



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:52 AM GMT

PDB ID : 2ULL
Title : MULTIPLE CONFORMATION STRUCTURE OF ALPHA-LYTIC PROTEASE AT 120 K
Authors : Rader, S.D.; Agard, D.A.
Deposited on : 1996-11-26
Resolution : 1.50 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

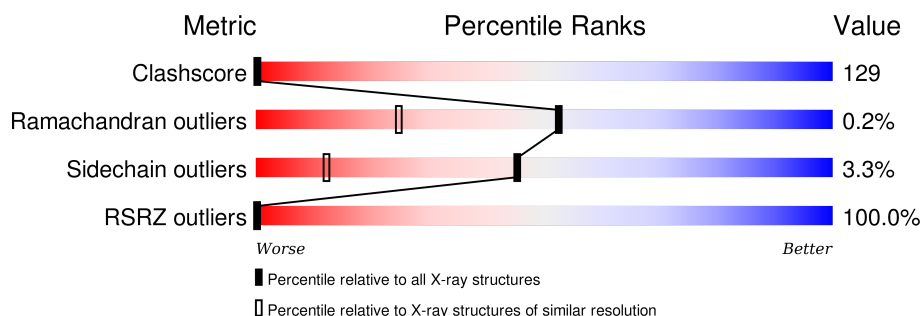
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	1-A	198	<div> <div>100%</div> <div>97%</div> </div>
1	10-A	198	<div> <div>100%</div> <div>97%</div> </div>
1	11-A	198	<div> <div>100%</div> <div>98%</div> </div>
1	12-A	198	<div> <div>100%</div> <div>97%</div> </div>
1	13-A	198	<div> <div>100%</div> <div>97%</div> </div>
1	14-A	198	<div> <div>100%</div> <div>97%</div> </div>
1	15-A	198	<div> <div>100%</div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
1	16-A	198	<div>100%</div> <div>97%</div>
1	2-A	198	<div>100%</div> <div>98%</div>
1	3-A	198	<div>100%</div> <div>98%</div>
1	4-A	198	<div>100%</div> <div>97%</div>
1	5-A	198	<div>100%</div> <div>96%</div>
1	6-A	198	<div>100%</div> <div>97%</div>
1	7-A	198	<div>100%</div> <div>97%</div>
1	8-A	198	<div>100%</div> <div>97%</div>
1	9-A	198	<div>100%</div> <div>97%</div>

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
2	SO4	1-A	3	-	-	-	X
2	SO4	1-A	4	-	X	-	X
2	SO4	10-A	2	-	-	-	X
2	SO4	10-A	3	-	-	-	X
2	SO4	10-A	4	-	X	-	X
2	SO4	11-A	3	-	-	-	X
2	SO4	11-A	4	-	X	-	X
2	SO4	12-A	3	-	-	-	X
2	SO4	12-A	4	-	X	-	X
2	SO4	13-A	3	-	-	-	X
2	SO4	13-A	4	-	X	-	X
2	SO4	14-A	2	-	-	-	X
2	SO4	14-A	3	-	-	-	X
2	SO4	14-A	4	-	X	-	X
2	SO4	15-A	3	-	-	-	X
2	SO4	15-A	4	-	X	-	X
2	SO4	16-A	3	-	-	-	X
2	SO4	16-A	4	-	X	-	X
2	SO4	2-A	3	-	-	-	X
2	SO4	2-A	4	-	X	-	X
2	SO4	3-A	2	-	-	-	X
2	SO4	3-A	3	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	3-A	4	-	X	-	X
2	SO4	4-A	2	-	-	-	X
2	SO4	4-A	3	-	-	-	X
2	SO4	4-A	4	-	X	-	X
2	SO4	5-A	3	-	-	-	X
2	SO4	5-A	4	-	X	-	X
2	SO4	6-A	3	-	-	-	X
2	SO4	6-A	4	-	X	-	X
2	SO4	7-A	3	-	-	-	X
2	SO4	7-A	4	-	X	-	X
2	SO4	8-A	3	-	-	-	X
2	SO4	8-A	4	-	X	-	X
2	SO4	9-A	3	-	-	-	X
2	SO4	9-A	4	-	X	-	X
3	TAM	1-A	1	-	-	-	X
3	TAM	10-A	1	-	-	-	X
3	TAM	11-A	1	-	-	-	X
3	TAM	12-A	1	-	-	-	X
3	TAM	13-A	1	-	-	-	X
3	TAM	14-A	1	-	-	-	X
3	TAM	15-A	1	-	-	-	X
3	TAM	16-A	1	-	-	-	X
3	TAM	2-A	1	-	-	-	X
3	TAM	3-A	1	-	-	-	X
3	TAM	4-A	1	-	-	-	X
3	TAM	5-A	1	-	-	-	X
3	TAM	6-A	1	-	-	-	X
3	TAM	7-A	1	-	-	-	X
3	TAM	8-A	1	-	-	-	X
3	TAM	9-A	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27440 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	2-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	3-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	4-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	5-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	6-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	7-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	8-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	9-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	10-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	11-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	12-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	13-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	14-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	15-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			
1	16-A	198	Total	C	N	O	S	0	0	0
			1391	846	262	275	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		

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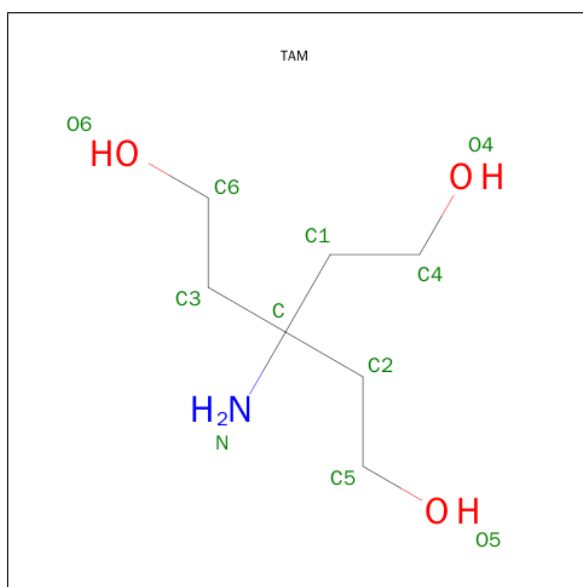
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C₇H₁₇NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	N	0	0
			8	7	1		
3	2-A	1	Total	C	N	0	0
			8	7	1		
3	3-A	1	Total	C	N	0	0
			8	7	1		
3	4-A	1	Total	C	N	0	0
			8	7	1		
3	5-A	1	Total	C	N	0	0
			8	7	1		
3	6-A	1	Total	C	N	0	0
			8	7	1		
3	7-A	1	Total	C	N	0	0
			8	7	1		
3	8-A	1	Total	C	N	0	0
			8	7	1		
3	9-A	1	Total	C	N	0	0
			8	7	1		
3	10-A	1	Total	C	N	0	0
			8	7	1		
3	11-A	1	Total	C	N	0	0
			8	7	1		
3	12-A	1	Total	C	N	0	0
			8	7	1		
3	13-A	1	Total	C	N	0	0
			8	7	1		
3	14-A	1	Total	C	N	0	0
			8	7	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-A	1	Total	C	N	0	0
			8	7	1		
3	16-A	1	Total	C	N	0	0
			8	7	1		

