLN LYS LEU THR GLU LYS ASP LYS ILE ASP VAL GLU PHE SER SER

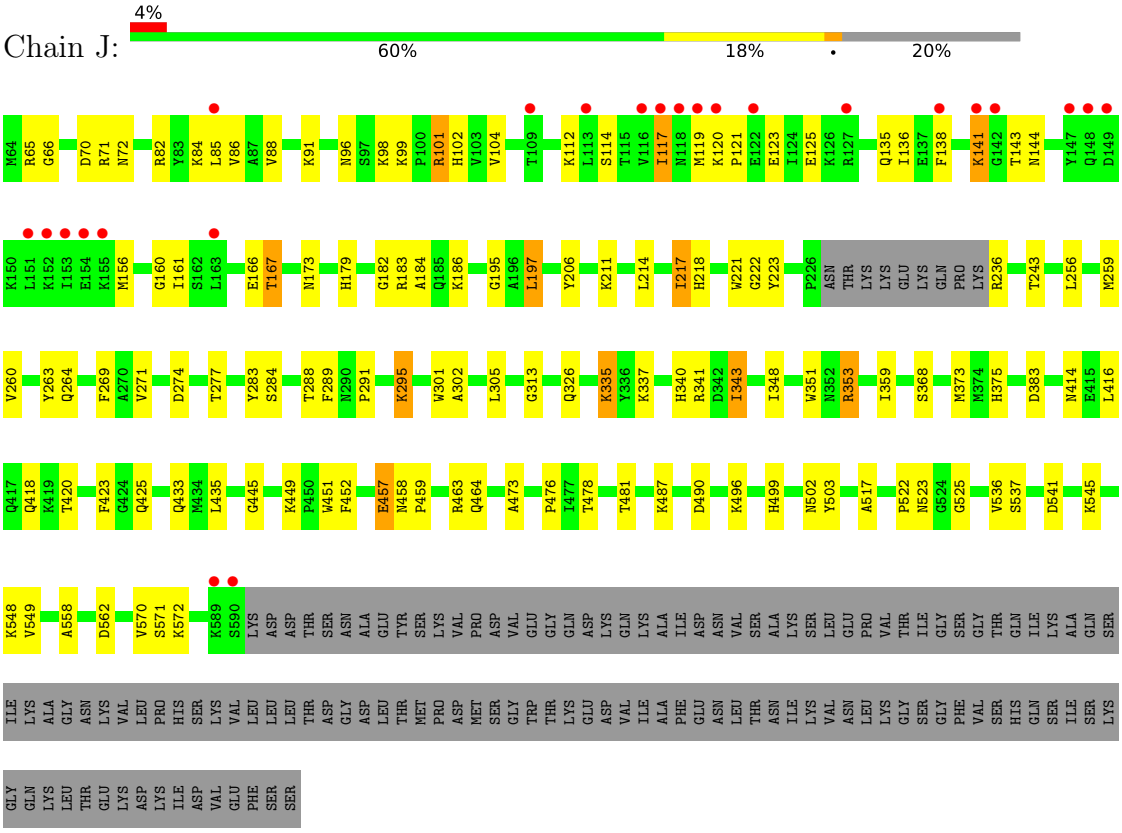
• Molecule 1: Penicillin-binding protein 1

Chain I:



