wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 11:20 PM EDT

PDB ID	:	4CG3
Title	:	Structural and functional studies on a thermostable polyethylene therephtalate degrading hydrolase from Thermobifida fusca
Authors	:	Roth, C.; Wei, R.; Oeser, T.; Then, J.; Foellner, C.; Zimmermann, W.; Straeter, N.
Deposited on	:	2013-11-20
Resolution	:	1.55 Å(reported)

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

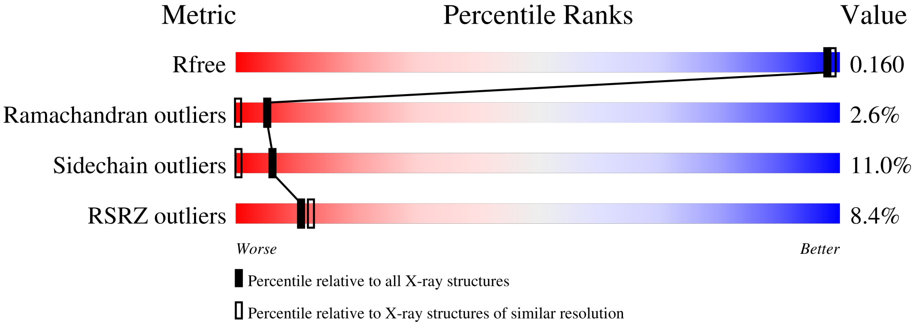
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

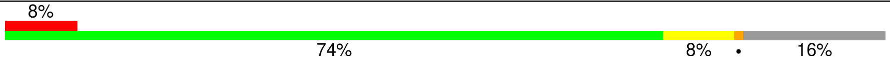
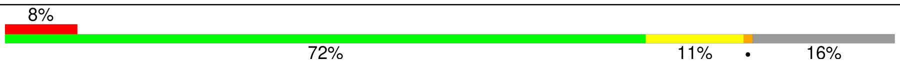
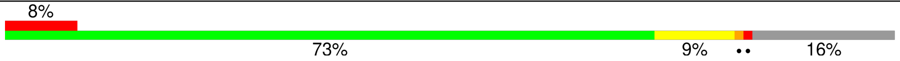
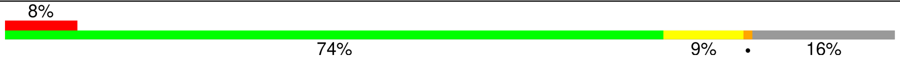
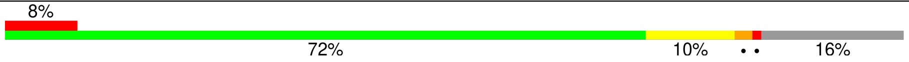
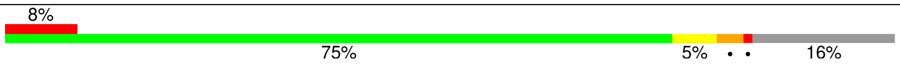
The reported resolution of this entry is 1.55 Å.