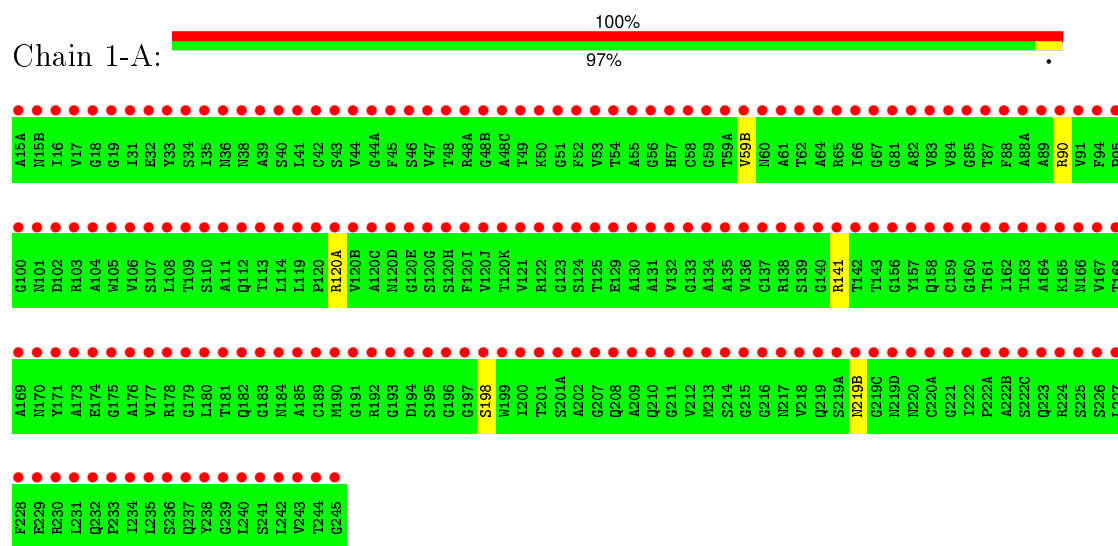
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	301	Total	O	2	0
			301	301		
4	2-A	301	Total	O	2	0
			301	301		
4	3-A	301	Total	O	2	0
			301	301		
4	4-A	301	Total	O	2	0
			301	301		
4	5-A	301	Total	O	2	0
			301	301		
4	6-A	301	Total	O	2	0
			301	301		
4	7-A	301	Total	O	2	0
			301	301		
4	8-A	301	Total	O	2	0
			301	301		
4	9-A	301	Total	O	2	0
			301	301		
4	10-A	301	Total	O	2	0
			301	301		
4	11-A	301	Total	O	2	0
			301	301		
4	12-A	301	Total	O	2	0
			301	301		
4	13-A	301	Total	O	2	0
			301	301		
4	14-A	301	Total	O	2	0
			301	301		
4	15-A	301	Total	O	2	0
			301	301		
4	16-A	301	Total	O	2	0
			301	301		

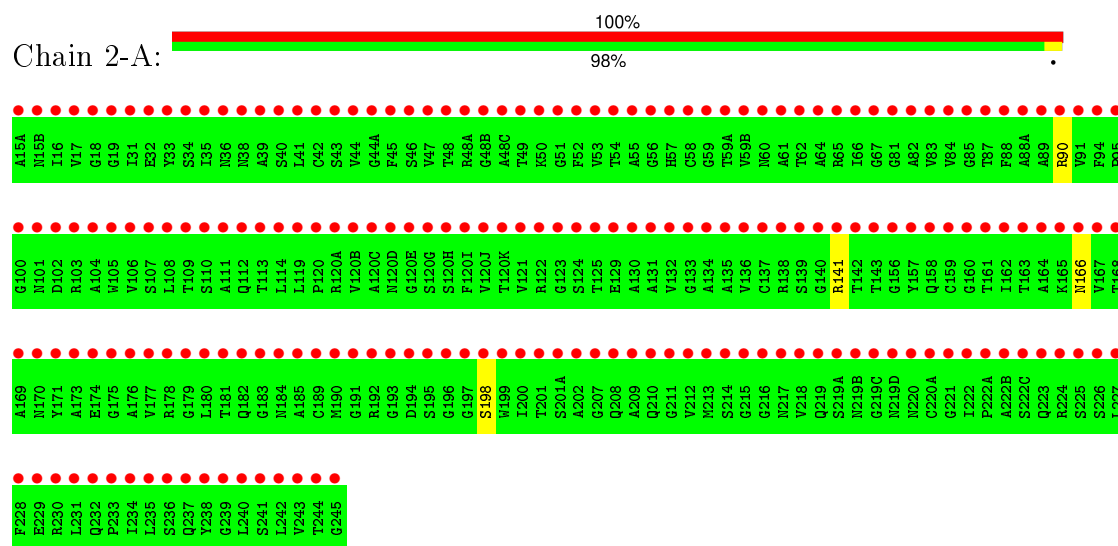
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ALPHA-LYTIC PROTEASE