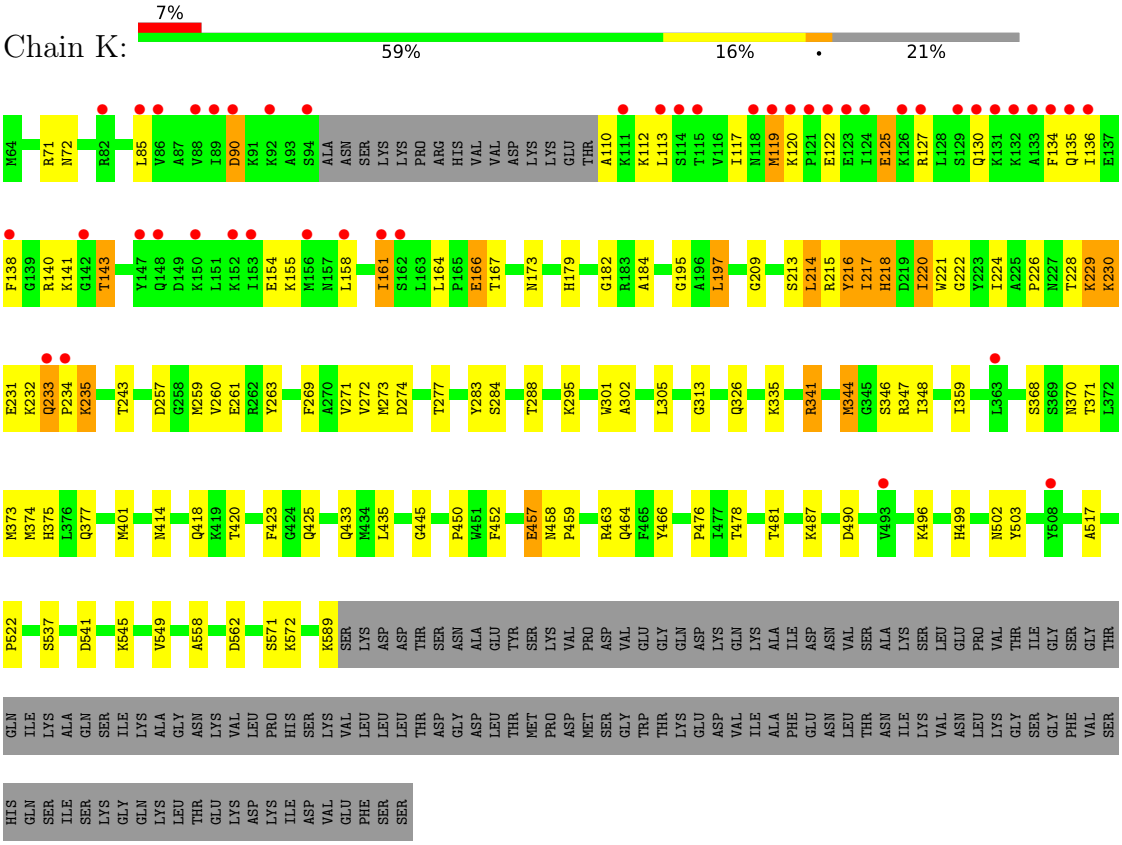
• Molecule 1: Penicillin-binding protein 1

Chain J:



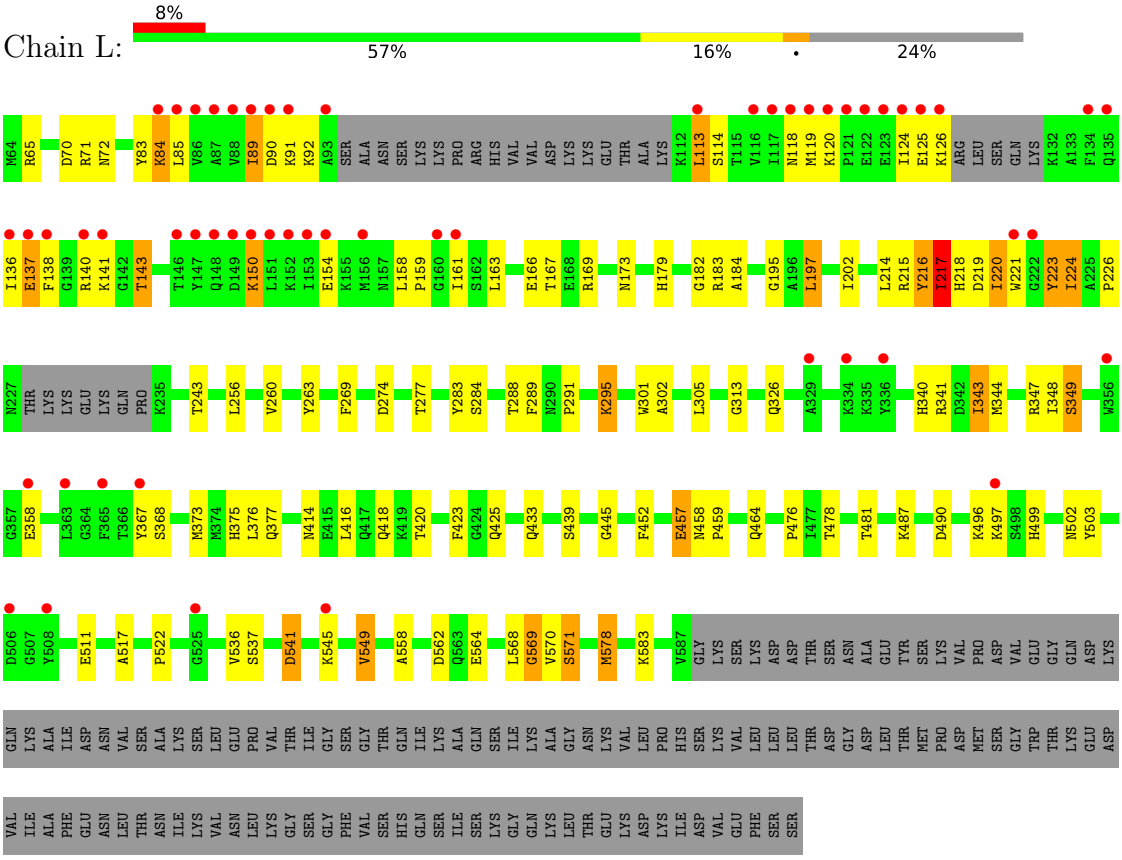
• Molecule 1: Penicillin-binding protein 1

