



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2016 – 01:33 PM EST

PDB ID : 5BP4
Title : Modifying region (DH-ER-KR) of a mycocerosic acid synthase-like (MAS-like) PKS
Authors : Herbst, D.A.; Jakob, P.R.; Zaehring, F.; Maier, T.
Deposited on : 2015-05-27
Resolution : 3.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

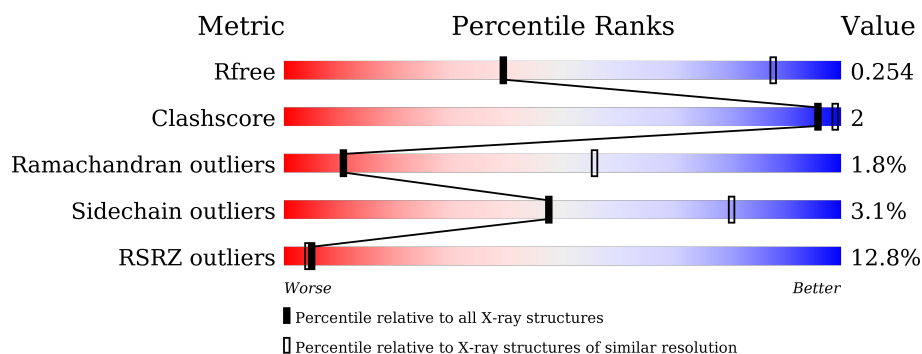
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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}	91344	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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	1140	<div> <div>10%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	B	1140	<div> <div>4%</div> <div>89%</div> <div>7%</div> <div>..</div> </div>
1	C	1140	<div> <div>8%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	1140	<div> <div>9%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	E	1140	<div> <div>21%</div> <div>89%</div> <div>6%</div> <div>.</div> </div>
1	F	1140	<div> <div>16%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	1140	
1	H	1140	
1	I	1140	
1	J	1140	
1	K	1140	
1	L	1140	
1	M	1140	
1	N	1140	
1	O	1140	
1	P	1140	
1	Q	1140	
1	R	1140	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 262498 atoms, of which 129384 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 Mycocerosic acid synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	B	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	C	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	D	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	E	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	F	1093	Total	C	H	N	O	S	0	0	0
			16142	5122	7965	1467	1564	24			
1	G	1088	Total	C	H	N	O	S	0	0	0
			16079	5102	7939	1462	1552	24			
1	H	1097	Total	C	H	N	O	S	0	0	0
			16195	5138	7991	1471	1571	24			
1	I	655	Total	C	H	N	O	S	0	0	0
			9680	3057	4801	872	935	15			
1	J	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	K	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	L	897	Total	C	H	N	O	S	0	0	0
			13209	4199	6535	1183	1272	20			
1	M	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	N	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	O	633	Total	C	H	N	O	S	0	0	0
			9327	2950	4625	839	898	15			
1	P	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	608	Total	C	H	N	O	S	0	0	0
			8979	2846	4455	804	859	15			
1	R	637	Total	C	H	N	O	S	0	0	0
			9417	2980	4669	844	909	15			

There are 54 discrepancies between the modelled and reference sequences:

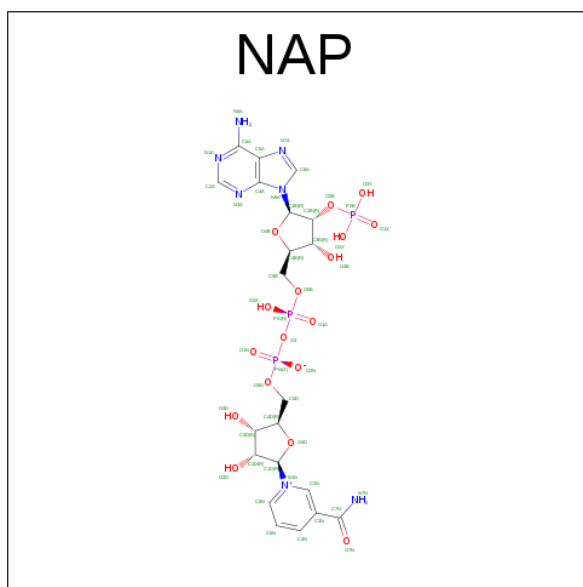
Chain	Residue	Modelled	Actual	Comment	Reference
A	882	SER	-	expression tag	UNP A0R1E8
A	883	MET	-	expression tag	UNP A0R1E8
A	2021	GLN	-	expression tag	UNP A0R1E8
B	882	SER	-	expression tag	UNP A0R1E8
B	883	MET	-	expression tag	UNP A0R1E8
B	2021	GLN	-	expression tag	UNP A0R1E8
C	882	SER	-	expression tag	UNP A0R1E8
C	883	MET	-	expression tag	UNP A0R1E8
C	2021	GLN	-	expression tag	UNP A0R1E8
D	882	SER	-	expression tag	UNP A0R1E8
D	883	MET	-	expression tag	UNP A0R1E8
D	2021	GLN	-	expression tag	UNP A0R1E8
E	882	SER	-	expression tag	UNP A0R1E8
E	883	MET	-	expression tag	UNP A0R1E8
E	2021	GLN	-	expression tag	UNP A0R1E8
F	882	SER	-	expression tag	UNP A0R1E8
F	883	MET	-	expression tag	UNP A0R1E8
F	2021	GLN	-	expression tag	UNP A0R1E8
G	882	SER	-	expression tag	UNP A0R1E8
G	883	MET	-	expression tag	UNP A0R1E8
G	2021	GLN	-	expression tag	UNP A0R1E8
H	882	SER	-	expression tag	UNP A0R1E8
H	883	MET	-	expression tag	UNP A0R1E8
H	2021	GLN	-	expression tag	UNP A0R1E8
I	882	SER	-	expression tag	UNP A0R1E8
I	883	MET	-	expression tag	UNP A0R1E8
I	2021	GLN	-	expression tag	UNP A0R1E8
J	882	SER	-	expression tag	UNP A0R1E8
J	883	MET	-	expression tag	UNP A0R1E8
J	2021	GLN	-	expression tag	UNP A0R1E8
K	882	SER	-	expression tag	UNP A0R1E8
K	883	MET	-	expression tag	UNP A0R1E8
K	2021	GLN	-	expression tag	UNP A0R1E8
L	882	SER	-	expression tag	UNP A0R1E8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	883	MET	-	expression tag	UNP A0R1E8
L	2021	GLN	-	expression tag	UNP A0R1E8
M	882	SER	-	expression tag	UNP A0R1E8
M	883	MET	-	expression tag	UNP A0R1E8
M	2021	GLN	-	expression tag	UNP A0R1E8
N	882	SER	-	expression tag	UNP A0R1E8
N	883	MET	-	expression tag	UNP A0R1E8
N	2021	GLN	-	expression tag	UNP A0R1E8
O	882	SER	-	expression tag	UNP A0R1E8
O	883	MET	-	expression tag	UNP A0R1E8
O	2021	GLN	-	expression tag	UNP A0R1E8
P	882	SER	-	expression tag	UNP A0R1E8
P	883	MET	-	expression tag	UNP A0R1E8
P	2021	GLN	-	expression tag	UNP A0R1E8
Q	882	SER	-	expression tag	UNP A0R1E8
Q	883	MET	-	expression tag	UNP A0R1E8
Q	2021	GLN	-	expression tag	UNP A0R1E8
R	882	SER	-	expression tag	UNP A0R1E8
R	883	MET	-	expression tag	UNP A0R1E8
R	2021	GLN	-	expression tag	UNP A0R1E8