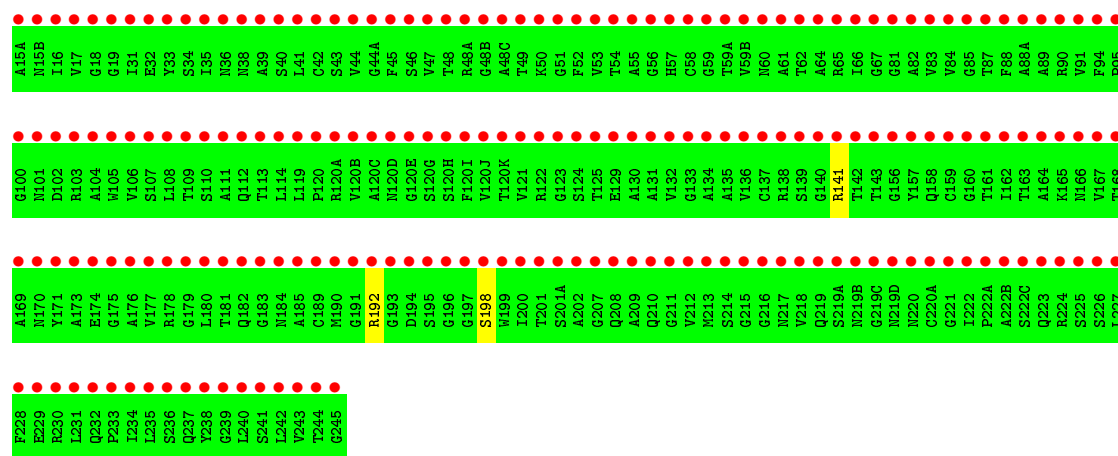


• Molecule 1: ALPHA-LYTIC PROTEASE

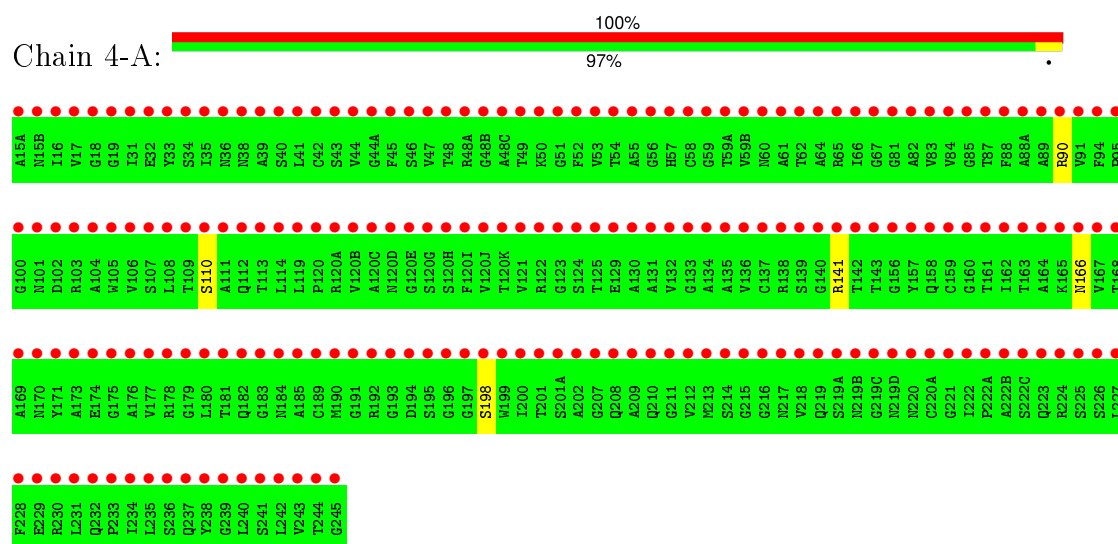


• Molecule 1: ALPHA-LYTIC PROTEASE

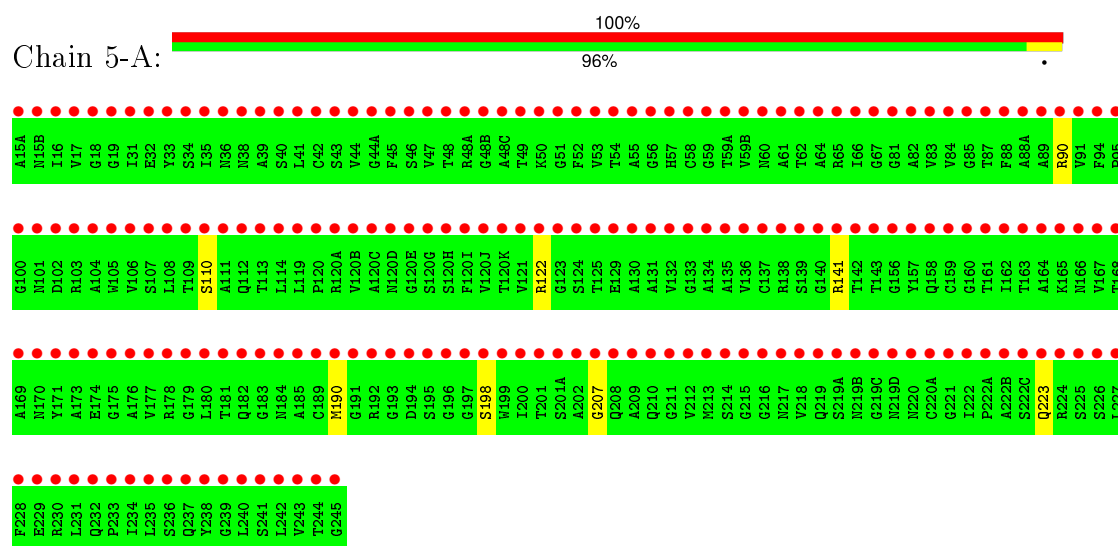




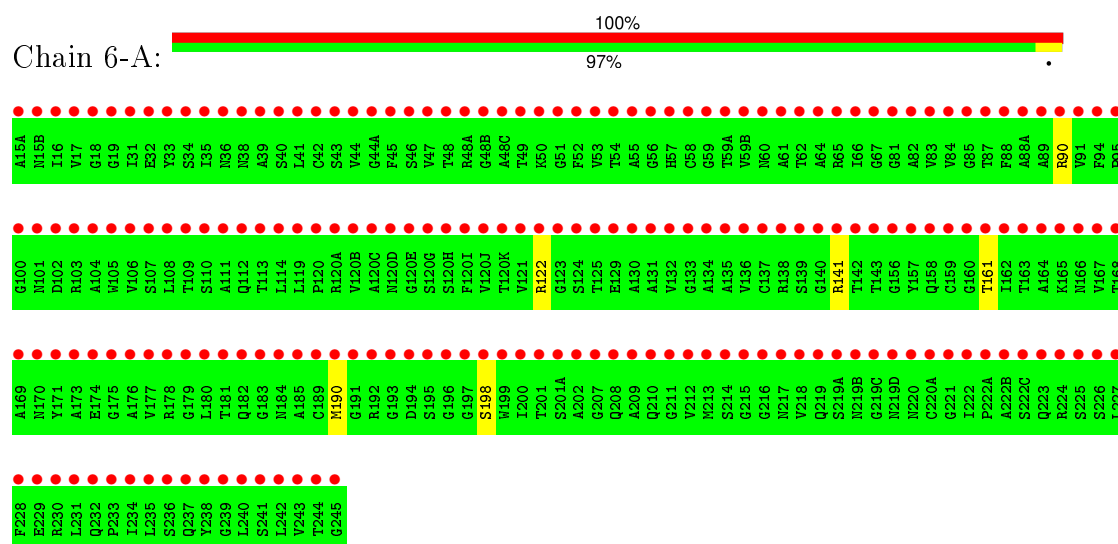
• Molecule 1: ALPHA-LYTIC PROTEASE



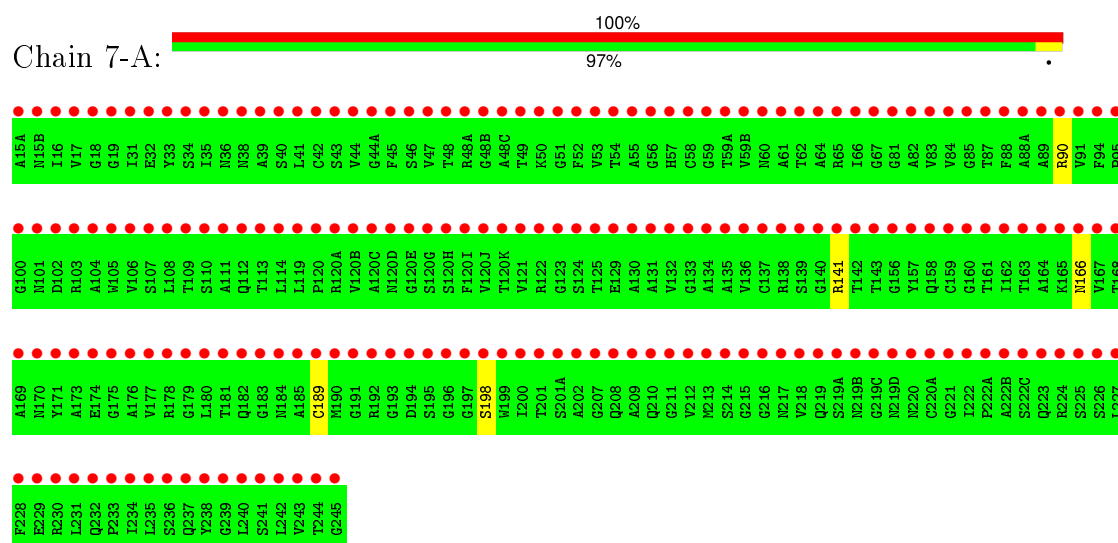
• Molecule 1: ALPHA-LYTIC PROTEASE



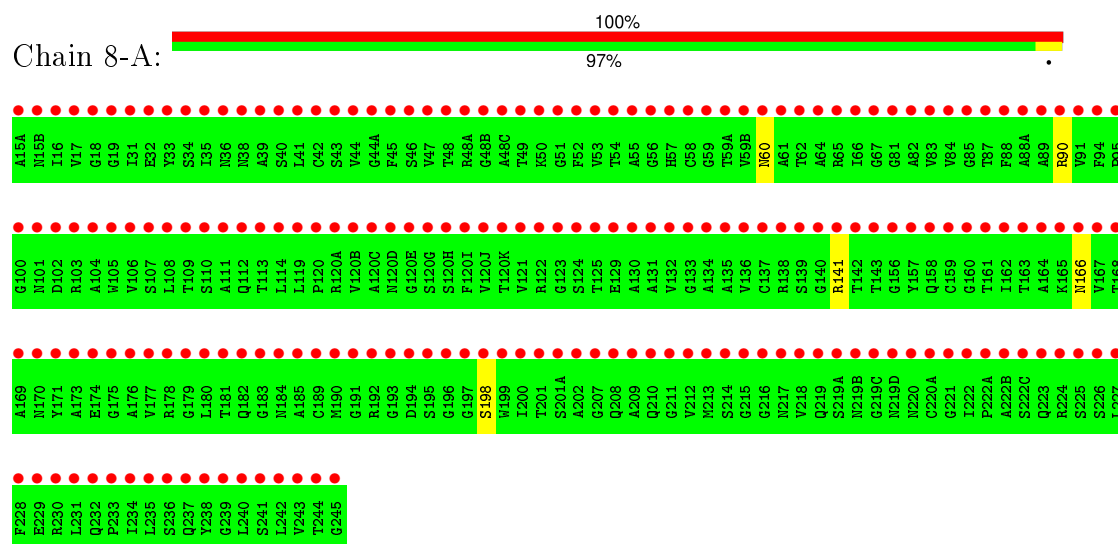
• Molecule 1: ALPHA-LYTIC PROTEASE



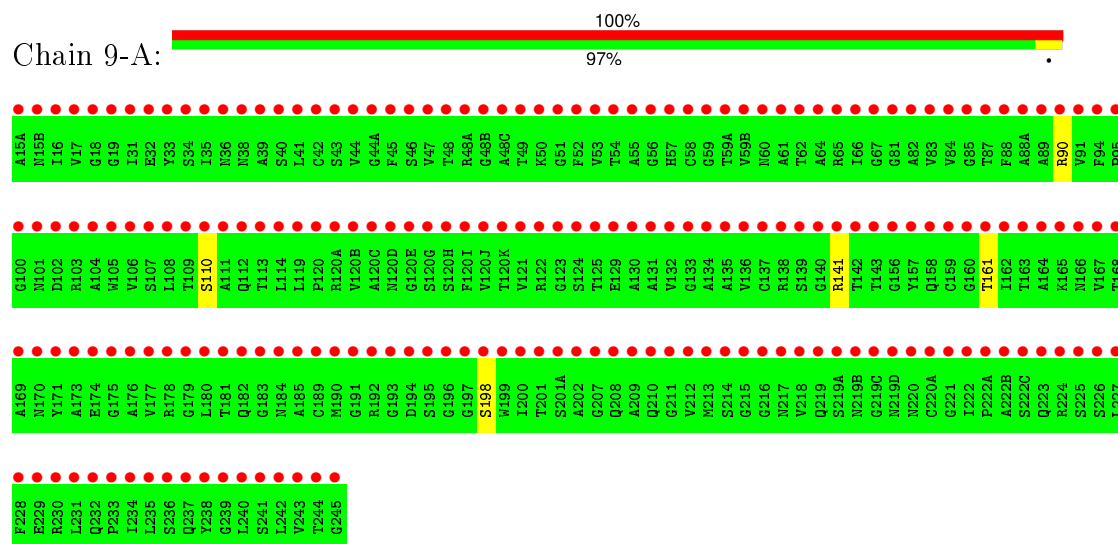
• Molecule 1: ALPHA-LYTIC PROTEASE



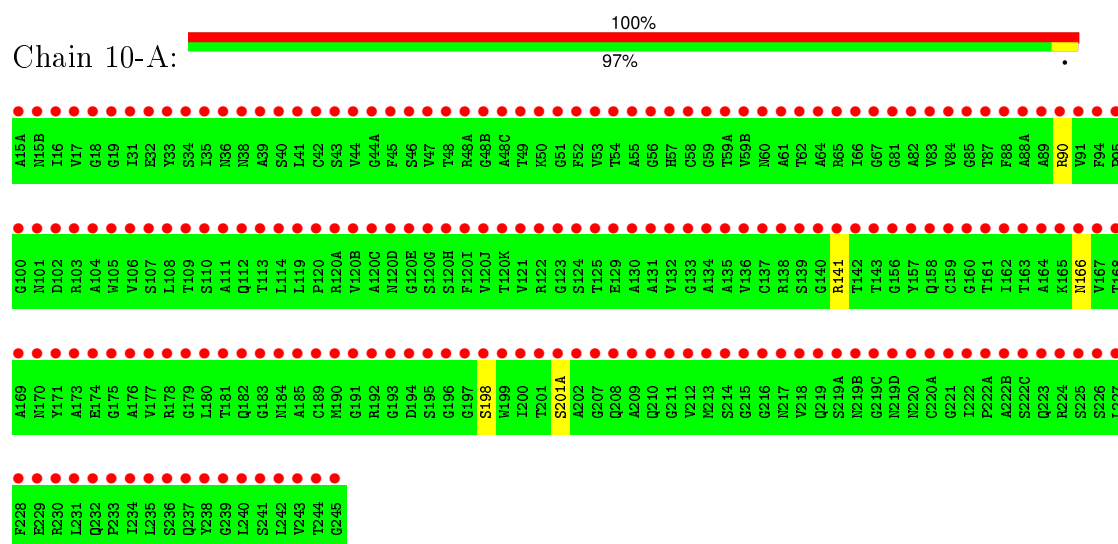
• Molecule 1: ALPHA-LYTIC PROTEASE



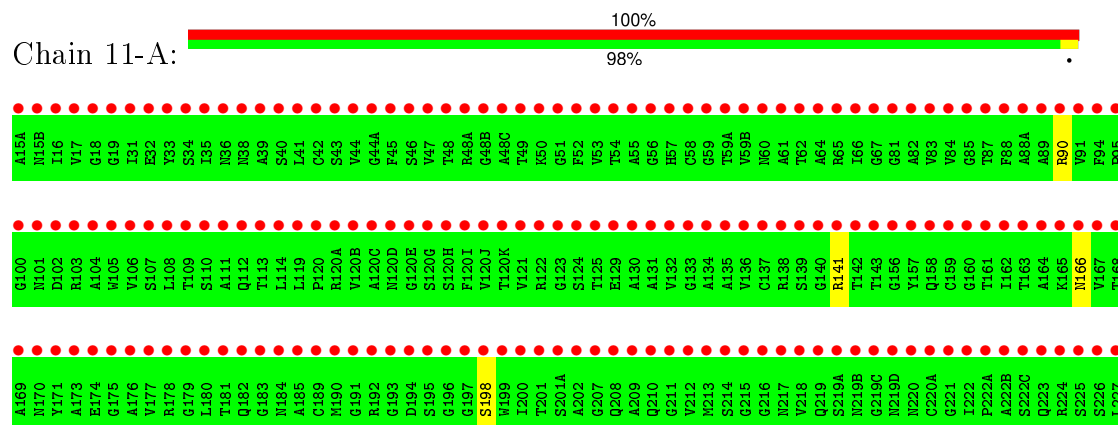
- Molecule 1: ALPHA-LYTIC PROTEASE



- Molecule 1: ALPHA-LYTIC PROTEASE