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	1483 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	1-A	313	 8% 72% 8% • • 16%
1	10-A	313	 8% 74% 8% • 16%
1	11-A	313	 8% 72% 11% • 16%
1	12-A	313	 8% 73% 9% • • 16%
1	13-A	313	 8% 74% 9% • 16%
1	14-A	313	 8% 72% 10% • • 16%
1	15-A	313	 8% 75% 5% • • 16%

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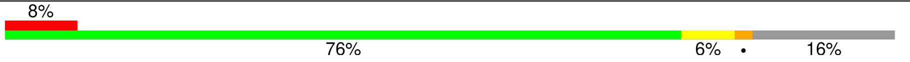
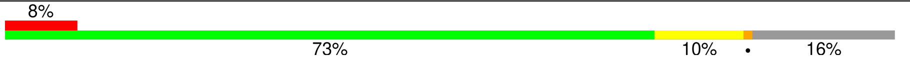
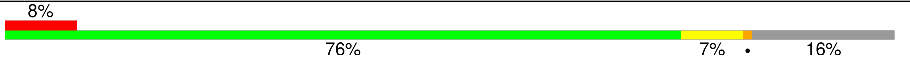
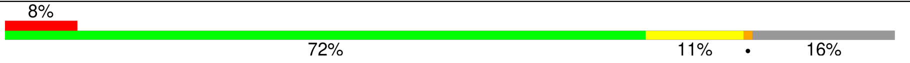
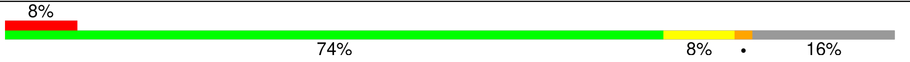
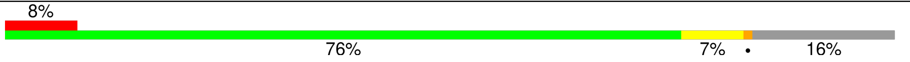
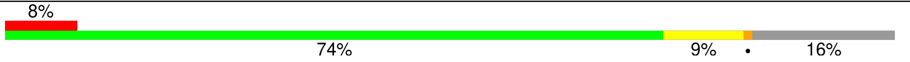
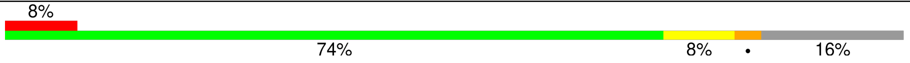
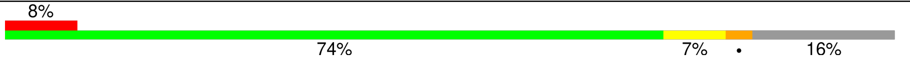
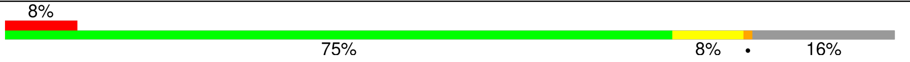
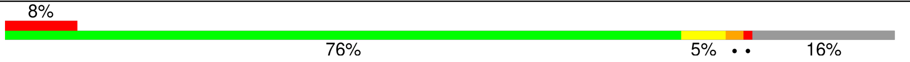
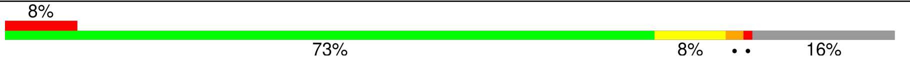
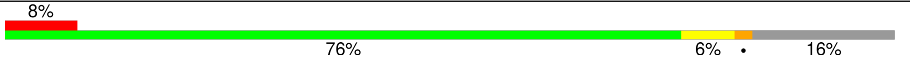
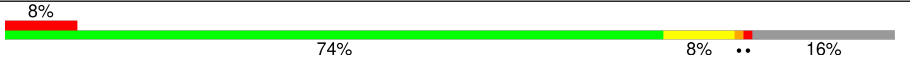
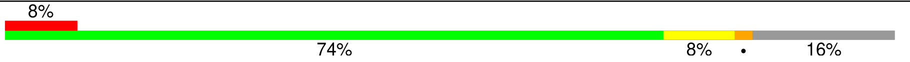
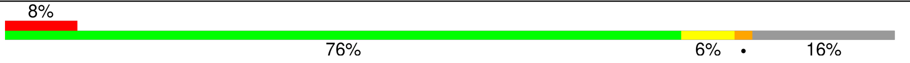
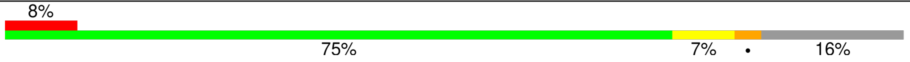
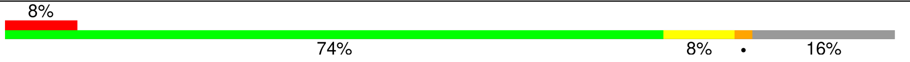