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			73	21	25	7	17		

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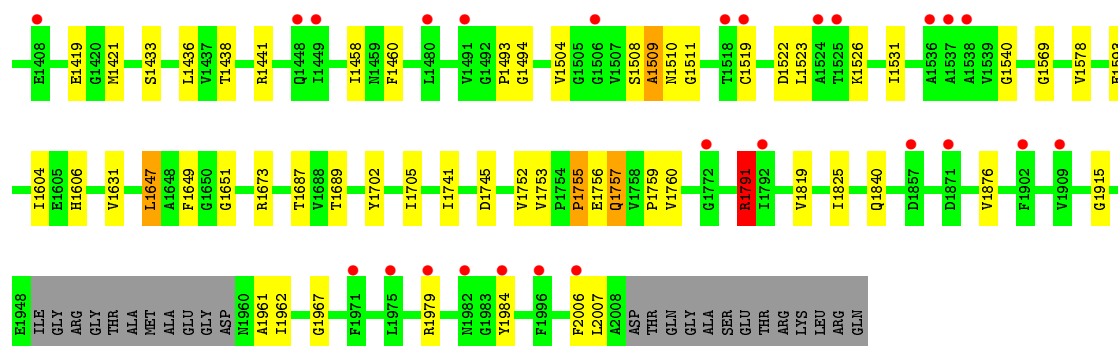
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	B	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	C	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	C	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	D	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	E	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	F	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	G	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	G	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	H	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	H	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	I	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	J	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	J	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	K	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	K	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	L	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	M	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

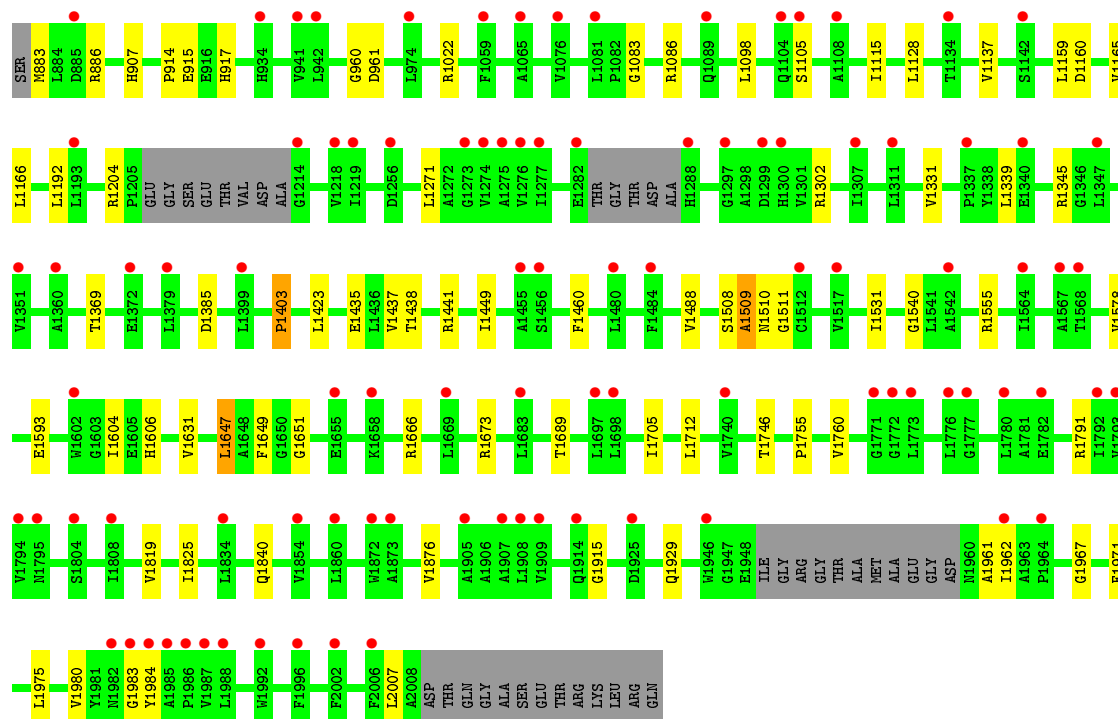
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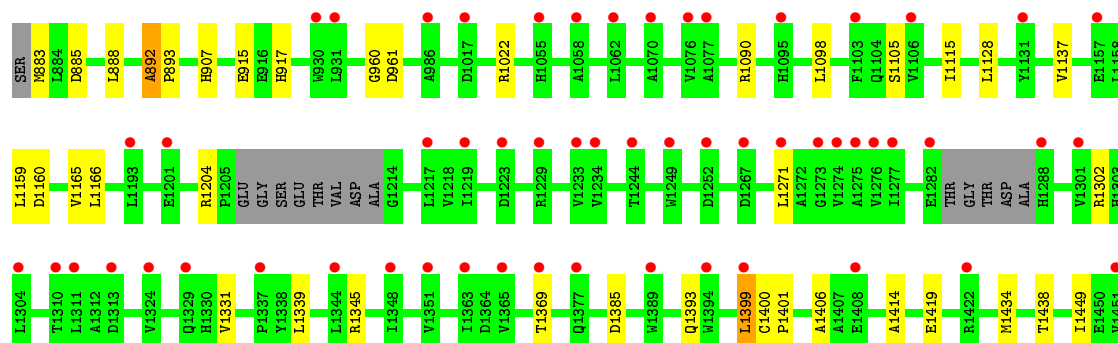
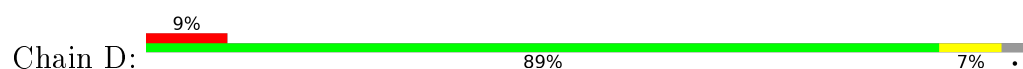
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	M	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	N	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	N	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	O	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	P	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	P	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	Q	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	R	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