- Molecule 1: ALPHA-LYTIC PROTEASE



F228
E229
R230
L231
Q232
P233
I234
L235
Q237
Y238
G239
L240
S241
L242
V243
T244
G245

• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 12-A:  100%
97%

A15A
N15B
I16
V17
G18
G19
I31
E32
Y33
S34
I35
N36
N38
A39
S40
L41
C42
S43
V44
G44A
F45
S46
V47
T48
R48A
F120I
G48B
A48C
T49
K50
G51
F52
V53
T54
A55
G56
H57
C58
G59
T59A
V59B
N60
A61
T62
A64
R65
I66
G67
G81
A82
V83
V84
G85
T87
F88
A88A
A89
R90
V91
F94
P95

G100
N101
D102
R103
A104
W105
V106
S107
L108
T109
S110
A111
N112
T113
L114
L119
P120
C121
R120A
V120B
A120C
M120D
G120E
S120G
S120H
F120I
V120J
T120K
V121
R122
G123
S124
T125
E129
A130
A131
V132
G133
A134
A135
V136
C137
R138
S139
G140
R141
T142
T143
G156
Y157
Q158
C159
G160
T161
I162
T163
A164
K165
M166
V167
T168

A169
M170
Y171
E174
G175
A176
V177
R178
G179
L180
T181
Q182
G183
M184
A185
C189
M190
G191
R192
G193
D194
S195
G196
S198
W199
L200
T201
S201A
A202
G207
Q208
A209
Q210
G211
V212
V213
S214
G215
G216
N217
V218
Q219
S219A
N219B
G219C
N219D
N220
C220A
G221
I222
P222A
F222B
S222C
Q223
R224
S225
S226
L227

F228
E229
R230
L231
Q232
P233
I234
L235
Q237
Y238
G239
L240
S241
L242
V243
T244
G245

• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 13-A:  100%
97%

A15A
N15B
I16
V17
G18
G19
I31
E32
Y33
S34
I35
N36
N38
A39
S40
L41
C42
S43
V44
G44A
F45
S46
V47
T48
R48A
F120I
G48B
A48C
T49
K50
G51
F52
V53
T54
A55
G56
H57
C58
G59
T59A
V59B
N60
A61
T62
A64
R65
I66
G67
G81
A82
V83
V84
G85
T87
F88
A88A
A89
R90
V91
F94
P95