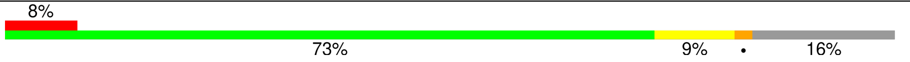
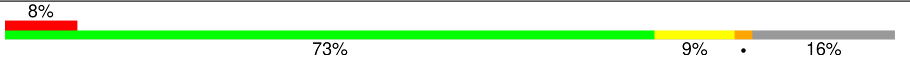
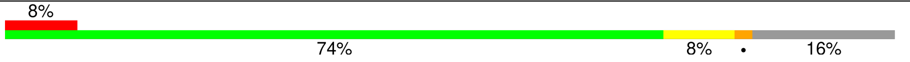
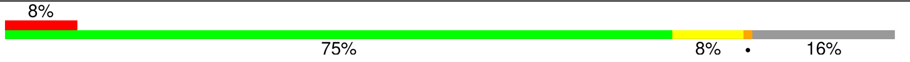
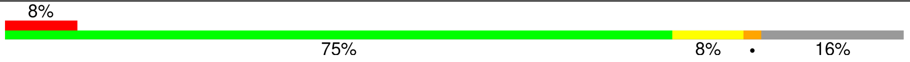
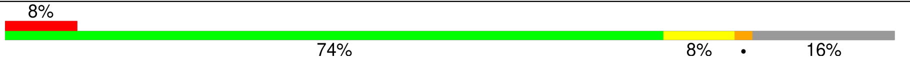
Mol	Chain	Length	Quality of chain
1	16-A	313	 8% 74% 9% • 16%
1	17-A	313	 8% 76% 6% • 16%
1	18-A	313	 8% 73% 10% • 16%
1	19-A	313	 8% 76% 7% • 16%
1	2-A	313	 8% 72% 11% • 16%
1	20-A	313	 8% 74% 8% • 16%
1	21-A	313	 8% 76% 7% • 16%
1	22-A	313	 8% 74% 9% • 16%
1	23-A	313	 8% 74% 8% • 16%
1	24-A	313	 8% 74% 7% • 16%
1	25-A	313	 8% 75% 8% • 16%
1	26-A	313	 8% 76% 5% • • 16%
1	27-A	313	 8% 73% 8% • • 16%
1	28-A	313	 8% 76% 6% • 16%
1	29-A	313	 8% 74% 8% •• 16%
1	3-A	313	 8% 74% 8% • 16%
1	30-A	313	 8% 76% 6% • 16%
1	31-A	313	 8% 75% 7% • 16%
1	32-A	313	 8% 74% 8% • 16%
1	33-A	313	 8% 73% 9% • 16%
1	34-A	313	 8% 73% 9% • 16%
1	35-A	313	 8% 74% 8% • 16%
1	36-A	313	 8% 75% 8% • 16%
1	37-A	313	 8% 75% 8% • 16%
1	38-A	313	 8% 74% 8% • 16%

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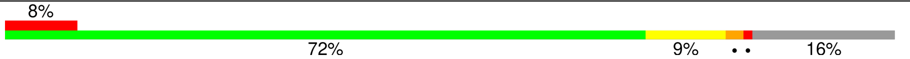