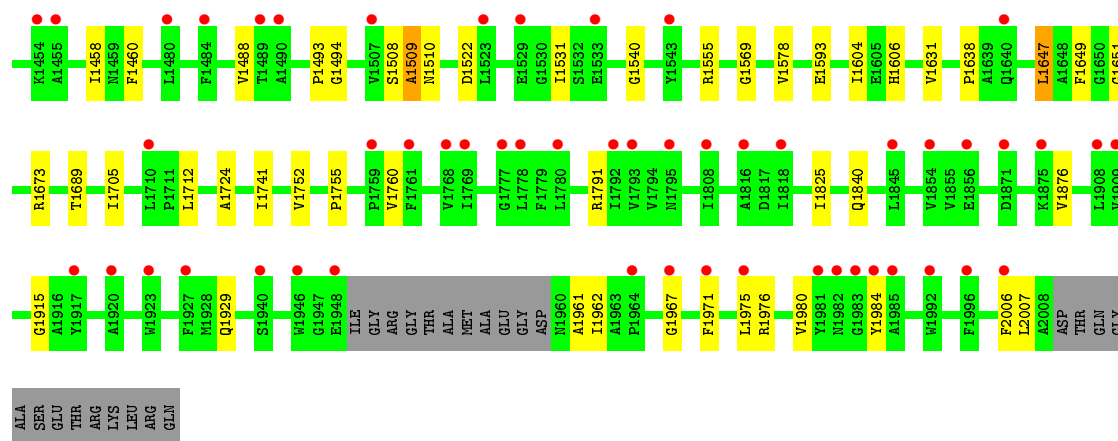


• Molecule 1: Mycocerosic acid synthase

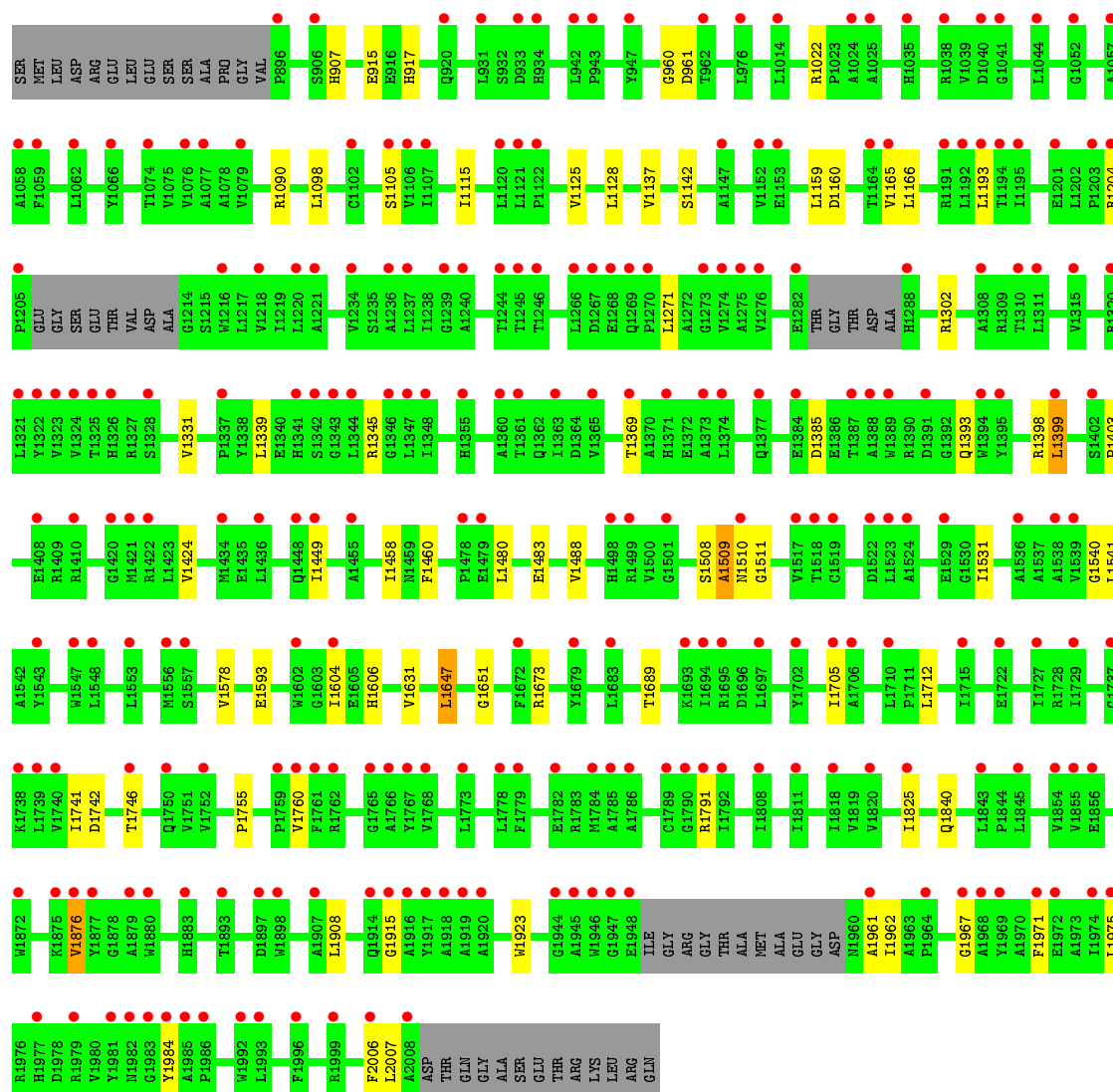
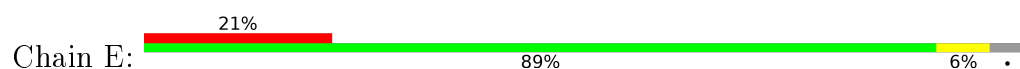