G100
N101
D102
R103
A104
W105
V106
S107
L108
T109
S110
A111
N112
T113
L114
L119
P120
C121
R120A
V120B
A120C
M120D
G120E
S120G
S120H
F120I
V120J
T120K
V121
R122
G123
S124
T125
E129
A130
A131
V132
G133
A134
A135
V136
C137
R138
S139
G140
R141
T142
T143
G156
Y157
Q158
C159
G160
T161
I162
T163
A164
K165
M166
V167
T168

A169
M170
Y171
E174
G175
A176
V177
R178
G179
L180
T181
Q182
G183
M184
A185
C189
M190
G191
R192
G193
D194
S195
G196
S198
W199
L200
T201
S201A
A202
G207
Q208
A209
Q210
G211
V212
V213
S214
G215
G216
N217
V218
Q219
S219A
N219B
G219C
N219D
N220
C220A
G221
I222
P222A
F222B
S222C
Q223
R224
S225
S226
L227

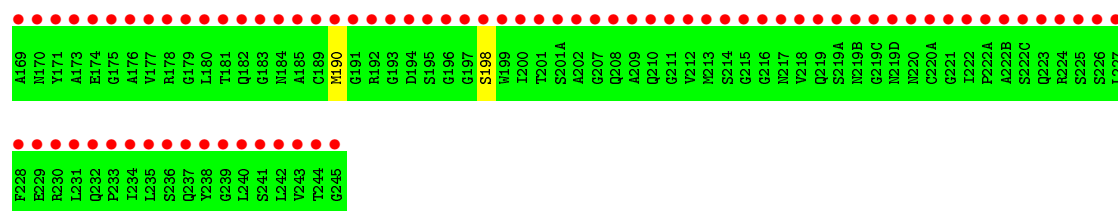
F228
E229
R230
L231
Q232
P233
I234
L235
Q237
Y238
G239
L240
S241
L242
V243
T244
G245

• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 14-A:  100%
97%

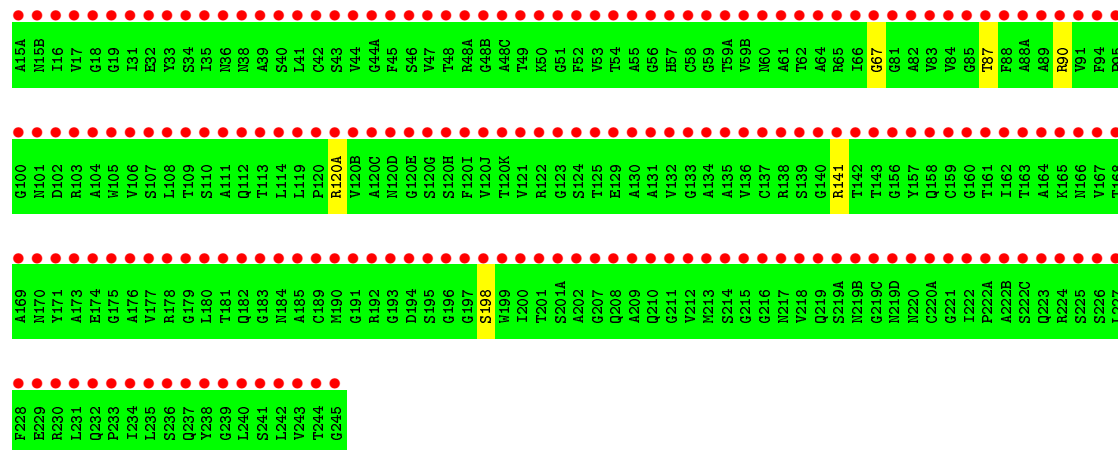
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N15B
I16
V17
G18
G19
I31
E32
Y33
S34
I35
N36
N38
A39
S40
L41
C42
S43
V44
G44A
F45
S46
V47
T48
R48A
F120I
G48B
A48C
T49
K50
G51
F52
V53
T54
A55
G56
H57
C58
G59
T59A
V59B
N60
A61
T62
A64
R65
I66
G67
G81
A82
V83
V84
G85
T87
F88
A88A
A89
R90
V91
F94
P95

G100
N101
D102
R103
A104
W105
V106
S107
L108
T109
S110
A111
N112
T113
L114
L119
P120
C121
R120A
V120B
A120C
M120D
G120E
S120G
S120H
F120I
V120J
T120K
V121
R122
G123
S124
T125
E129
A130
A131
V132
G133
A134
A135
V136
C137
R138
S139
G140
R141
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G160
T161
I162
T163
A164
K165
M166
V167
T168



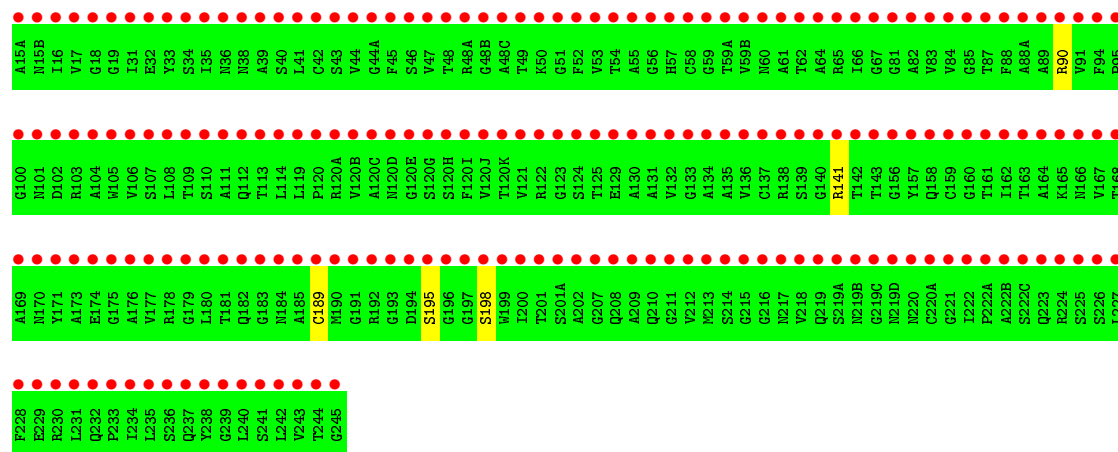
• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 15-A: 100%
97%



• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 16-A: 100%
97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	65.80 Å 65.80 Å 79.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.50 13.57 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (6.00-1.50) 98.5 (13.57-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 1.48 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.165 , 0.192 0.501 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	5.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.38 , 7.5	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 33422 reflections	Xtriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	27440	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TAM, SO4

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	1-A	0.34	0/1409	0.69	0/1909
1	2-A	0.34	0/1409	0.69	0/1909
1	3-A	0.34	0/1409	0.68	0/1909
1	4-A	0.34	0/1409	0.70	0/1909
1	5-A	0.34	0/1409	0.70	1/1909 (0.1%)
1	6-A	0.36	0/1409	0.80	2/1909 (0.1%)
1	7-A	0.36	0/1409	0.69	0/1909
1	8-A	0.34	0/1409	0.69	0/1909
1	9-A	0.34	0/1409	0.69	0/1909
1	10-A	0.34	0/1409	0.69	0/1909
1	11-A	0.34	0/1409	0.69	0/1909
1	12-A	0.34	0/1409	0.67	0/1909
1	13-A	0.37	1/1409 (0.1%)	0.74	2/1909 (0.1%)
1	14-A	0.35	0/1409	0.70	0/1909
1	15-A	0.34	0/1409	0.71	1/1909 (0.1%)
1	16-A	0.34	0/1409	0.70	0/1909
All	All	0.35	1/22544 (0.0%)	0.70	6/30544 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	48(A)	ARG	CZ-NH2	-5.97	1.25	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	122	ARG	NE-CZ-NH2	-14.31	113.14	120.30
1	13-A	48(A)	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	6-A	122	ARG	NH1-CZ-NH2	6.68	126.75	119.40
1	13-A	48(A)	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	15-A	120(A)	ARG	NE-CZ-NH2	-5.44	117.58	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	1-A	1391	0	1363	0	0
1	2-A	1391	0	1361	0	0
1	3-A	1391	0	1363	0	0
1	4-A	1391	0	1361	0	0
1	5-A	1391	0	1363	0	0
1	6-A	1391	0	1363	0	0
1	7-A	1391	0	1365	0	0
1	8-A	1391	0	1361	0	0
1	9-A	1391	0	1363	0	0
1	10-A	1391	0	1363	0	0
1	11-A	1391	0	1361	0	0
1	12-A	1391	0	1361	0	0
1	13-A	1391	0	1363	0	0
1	14-A	1391	0	1361	0	0
1	15-A	1391	0	1361	0	0
1	16-A	1391	0	1363	0	0
2	1-A	15	0	0	0	0
2	2-A	15	0	0	0	0
2	3-A	15	0	0	0	0
2	4-A	15	0	0	0	0
2	5-A	15	0	0	0	0
2	6-A	15	0	0	0	0
2	7-A	15	0	0	0	0
2	8-A	15	0	0	0	0
2	9-A	15	0	0	0	0
2	10-A	15	0	0	0	0
2	11-A	15	0	0	0	0
2	12-A	15	0	0	0	0
2	13-A	15	0	0	0	0
2	14-A	15	0	0	0	0
2	15-A	15	0	0	0	0
2	16-A	15	0	0	0	0
3	1-A	8	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-A	8	0	8	4	0
3	3-A	8	0	8	4	0
3	4-A	8	0	8	4	0
3	5-A	8	0	8	4	0
3	6-A	8	0	8	4	0
3	7-A	8	0	8	4	0
3	8-A	8	0	8	4	0
3	9-A	8	0	8	4	0
3	10-A	8	0	8	4	0
3	11-A	8	0	8	4	0
3	12-A	8	0	8	4	0
3	13-A	8	0	8	4	0
3	14-A	8	0	8	4	0
3	15-A	8	0	8	4	0
3	16-A	8	0	8	4	0
4	1-A	301	0	0	4	0
4	2-A	301	0	0	4	0
4	3-A	301	0	0	4	0
4	4-A	301	0	0	4	0
4	5-A	301	0	0	4	0
4	6-A	301	0	0	4	0
4	7-A	301	0	0	4	0
4	8-A	301	0	0	4	0
4	9-A	301	0	0	4	0
4	10-A	301	0	0	4	0
4	11-A	301	0	0	4	0
4	12-A	301	0	0	4	0
4	13-A	301	0	0	4	0
4	14-A	301	0	0	4	0
4	15-A	301	0	0	4	0
4	16-A	301	0	0	4	0
All	All	27440	0	21924	64	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 129.

The worst 5 of 64 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)
3:A:1:TAM:C4	4:A:339:HOH:O	2.36	0.74
3:A:1:TAM:C4	4:A:339:HOH:O	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1:TAM:C4	4:A:339:HOH:O	2.36	0.74
3:A:1:TAM:C4	4:A:339:HOH:O	2.36	0.74
3:A:1:TAM:C4	4:A:339:HOH:O	2.36	0.74

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	1-A	196/198 (99%)	183 (93%)	12 (6%)	1 (0%)	34	10
1	2-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	3-A	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	34	10
1	4-A	196/198 (99%)	182 (93%)	13 (7%)	1 (0%)	34	10
1	5-A	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	34	10
1	6-A	196/198 (99%)	185 (94%)	11 (6%)	0	100	100
1	7-A	196/198 (99%)	180 (92%)	16 (8%)	0	100	100
1	8-A	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
1	9-A	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
1	10-A	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
1	11-A	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
1	12-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	13-A	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
1	14-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	15-A	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	34	10
1	16-A	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
All	All	3136/3168 (99%)	2952 (94%)	179 (6%)	5 (0%)	52	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5-A	110	SER
1	15-A	67	GLY
1	4-A	110	SER
1	3-A	192	ARG
1	1-A	59(B)	VAL

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	1-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	2-A	142/142 (100%)	138 (97%)	4 (3%)	51	17
1	3-A	142/142 (100%)	140 (99%)	2 (1%)	74	47
1	4-A	142/142 (100%)	138 (97%)	4 (3%)	51	17
1	5-A	142/142 (100%)	136 (96%)	6 (4%)	36	7
1	6-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	7-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	8-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	9-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	10-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	11-A	142/142 (100%)	138 (97%)	4 (3%)	51	17
1	12-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	13-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	14-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
1	15-A	142/142 (100%)	138 (97%)	4 (3%)	51	17
1	16-A	142/142 (100%)	137 (96%)	5 (4%)	43	11
All	All	2272/2272 (100%)	2198 (97%)	74 (3%)	45	12