Chain K:



• Molecule 1: Penicillin-binding protein 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	311.86Å 197.15Å 221.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.03 49.01 – 3.03	Depositor EDS
% Data completeness (in resolution range)	55.2 (49.00-3.03) 55.3 (49.01-3.03)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.246 0.213 , 0.244	Depositor DCC
R_{free} test set	7237 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	81.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	48707	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EPE, CD

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	0/4195	0.87	0/5641
1	B	0.70	0/4247	0.87	0/5712
1	C	0.69	0/4188	0.87	0/5633
1	D	0.69	0/4044	0.85	0/5440
1	E	0.70	0/4210	0.85	0/5662
1	F	0.71	0/4256	0.86	0/5723
1	G	0.68	0/4188	0.85	0/5633
1	H	0.71	0/3787	0.86	0/5099
1	I	0.69	0/4172	0.84	0/5611
1	J	0.70	0/4169	0.85	0/5608
1	K	0.71	0/4117	0.85	0/5537
1	L	0.74	0/3979	0.87	0/5354
All	All	0.70	0/49552	0.86	0/66653

There are no bond length outliers.

There are no bond angle outliers.

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	4105	0	4096	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4156	0	4149	74	0
1	C	4098	0	4084	58	0
1	D	3958	0	3928	61	0
1	E	4120	0	4109	78	0
1	F	4165	0	4162	74	0
1	G	4098	0	4084	68	0
1	H	3703	0	3646	62	0
1	I	4083	0	4070	54	0
1	J	4080	0	4062	60	0
1	K	4029	0	4013	72	0
1	L	3894	0	3855	56	0
2	A	15	0	18	0	0
2	B	15	0	18	0	0
2	C	15	0	17	0	0
2	D	15	0	17	0	0
2	E	15	0	17	0	0
2	F	15	0	17	1	0
2	G	15	0	17	0	0
2	H	15	0	18	1	0
2	I	15	0	18	1	0
2	J	15	0	18	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	C	1	0	0	2	0
4	D	1	0	0	1	0
4	E	1	0	0	2	0
4	F	1	0	0	1	0
4	H	1	0	0	1	0
4	J	1	0	0	1	0
4	K	1	0	0	2	0
4	L	1	0	0	1	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	3	0	0	1	0
5	E	7	0	0	0	0
5	F	8	0	0	1	0
5	G	5	0	0	0	0
5	H	3	0	0	0	0
5	I	4	0	0	1	0
5	J	4	0	0	1	0
5	K	3	0	0	1	0
5	L	1	0	0	0	0
All	All	48707	0	48433	745	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 8.

The worst 5 of 745 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:E:343:ILE:HG21	1:E:348:ILE:HD11	1.16	1.15
1:J:117:ILE:HD11	1:J:141:LYS:O	1.51	1.11
1:H:85:LEU:HD12	1:H:163:LEU:HD21	1.40	1.02
1:F:223:TYR:O	1:F:224:ILE:HG12	1.58	1.01
1:A:392:PHE:HA	1:A:447:MET:HE3	1.43	0.98