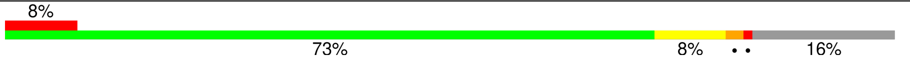
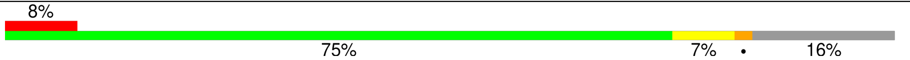
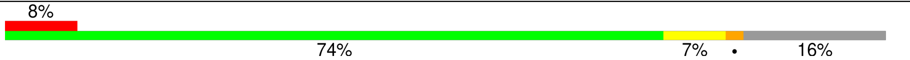
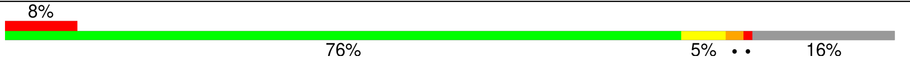
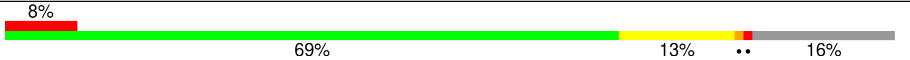
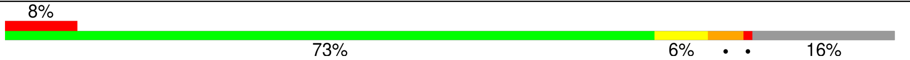
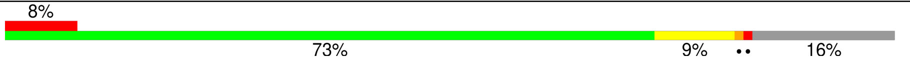
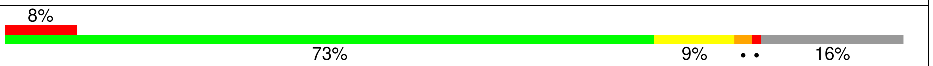
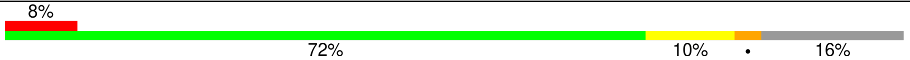
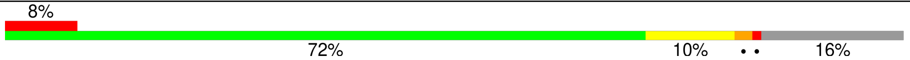
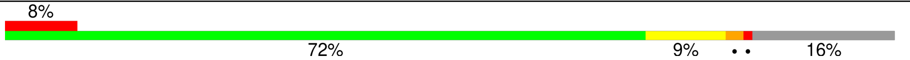
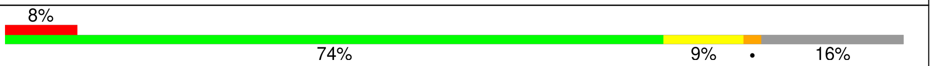
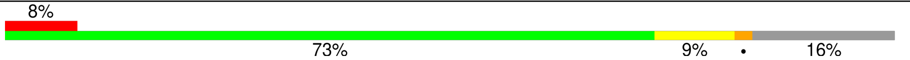
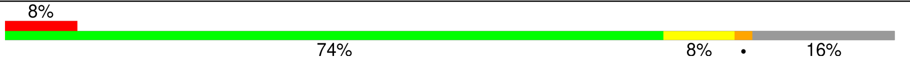
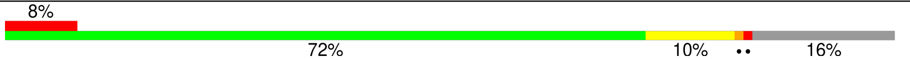
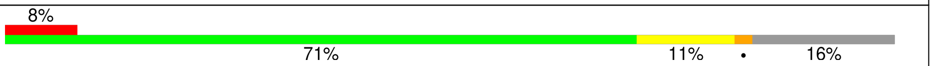
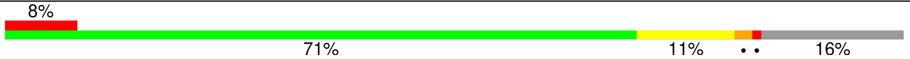
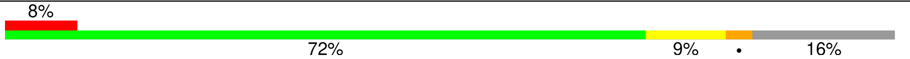
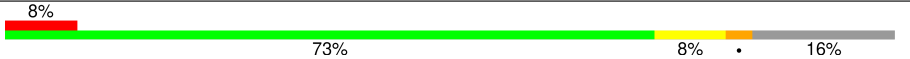
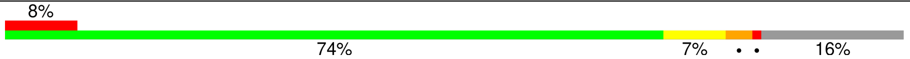
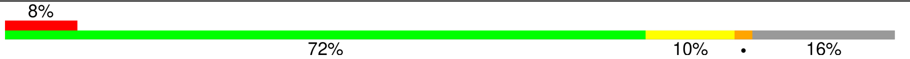
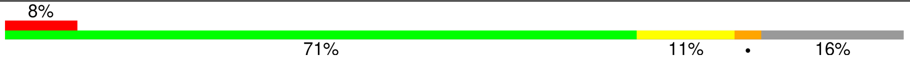
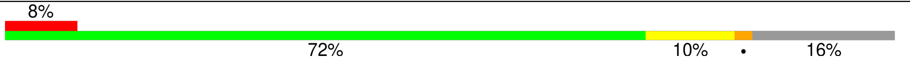
Mol	Chain	Length	Quality of chain
1	39-A	313	
1	4-A	313	
1	40-A	313	
1	41-A	313	
1	42-A	313	
1	43-A	313	
1	44-A	313	
1	45-A	313	
1	46-A	313	
1	47-A	313	