• Molecule 1: Mycocerosic acid synthase

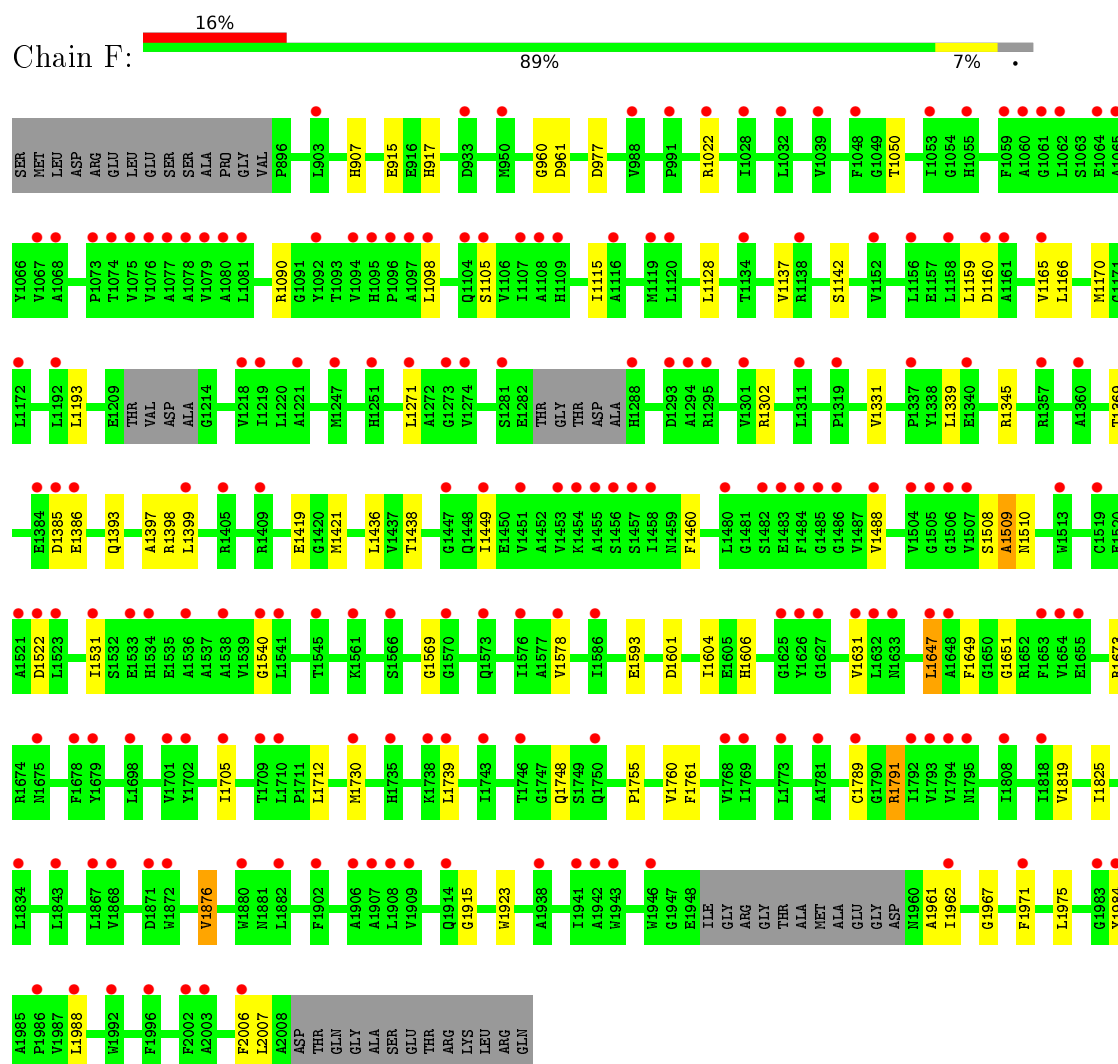




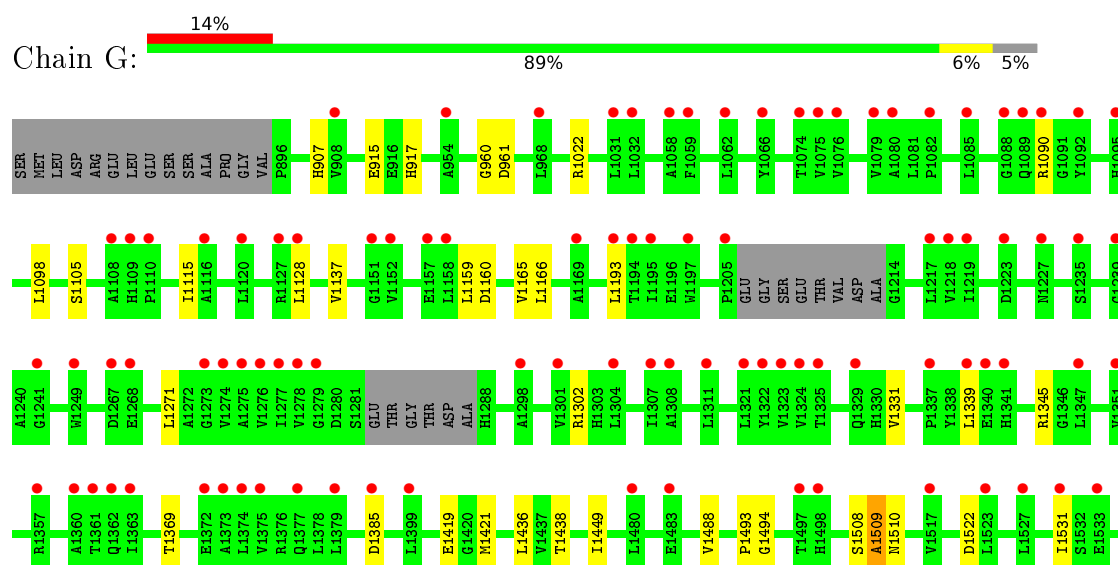
• Molecule 1: Mycocerosic acid synthase

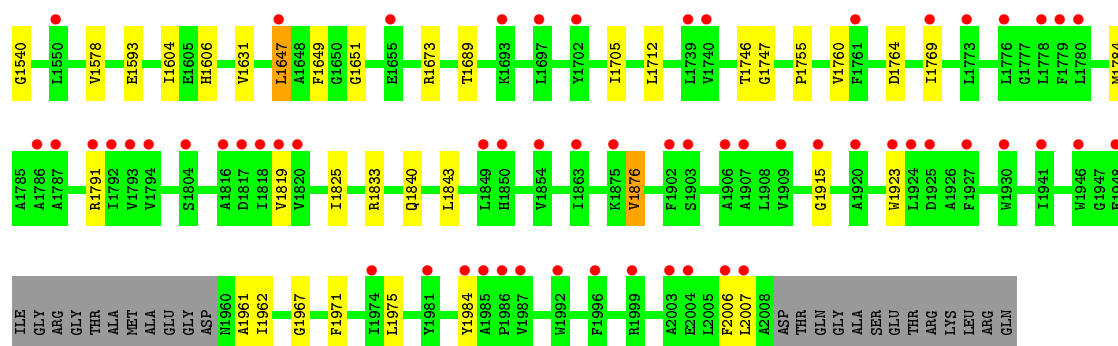


• Molecule 1: Mycocerosic acid synthase

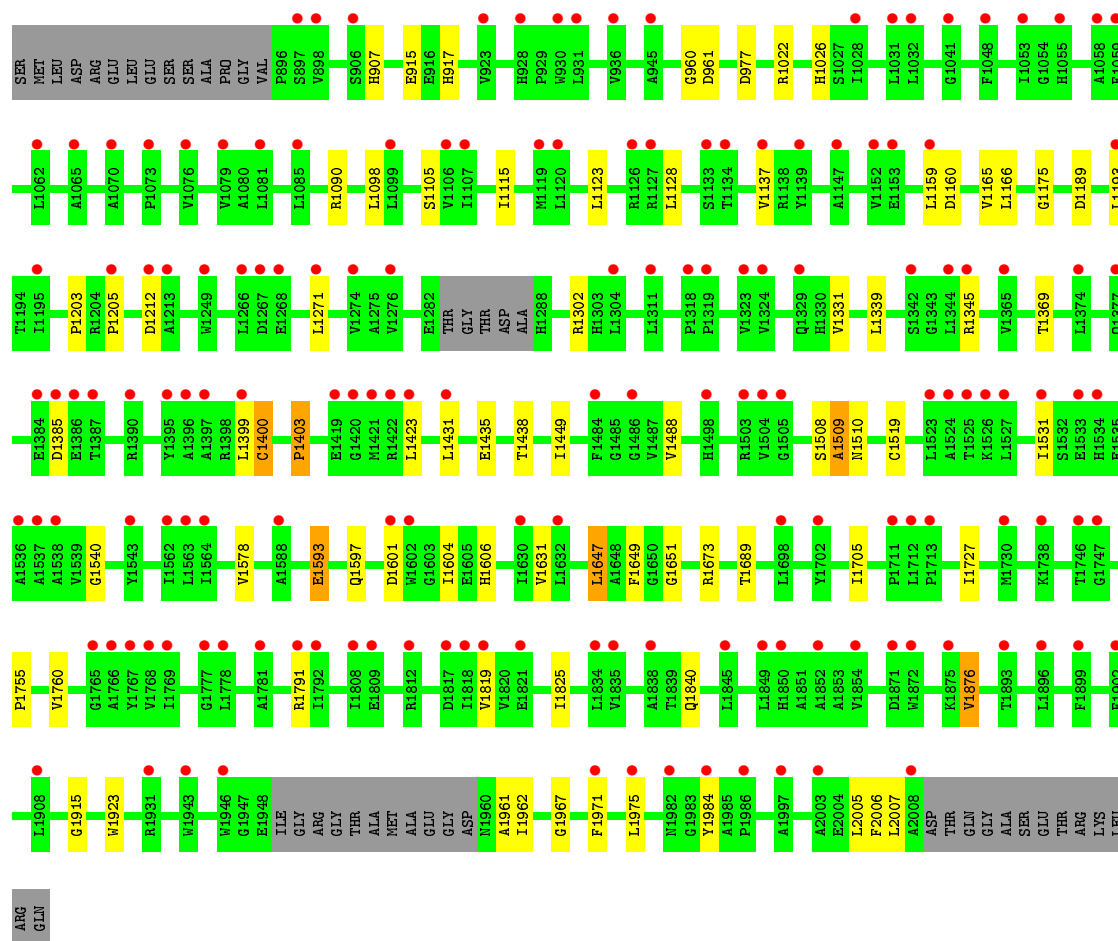


• Molecule 1: Mycroceroic acid synthase