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	517/650 (80%)	454 (88%)	59 (11%)	4 (1%)	19 54
1	B	525/650 (81%)	455 (87%)	63 (12%)	7 (1%)	12 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	516/650 (79%)	452 (88%)	59 (11%)	5 (1%)	15	49
1	D	496/650 (76%)	429 (86%)	59 (12%)	8 (2%)	9	37
1	E	519/650 (80%)	456 (88%)	56 (11%)	7 (1%)	12	42
1	F	526/650 (81%)	456 (87%)	61 (12%)	9 (2%)	9	35
1	G	516/650 (79%)	453 (88%)	59 (11%)	4 (1%)	19	54
1	H	465/650 (72%)	403 (87%)	57 (12%)	5 (1%)	14	47
1	I	514/650 (79%)	449 (87%)	59 (12%)	6 (1%)	13	44
1	J	514/650 (79%)	449 (87%)	61 (12%)	4 (1%)	19	54
1	K	507/650 (78%)	438 (86%)	63 (12%)	6 (1%)	13	44
1	L	486/650 (75%)	424 (87%)	53 (11%)	9 (2%)	8	33
All	All	6101/7800 (78%)	5318 (87%)	709 (12%)	74 (1%)	13	44

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	SER
1	D	232	LYS
1	F	97	SER
1	F	214	LEU
1	F	233	GLN

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	438/552 (79%)	387 (88%)	51 (12%)	5	21
1	B	444/552 (80%)	391 (88%)	53 (12%)	5	20
1	C	437/552 (79%)	389 (89%)	48 (11%)	6	23
1	D	422/552 (76%)	368 (87%)	54 (13%)	4	18
1	E	440/552 (80%)	385 (88%)	55 (12%)	4	18
1	F	445/552 (81%)	390 (88%)	55 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	437/552 (79%)	396 (91%)	41 (9%)	8	30
1	H	392/552 (71%)	347 (88%)	45 (12%)	5	22
1	I	435/552 (79%)	397 (91%)	38 (9%)	10	34
1	J	435/552 (79%)	382 (88%)	53 (12%)	5	19
1	K	429/552 (78%)	376 (88%)	53 (12%)	4	19
1	L	414/552 (75%)	352 (85%)	62 (15%)	3	13
All	All	5168/6624 (78%)	4560 (88%)	608 (12%)	5	20

5 of 608 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	197	LEU
1	L	220	ILE
1	J	383	ASP
1	J	179	HIS
1	K	231	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	436	GLN
1	K	377	GLN
1	H	218	HIS
1	L	377	GLN
1	I	518	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
2	EPE	F	801	-	15,15,15	1.01	1 (6%)	18,20,20	0.98	2 (11%)
2	EPE	I	801	-	15,15,15	0.79	1 (6%)	18,20,20	0.88	0
2	EPE	E	801	-	15,15,15	0.97	1 (6%)	18,20,20	1.03	2 (11%)
2	EPE	H	801	-	15,15,15	0.62	1 (6%)	18,20,20	0.66	0
2	EPE	B	801	-	15,15,15	0.63	1 (6%)	18,20,20	0.84	1 (5%)
2	EPE	C	801	-	15,15,15	1.03	1 (6%)	18,20,20	1.21	1 (5%)
2	EPE	J	801	-	15,15,15	0.69	1 (6%)	18,20,20	0.88	0
2	EPE	D	801	-	15,15,15	1.12	1 (6%)	18,20,20	1.32	2 (11%)
2	EPE	A	801	-	15,15,15	0.67	1 (6%)	18,20,20	0.66	0
2	EPE	G	801	-	15,15,15	1.01	1 (6%)	18,20,20	1.17	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	F	801	-	-	5/9/19/19	0/1/1/1
2	EPE	I	801	-	-	5/9/19/19	0/1/1/1
2	EPE	E	801	-	-	6/9/19/19	0/1/1/1
2	EPE	H	801	-	-	6/9/19/19	0/1/1/1
2	EPE	B	801	-	-	7/9/19/19	0/1/1/1
2	EPE	C	801	-	-	6/9/19/19	0/1/1/1
2	EPE	J	801	-	-	5/9/19/19	0/1/1/1
2	EPE	D	801	-	-	4/9/19/19	0/1/1/1
2	EPE	A	801	-	-	5/9/19/19	0/1/1/1
2	EPE	G	801	-	-	3/9/19/19	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	EPE	O1S-S	3.62	1.55	1.45
2	G	801	EPE	O1S-S	3.53	1.55	1.45
2	F	801	EPE	O2S-S	3.52	1.55	1.45
2	E	801	EPE	O2S-S	3.46	1.55	1.45
2	D	801	EPE	O1S-S	3.46	1.55	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	EPE	O3S-S-O2S	3.25	119.22	111.27
2	G	801	EPE	O1S-S-C10	-2.98	103.33	106.92
2	F	801	EPE	O3S-S-O1S	2.84	118.20	111.27
2	E	801	EPE	O3S-S-O1S	2.78	118.06	111.27
2	E	801	EPE	O2S-S-C10	-2.70	103.67	106.92