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8-A	141	ARG
1	10-A	90	ARG
1	15-A	198	SER
1	8-A	166	ASN
1	9-A	110	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-A	101	ASN
1	11-A	101	ASN
1	15-A	232	GLN
1	10-A	60	ASN
1	11-A	158	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

64 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAM	1-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	1-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	1-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	1-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	10-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	10-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	10-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	10-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	11-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	11-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	11-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	11-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	12-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	12-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	12-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	12-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	13-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	13-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	13-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	13-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	14-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	14-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	14-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	14-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	15-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	15-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	15-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	15-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	16-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	16-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	16-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	16-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	2-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	2-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	2-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	2-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	3-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	3-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	3-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	3-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	4-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	4-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	4-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	4-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	5-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	5-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	5-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	5-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	6-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	6-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	6-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	6-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	7-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	7-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	7-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	7-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	8-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	8-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	8-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	8-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)
3	TAM	9-A	1	-	7,7,10	1.76	3 (42%)	6,9,12	6.35	4 (66%)
2	SO4	9-A	2	-	4,4,4	1.96	1 (25%)	6,6,6	1.50	1 (16%)
2	SO4	9-A	3	-	4,4,4	2.64	3 (75%)	6,6,6	0.68	0
2	SO4	9-A	4	-	4,4,4	3.21	3 (75%)	6,6,6	4.06	4 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAM	1-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	1-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	10-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	10-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	11-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	11-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	12-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	12-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	13-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	13-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	14-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	14-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	15-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	15-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	16-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	16-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	2-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	2-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	3-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	3-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	4-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	4-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	3	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	4-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	5-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	5-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	6-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	6-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	7-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	7-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	8-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	8-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	4	-	-	0/0/0/0	0/0/0/0
3	TAM	9-A	1	-	-	0/9/9/12	0/0/0/0
2	SO4	9-A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	4	-	-	0/0/0/0	0/0/0/0

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-A	4	SO4	O2-S	-4.22	1.32	1.47
2	6-A	4	SO4	O2-S	-4.22	1.32	1.47
2	12-A	4	SO4	O2-S	-4.22	1.32	1.47
2	3-A	4	SO4	O2-S	-4.22	1.32	1.47
2	8-A	4	SO4	O2-S	-4.22	1.32	1.47

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-A	4	SO4	O2-S-O1	-5.86	90.91	109.50
2	6-A	4	SO4	O2-S-O1	-5.86	90.91	109.50
2	12-A	4	SO4	O2-S-O1	-5.86	90.91	109.50
2	3-A	4	SO4	O2-S-O1	-5.86	90.91	109.50
2	8-A	4	SO4	O2-S-O1	-5.86	90.91	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	1	TAM	4	0
3	10-A	1	TAM	4	0
3	11-A	1	TAM	4	0
3	12-A	1	TAM	4	0
3	13-A	1	TAM	4	0
3	14-A	1	TAM	4	0
3	15-A	1	TAM	4	0
3	16-A	1	TAM	4	0
3	2-A	1	TAM	4	0
3	3-A	1	TAM	4	0
3	4-A	1	TAM	4	0
3	5-A	1	TAM	4	0
3	6-A	1	TAM	4	0
3	7-A	1	TAM	4	0
3	8-A	1	TAM	4	0
3	9-A	1	TAM	4	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	1-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	2-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	3-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	4-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	5-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	6-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	7-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	8-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	9-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	10-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	11-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	12-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	13-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	14-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	15-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
1	16-A	198/198 (100%)	11.63	198 (100%)	0	0	3, 3, 3, 3	198 (100%)
All	All	3168/3168 (100%)	11.63	3168 (100%)	0	0	3, 3, 3, 3	3168 (100%)

The worst 5 of 3168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	173	ALA	23.5
1	2-A	173	ALA	23.5
1	3-A	173	ALA	23.5
1	4-A	173	ALA	23.5
1	5-A	173	ALA	23.5

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	SO4	8-A	4	5/5	0.85	0.69	0.31	18,18,19,19	5
2	SO4	2-A	4	5/5	0.85	0.69	0.28	18,18,19,19	5
2	SO4	10-A	4	5/5	0.85	0.69	0.26	18,18,19,19	5
2	SO4	6-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	13-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	11-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	5-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	4-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	7-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	3-A	4	5/5	0.85	0.69	0.12	18,18,19,19	5
2	SO4	12-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
2	SO4	16-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
2	SO4	1-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
2	SO4	15-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
2	SO4	9-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
2	SO4	14-A	4	5/5	0.85	0.69	-0.04	18,18,19,19	5
3	TAM	16-A	1	8/11	0.69	0.50	-0.92	7,8,10,11	8
3	TAM	15-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	3-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	1-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	7-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	14-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	8-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	9-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	12-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TAM	13-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
3	TAM	4-A	1	8/11	0.69	0.50	-0.98	7,8,10,11	8
2	SO4	10-A	2	5/5	0.91	0.46	-1.31	9,9,10,10	5
2	SO4	3-A	2	5/5	0.91	0.46	-1.31	9,9,10,10	5
2	SO4	4-A	2	5/5	0.91	0.46	-1.31	9,9,10,10	5
2	SO4	14-A	2	5/5	0.91	0.46	-1.31	9,9,10,10	5
3	TAM	11-A	1	8/11	0.69	0.50	-1.44	7,8,10,11	8
3	TAM	10-A	1	8/11	0.69	0.50	-1.44	7,8,10,11	8
3	TAM	2-A	1	8/11	0.69	0.50	-1.44	7,8,10,11	8
3	TAM	6-A	1	8/11	0.69	0.50	-1.44	7,8,10,11	8
3	TAM	5-A	1	8/11	0.69	0.50	-1.44	7,8,10,11	8
2	SO4	5-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	1-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	13-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	6-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	16-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	9-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	8-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	7-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	2-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	15-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	14-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	3-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	12-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	4-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	11-A	3	5/5	0.98	0.46	-2.46	6,6,6,7	5
2	SO4	10-A	3	5/5	0.98	0.46	-2.47	6,6,6,7	5
2	SO4	12-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	2-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	7-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	16-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	1-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	9-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	5-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	13-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	8-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	15-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	11-A	2	5/5	0.91	0.46	-	9,9,10,10	5
2	SO4	6-A	2	5/5	0.91	0.46	-	9,9,10,10	5

6.5 Other polymers [i](#)

There are no such residues in this entry.