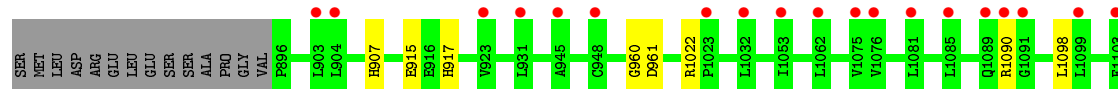




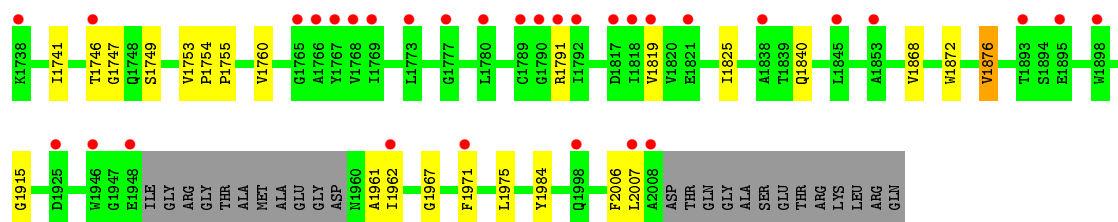
• Molecule 1: Mycocerosic acid synthase



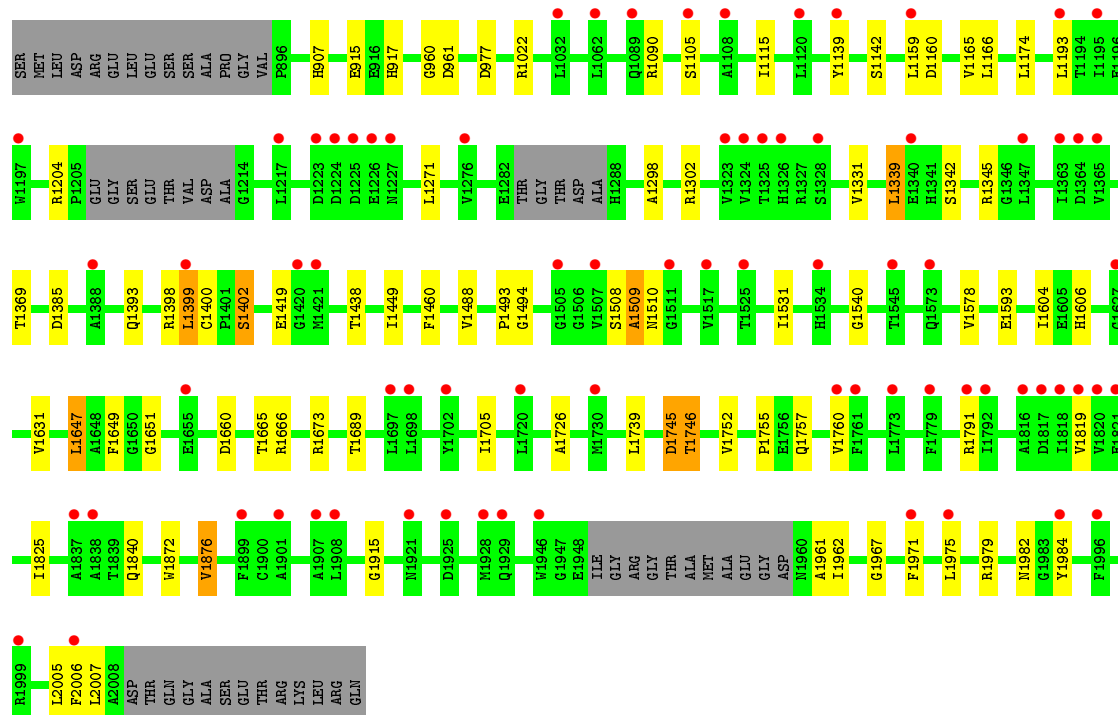
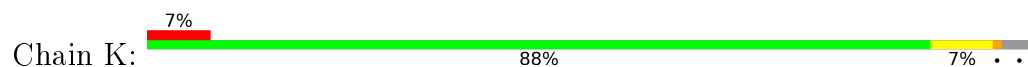
• Molecule 1: Mycocerosic acid synthase



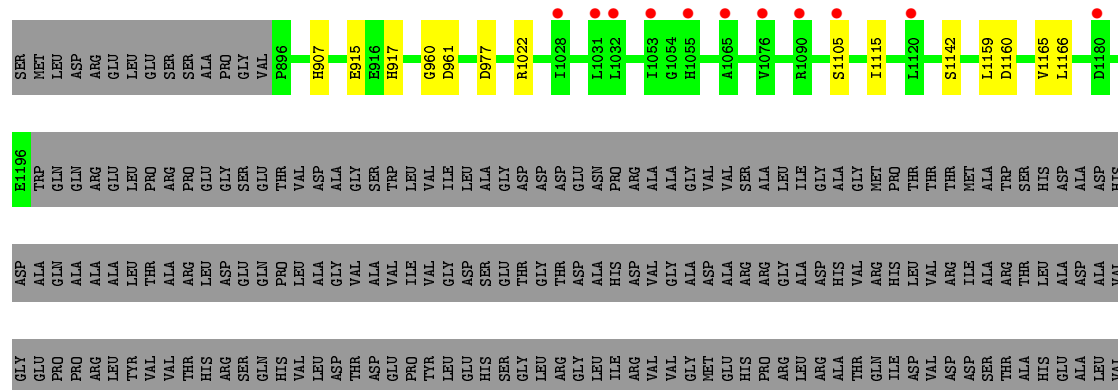
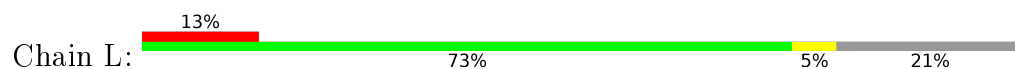