1	48-A	313	
1	49-A	313	
1	5-A	313	
1	50-A	313	
1	51-A	313	
1	52-A	313	
1	53-A	313	
1	54-A	313	
1	55-A	313	
1	56-A	313	
1	57-A	313	
1	58-A	313	
1	59-A	313	
1	6-A	313	
1	60-A	313	

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Mol	Chain	Length	Quality of chain
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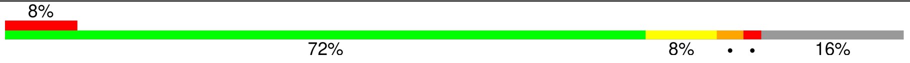
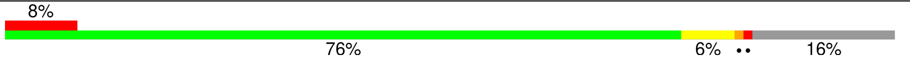
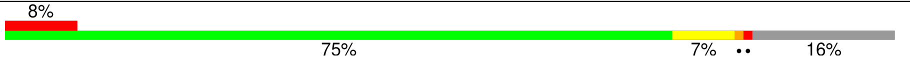
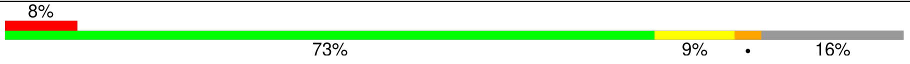
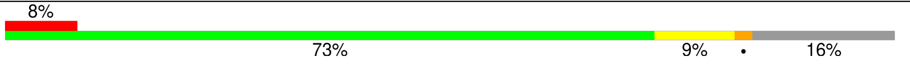
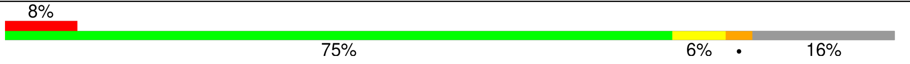
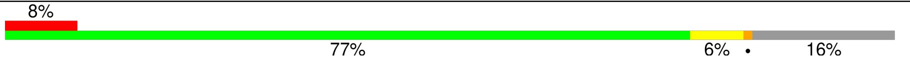
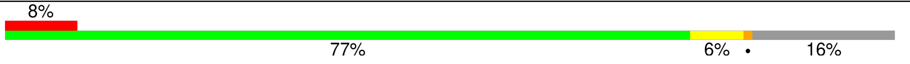
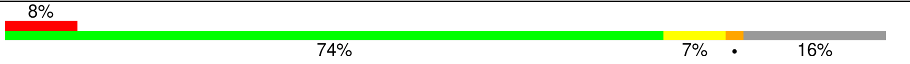
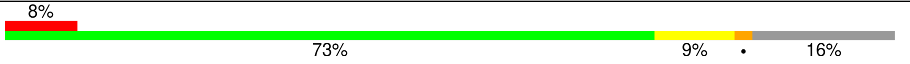
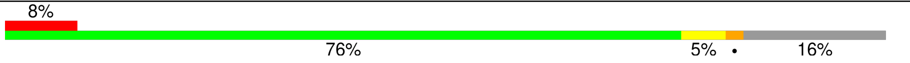
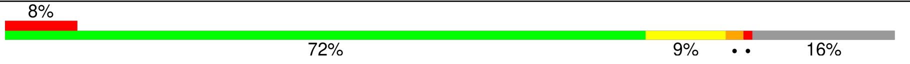
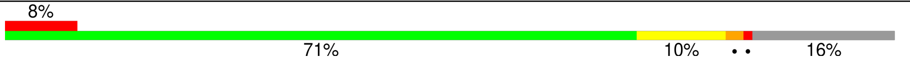
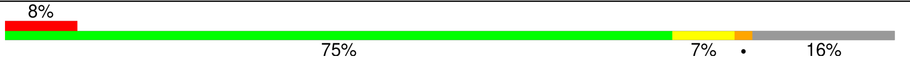
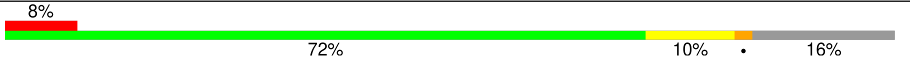
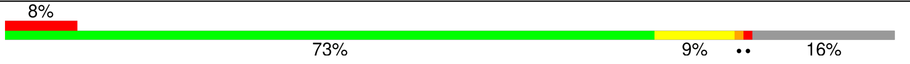
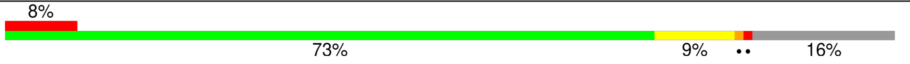
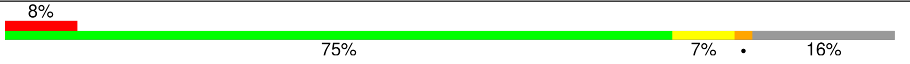
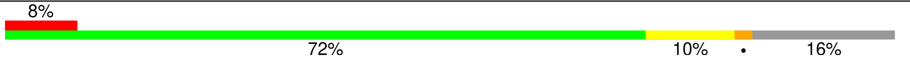