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	EPE	C10-C9-N1-C2
2	A	801	EPE	C10-C9-N1-C6
2	A	801	EPE	C8-C7-N4-C5
2	A	801	EPE	S-C10-C9-N1
2	B	801	EPE	S-C10-C9-N1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	EPE	1	0
2	I	801	EPE	1	0
2	H	801	EPE	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	521/650 (80%)	-0.13	11 (2%)	63	34	42, 79, 150, 203	0
1	B	527/650 (81%)	-0.23	5 (0%)	84	62	44, 82, 132, 200	1 (0%)
1	C	520/650 (80%)	-0.14	9 (1%)	70	42	44, 86, 162, 191	0
1	D	502/650 (77%)	0.07	40 (7%)	12	4	41, 83, 199, 280	0
1	E	523/650 (80%)	-0.17	5 (0%)	82	59	43, 90, 135, 185	1 (0%)
1	F	528/650 (81%)	-0.08	21 (3%)	38	16	46, 93, 164, 196	1 (0%)
1	G	520/650 (80%)	-0.23	6 (1%)	79	53	50, 84, 136, 198	0
1	H	471/650 (72%)	-0.11	29 (6%)	20	7	46, 85, 166, 213	0
1	I	518/650 (79%)	-0.21	6 (1%)	79	53	42, 88, 134, 186	0
1	J	518/650 (79%)	-0.07	24 (4%)	32	12	40, 93, 174, 230	0
1	K	511/650 (78%)	0.24	45 (8%)	10	3	49, 110, 192, 273	0
1	L	494/650 (76%)	0.36	55 (11%)	5	1	64, 122, 194, 253	0
All	All	6153/7800 (78%)	-0.06	256 (4%)	36	14	40, 90, 166, 280	3 (0%)

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	THR	8.8
1	D	161	ILE	7.1
1	D	160	GLY	6.9
1	L	138	PHE	6.7
1	J	118	ASN	6.6

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 monosaccharides 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
2	EPE	F	801	15/15	0.80	0.34	144,157,176,177	0
2	EPE	J	801	15/15	0.84	0.25	83,113,191,192	0
2	EPE	I	801	15/15	0.85	0.28	73,111,167,179	0
2	EPE	D	801	15/15	0.85	0.24	79,123,194,197	0
2	EPE	G	801	15/15	0.87	0.26	86,121,204,211	0
2	EPE	C	801	15/15	0.88	0.23	86,113,196,197	0
2	EPE	E	801	15/15	0.88	0.28	85,140,193,198	0
2	EPE	H	801	15/15	0.89	0.24	96,123,197,213	0
2	EPE	B	801	15/15	0.89	0.26	89,134,175,176	0
2	EPE	A	801	15/15	0.89	0.26	100,111,190,196	0
3	CD	G	802	1/1	0.91	0.17	108,108,108,108	0
4	CL	H	802	1/1	0.92	0.11	76,76,76,76	0
4	CL	D	802	1/1	0.94	0.06	82,82,82,82	0
4	CL	J	802	1/1	0.94	0.06	70,70,70,70	0
4	CL	K	801	1/1	0.94	0.06	93,93,93,93	0
4	CL	L	801	1/1	0.94	0.06	87,87,87,87	0
4	CL	C	802	1/1	0.95	0.06	72,72,72,72	0
4	CL	F	802	1/1	0.95	0.07	88,88,88,88	0
3	CD	H	803	1/1	0.96	0.06	37,37,37,37	0
3	CD	A	802	1/1	0.96	0.16	98,98,98,98	0
4	CL	E	802	1/1	0.97	0.13	102,102,102,102	0
3	CD	B	802	1/1	0.98	0.09	131,131,131,131	0
3	CD	C	803	1/1	0.98	0.17	94,94,94,94	0
3	CD	E	803	1/1	0.99	0.12	110,110,110,110	0
3	CD	F	803	1/1	0.99	0.10	131,131,131,131	0
3	CD	I	802	1/1	0.99	0.10	101,101,101,101	0
3	CD	J	803	1/1	0.99	0.15	102,102,102,102	0
3	CD	D	803	1/1	1.00	0.17	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.