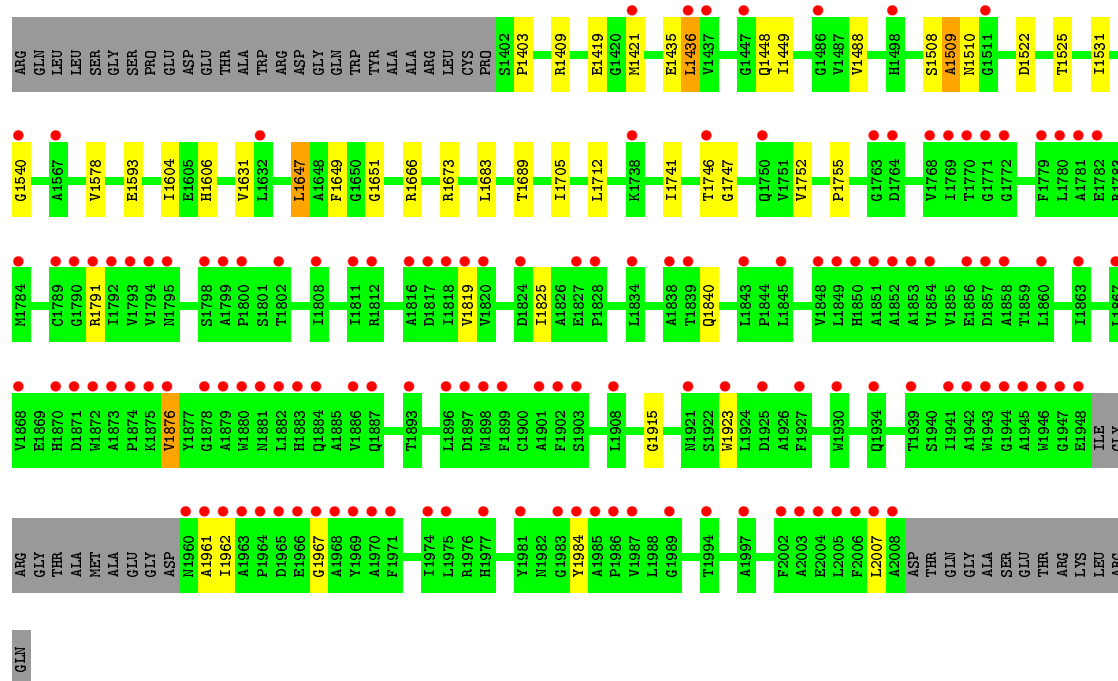


• Molecule 1: Mycocerosic acid synthase

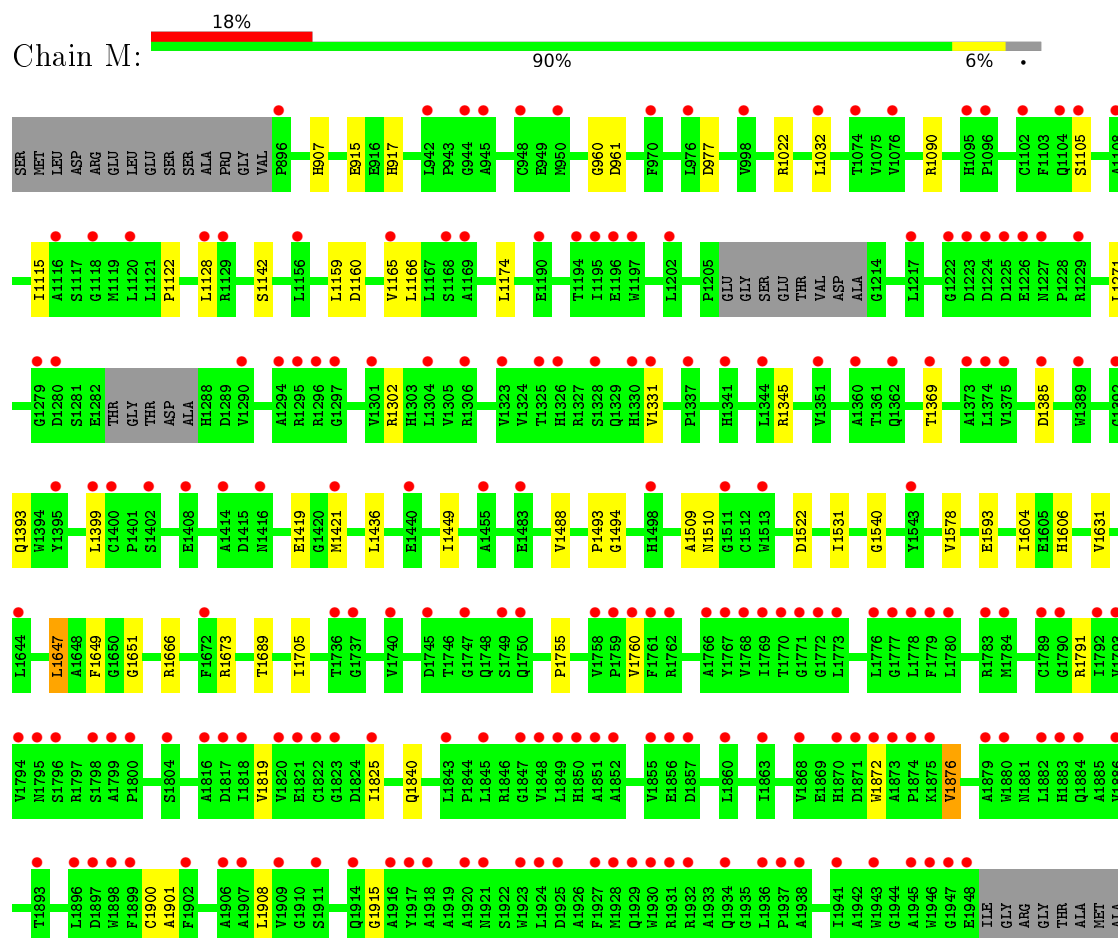


• Molecule 1: Mycocerosic acid synthase

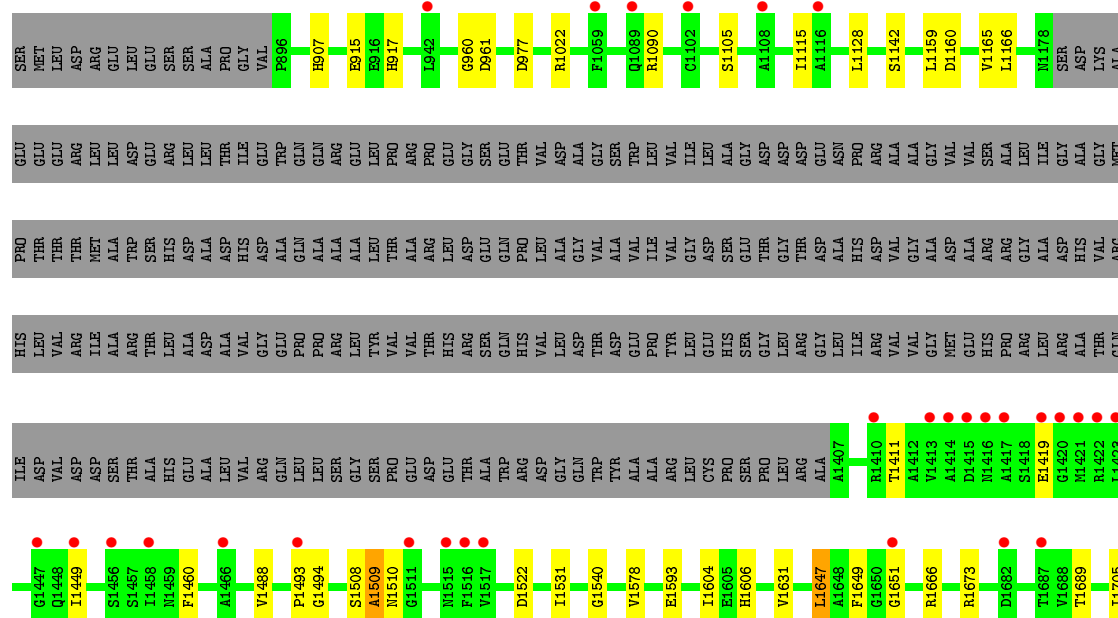


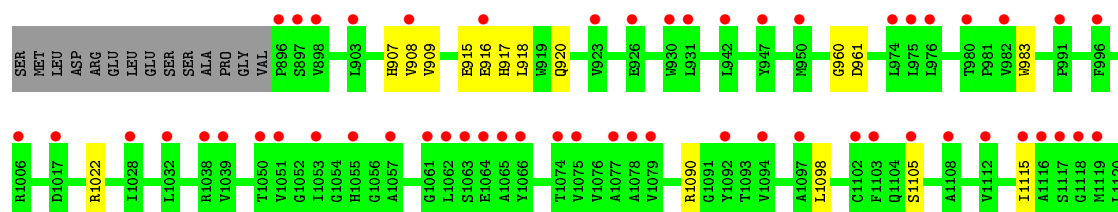


- Molecule 1: Mycocerosic acid synthase



Chain N: 8% 88% 7% 7%







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	151.38Å 190.37Å 270.84Å 95.58° 91.92° 103.65°	Depositor
Resolution (Å)	78.62 – 3.75 78.62 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (78.62-3.75) 95.4 (78.62-3.75)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.78Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.230 , 0.240 0.247 , 0.254	Depositor DCC
R_{free} test set	2985 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 132.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	262498	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.51	0/8420	0.65	0/11488
1	B	0.45	0/8420	0.62	1/11488 (0.0%)
1	C	0.41	0/8420	0.59	0/11488
1	D	0.41	0/8420	0.59	0/11488
1	E	0.40	0/8323	0.58	0/11356
1	F	0.39	0/8351	0.58	0/11393
1	G	0.42	0/8314	0.59	0/11344
1	H	0.41	0/8379	0.59	0/11434
1	I	0.40	0/4977	0.59	0/6783
1	J	0.42	0/8323	0.59	0/11356
1	K	0.44	0/8323	0.60	0/11356
1	L	0.44	0/6815	0.61	0/9296
1	M	0.40	0/8323	0.58	0/11356
1	N	0.42	0/8323	0.61	0/11356
1	O	0.44	0/4797	0.61	0/6540
1	P	0.43	0/8323	0.60	0/11356
1	Q	0.39	0/4617	0.58	0/6293
1	R	0.40	0/4844	0.60	0/6602
All	All	0.42	0/134712	0.60	1/183773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1178	ASN	C-N-CA	5.23	134.78	121.70

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	8245	8038	8072	32	0
1	B	8245	8038	8072	33	0
1	C	8245	8038	8072	22	1
1	D	8245	8038	8072	26	0
1	E	8149	7945	7979	23	0
1	F	8177	7965	7999	27	0
1	G	8140	7939	7973	23	0
1	H	8204	7991	8025	35	0
1	I	4879	4801	4822	12	0
1	J	8149	7945	7979	30	1
1	K	8149	7945	7979	30	0
1	L	6674	6535	6560	19	0
1	M	8149	7945	7979	19	0
1	N	8149	7945	7979	24	0
1	O	4702	4625	4646	14	0
1	P	8149	7945	7979	28	0
1	Q	4524	4455	4476	31	0
1	R	4748	4669	4690	23	0
2	A	75	36	36	2	0
2	B	75	36	36	2	0
2	C	79	36	36	1	0
2	D	75	36	36	2	0
2	E	48	25	25	1	0
2	F	75	36	36	2	0
2	G	75	36	36	0	0
2	H	75	36	36	0	0
2	I	48	25	25	1	0
2	J	75	36	36	0	0
2	K	75	36	36	2	0
2	L	48	25	25	1	0
2	M	75	36	36	0	0
2	N	75	36	36	0	0
2	O	48	25	25	1	0
2	P	75	36	36	0	0
2	Q	48	25	25	0	0
2	R	48	25	25	0	0
All	All	133114	129384	129935	406	1

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 2.

The worst 5 of 406 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:N:1348:ILE:CD1	1:N:1348:ILE:CG1	1.80	1.59
1:Q:908:VAL:HG13	1:R:920:GLN:HB2	1.68	0.75
1:N:1193:LEU:HD22	1:N:1399:LEU:HD22	1.70	0.73
1:C:914:PRO:HD3	1:D:1638:PRO:HG3	1.71	0.73
1:Q:909:VAL:O	1:R:983:TRP:NE1	2.21	0.71

All (1) 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:C:1083:GLY:HA2	1:J:1264:ALA:HB1[1_565]	1.34	0.26

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	1094/1140 (96%)	995 (91%)	79 (7%)	20 (2%)	11	56
1	B	1094/1140 (96%)	1002 (92%)	69 (6%)	23 (2%)	9	53
1	C	1094/1140 (96%)	1002 (92%)	73 (7%)	19 (2%)	11	57
1	D	1094/1140 (96%)	1001 (92%)	72 (7%)	21 (2%)	10	55
1	E	1081/1140 (95%)	993 (92%)	68 (6%)	20 (2%)	10	55
1	F	1085/1140 (95%)	995 (92%)	74 (7%)	16 (2%)	13	59
1	G	1080/1140 (95%)	990 (92%)	72 (7%)	18 (2%)	11	57
1	H	1091/1140 (96%)	996 (91%)	76 (7%)	19 (2%)	11	57
1	I	651/1140 (57%)	601 (92%)	39 (6%)	11 (2%)	11	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	1081/1140 (95%)	991 (92%)	68 (6%)	22 (2%)	9	54
1	K	1081/1140 (95%)	990 (92%)	71 (7%)	20 (2%)	10	55
1	L	891/1140 (78%)	815 (92%)	61 (7%)	15 (2%)	11	57
1	M	1081/1140 (95%)	995 (92%)	71 (7%)	15 (1%)	14	59
1	N	1081/1140 (95%)	982 (91%)	76 (7%)	23 (2%)	9	53
1	O	629/1140 (55%)	580 (92%)	37 (6%)	12 (2%)	10	55
1	P	1081/1140 (95%)	986 (91%)	72 (7%)	23 (2%)	9	53
1	Q	604/1140 (53%)	562 (93%)	35 (6%)	7 (1%)	16	63
1	R	633/1140 (56%)	582 (92%)	39 (6%)	12 (2%)	10	55
All	All	17526/20520 (85%)	16058 (92%)	1152 (7%)	316 (2%)	11	56

5 of 316 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1755	PRO
1	B	892	ALA
1	B	1179	SER
1	C	1755	PRO
1	D	892	ALA

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	836/863 (97%)	802 (96%)	34 (4%)	37	75
1	B	836/863 (97%)	808 (97%)	28 (3%)	45	79
1	C	836/863 (97%)	811 (97%)	25 (3%)	48	80
1	D	836/863 (97%)	809 (97%)	27 (3%)	46	79
1	E	825/863 (96%)	802 (97%)	23 (3%)	51	82
1	F	828/863 (96%)	801 (97%)	27 (3%)	45	79
1	G	824/863 (96%)	802 (97%)	22 (3%)	52	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	831/863 (96%)	809 (97%)	22 (3%)	54	83
1	I	503/863 (58%)	487 (97%)	16 (3%)	46	79
1	J	825/863 (96%)	795 (96%)	30 (4%)	42	77
1	K	825/863 (96%)	800 (97%)	25 (3%)	48	80
1	L	674/863 (78%)	653 (97%)	21 (3%)	47	80
1	M	825/863 (96%)	803 (97%)	22 (3%)	52	82
1	N	825/863 (96%)	795 (96%)	30 (4%)	42	77
1	O	483/863 (56%)	467 (97%)	16 (3%)	45	79
1	P	825/863 (96%)	796 (96%)	29 (4%)	43	78
1	Q	464/863 (54%)	452 (97%)	12 (3%)	54	83
1	R	490/863 (57%)	478 (98%)	12 (2%)	57	84
All	All	13391/15534 (86%)	12970 (97%)	421 (3%)	47	80

5 of 421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1128	LEU
1	J	1393	GLN
1	P	1712	LEU
1	H	1400	CYS
1	I	1438	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1597	GLN
1	J	1459	ASN
1	P	1633	ASN
1	H	1633	ASN
1	D	1459	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 ⓘ

30 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$
2	NAP	A	3001	-	45,52,52	0.95	1 (2%)	55,80,80	1.07	6 (10%)
2	NAP	A	3002	-	25,29,52	0.70	0	31,45,80	1.23	4 (12%)
2	NAP	B	3001	-	45,52,52	0.91	3 (6%)	55,80,80	1.34	4 (7%)
2	NAP	B	3002	-	25,29,52	0.83	0	31,45,80	1.50	6 (19%)
2	NAP	C	3001	-	45,52,52	0.78	2 (4%)	55,80,80	0.86	2 (3%)
2	NAP	C	3002	-	28,33,52	0.68	0	35,52,80	1.07	2 (5%)
2	NAP	D	3001	-	45,52,52	0.84	2 (4%)	55,80,80	1.01	4 (7%)
2	NAP	D	3002	-	25,29,52	0.76	0	31,45,80	1.34	4 (12%)
2	NAP	E	3001	-	45,52,52	0.87	3 (6%)	55,80,80	0.92	4 (7%)
2	NAP	F	3001	-	45,52,52	1.03	3 (6%)	55,80,80	1.01	4 (7%)
2	NAP	F	3002	-	25,29,52	0.76	0	31,45,80	1.29	3 (9%)
2	NAP	G	3001	-	45,52,52	0.82	1 (2%)	55,80,80	1.01	5 (9%)
2	NAP	G	3002	-	25,29,52	0.69	0	31,45,80	1.31	2 (6%)
2	NAP	H	3001	-	45,52,52	0.74	1 (2%)	55,80,80	0.79	1 (1%)
2	NAP	H	3002	-	25,29,52	0.76	0	31,45,80	1.30	5 (16%)
2	NAP	I	3001	-	45,52,52	0.81	1 (2%)	55,80,80	0.78	2 (3%)
2	NAP	J	3001	-	45,52,52	0.78	2 (4%)	55,80,80	1.18	3 (5%)
2	NAP	J	3002	-	25,29,52	0.80	0	31,45,80	1.32	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	K	3001	-	45,52,52	1.34	3 (6%)	55,80,80	1.22	5 (9%)
2	NAP	K	3002	-	25,29,52	0.65	0	31,45,80	1.39	5 (16%)
2	NAP	L	3001	-	45,52,52	0.90	2 (4%)	55,80,80	1.17	5 (9%)
2	NAP	M	3001	-	45,52,52	0.90	3 (6%)	55,80,80	1.07	5 (9%)
2	NAP	M	3002	-	25,29,52	0.91	1 (4%)	31,45,80	1.19	3 (9%)
2	NAP	N	3001	-	45,52,52	0.91	2 (4%)	55,80,80	1.05	5 (9%)
2	NAP	N	3002	-	25,29,52	0.88	1 (4%)	31,45,80	1.62	5 (16%)
2	NAP	O	3001	-	45,52,52	0.96	2 (4%)	55,80,80	1.46	5 (9%)
2	NAP	P	3001	-	45,52,52	0.86	2 (4%)	55,80,80	1.04	4 (7%)
2	NAP	P	3002	-	25,29,52	0.77	0	31,45,80	1.38	4 (12%)
2	NAP	Q	3001	-	45,52,52	0.87	1 (2%)	55,80,80	1.12	5 (9%)
2	NAP	R	3001	-	45,52,52	0.69	1 (2%)	55,80,80	0.87	3 (5%)

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	NAP	A	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	A	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	B	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	C	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	C	3002	-	-	0/17/37/67	0/3/3/5
2	NAP	D	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	D	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	E	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	F	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	F	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	G	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	G	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	H	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	H	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	I	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	J	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	J	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	K	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	K	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	L	3001	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	M	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	M	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	N	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	N	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	O	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	P	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	P	3002	-	-	0/11/31/67	0/3/3/5
2	NAP	Q	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	R	3001	-	-	0/27/67/67	0/5/5/5

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	NAP	O4D-C1D	-3.05	1.36	1.41
2	N	3001	NAP	O4D-C1D	-2.96	1.37	1.41
2	K	3001	NAP	O7N-C7N	-2.86	1.18	1.24
2	M	3001	NAP	O4D-C1D	-2.79	1.37	1.41
2	M	3001	NAP	C7N-N7N	-2.78	1.27	1.33

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3001	NAP	O4D-C1D-N1N	-6.68	100.89	108.10
2	N	3002	NAP	O2B-P2B-O1X	-6.22	92.64	107.48
2	B	3001	NAP	O4D-C1D-N1N	-6.10	101.52	108.10
2	J	3001	NAP	O2A-PA-O3	-5.54	81.52	105.27
2	P	3002	NAP	O2B-P2B-O1X	-4.93	95.72	107.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	NAP	2	0
2	B	3001	NAP	2	0
2	C	3001	NAP	1	0
2	D	3001	NAP	2	0
2	E	3001	NAP	1	0
2	F	3001	NAP	2	0
2	I	3001	NAP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	3001	NAP	2	0
2	L	3001	NAP	1	0
2	O	3001	NAP	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

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	1102/1140 (96%)	0.77	114 (10%) 9 6	84, 166, 265, 278	0
1	B	1102/1140 (96%)	0.61	51 (4%) 36 24	85, 136, 221, 240	0
1	C	1102/1140 (96%)	0.66	96 (8%) 13 8	89, 162, 233, 261	0
1	D	1102/1140 (96%)	0.70	108 (9%) 10 6	92, 173, 262, 282	0
1	E	1089/1140 (95%)	1.14	243 (22%) 1 1	127, 204, 264, 278	0
1	F	1093/1140 (95%)	0.97	187 (17%) 2 2	125, 193, 236, 259	0
1	G	1088/1140 (95%)	0.82	156 (14%) 4 3	108, 174, 224, 261	0
1	H	1097/1140 (96%)	0.85	160 (14%) 3 3	113, 180, 220, 255	0
1	I	655/1140 (57%)	0.80	66 (10%) 9 6	96, 167, 220, 254	0
1	J	1089/1140 (95%)	0.68	82 (7%) 17 11	95, 166, 213, 252	0
1	K	1089/1140 (95%)	0.68	76 (6%) 19 11	85, 138, 187, 226	0
1	L	897/1140 (78%)	1.13	148 (16%) 2 2	81, 145, 244, 264	0
1	M	1089/1140 (95%)	1.06	207 (19%) 2 1	111, 175, 239, 265	0
1	N	1089/1140 (95%)	0.66	94 (8%) 13 9	107, 157, 205, 254	0
1	O	633/1140 (55%)	0.69	39 (6%) 24 14	84, 131, 183, 222	0
1	P	1089/1140 (95%)	0.72	97 (8%) 12 7	85, 150, 211, 247	0
1	Q	608/1140 (53%)	1.75	200 (32%) 0 1	180, 229, 263, 279	0
1	R	637/1140 (55%)	1.10	140 (21%) 1 1	158, 210, 247, 266	0
All	All	17650/20520 (86%)	0.85	2264 (12%) 5 4	81, 170, 243, 282	0

The worst 5 of 2264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	1074	THR	18.2
1	L	1871	ASP	17.4
1	Q	1073	PRO	13.6

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Mol	Chain	Res	Type	RSRZ
1	Q	943	PRO	13.1
1	Q	942	LEU	12.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAP	L	3001	48/48	0.91	0.37	-0.03	110,118,130,134	0
2	NAP	M	3001	48/48	0.89	0.36	-0.13	132,144,158,161	0
2	NAP	A	3001	48/48	0.92	0.35	-0.14	104,124,136,137	0
2	NAP	E	3001	48/48	0.82	0.34	-0.21	181,193,197,198	0
2	NAP	K	3002	27/48	0.75	0.31	-0.21	135,151,159,161	0
2	NAP	J	3002	27/48	0.68	0.30	-0.23	166,169,175,176	0
2	NAP	B	3001	48/48	0.92	0.34	-0.25	103,111,127,129	0
2	NAP	P	3001	48/48	0.93	0.33	-0.31	106,124,132,136	0
2	NAP	N	3001	48/48	0.89	0.32	-0.33	141,152,175,175	0
2	NAP	Q	3001	48/48	0.61	0.40	-0.33	222,225,232,235	0
2	NAP	K	3001	48/48	0.94	0.34	-0.35	109,123,141,145	0
2	NAP	O	3001	48/48	0.92	0.35	-0.36	101,113,135,138	0
2	NAP	H	3001	48/48	0.85	0.32	-0.38	129,146,170,171	0
2	NAP	D	3002	27/48	0.68	0.28	-0.38	193,197,199,199	0
2	NAP	D	3001	48/48	0.90	0.31	-0.39	114,124,138,139	0
2	NAP	H	3002	27/48	0.64	0.30	-0.46	179,187,190,190	0
2	NAP	F	3002	27/48	0.67	0.28	-0.47	164,168,171,171	0
2	NAP	G	3001	48/48	0.90	0.31	-0.48	117,132,158,158	0
2	NAP	I	3001	48/48	0.87	0.33	-0.49	133,144,150,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	B	3002	27/48	0.78	0.29	-0.53	120,134,148,148	0
2	NAP	C	3001	48/48	0.91	0.33	-0.55	110,132,150,153	0
2	NAP	F	3001	48/48	0.85	0.33	-0.58	165,176,183,184	0
2	NAP	J	3001	48/48	0.92	0.30	-0.66	115,126,149,153	0
2	NAP	G	3002	27/48	0.70	0.20	-0.67	195,201,205,205	0
2	NAP	A	3002	27/48	0.61	0.26	-0.69	229,235,241,242	0
2	NAP	C	3002	31/48	0.73	0.27	-0.71	141,162,203,205	0
2	NAP	N	3002	27/48	0.58	0.25	-0.79	156,165,181,182	0
2	NAP	R	3001	48/48	0.77	0.23	-0.96	210,221,233,234	0
2	NAP	P	3002	27/48	0.61	0.21	-1.12	191,203,209,210	0
2	NAP	M	3002	27/48	0.54	0.28	-1.38	233,235,240,240	0

6.5 Other polymers [i](#)

There are no such residues in this entry.