1	62-A	313	
1	63-A	313	
1	64-A	313	
1	65-A	313	
1	66-A	313	
1	67-A	313	
1	68-A	313	
1	69-A	313	
1	7-A	313	
1	70-A	313	
1	71-A	313	
1	72-A	313	
1	73-A	313	
1	74-A	313	
1	75-A	313	
1	76-A	313	
1	77-A	313	
1	8-A	313	
1	9-A	313	

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	1001	-	-	-	X
2	SO4	10-A	1001	-	-	-	X
2	SO4	11-A	1001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	12-A	1001	-	-	-	X
2	SO4	13-A	1001	-	-	-	X
2	SO4	14-A	1001	-	-	-	X
2	SO4	15-A	1001	-	-	-	X
2	SO4	16-A	1001	-	-	-	X
2	SO4	17-A	1001	-	-	-	X
2	SO4	18-A	1001	-	-	-	X
2	SO4	19-A	1001	-	-	-	X
2	SO4	2-A	1001	-	-	-	X
2	SO4	20-A	1001	-	-	-	X
2	SO4	21-A	1001	-	-	-	X
2	SO4	22-A	1001	-	-	-	X
2	SO4	23-A	1001	-	-	-	X
2	SO4	24-A	1001	-	-	-	X
2	SO4	25-A	1001	-	-	-	X
2	SO4	26-A	1001	-	-	-	X
2	SO4	27-A	1001	-	-	-	X
2	SO4	28-A	1001	-	-	-	X
2	SO4	29-A	1001	-	-	-	X
2	SO4	3-A	1001	-	-	-	X
2	SO4	30-A	1001	-	-	-	X
2	SO4	31-A	1001	-	-	-	X
2	SO4	32-A	1001	-	-	-	X
2	SO4	33-A	1001	-	-	-	X
2	SO4	34-A	1001	-	-	-	X
2	SO4	35-A	1001	-	-	-	X
2	SO4	36-A	1001	-	-	-	X
2	SO4	37-A	1001	-	-	-	X
2	SO4	38-A	1001	-	-	-	X
2	SO4	39-A	1001	-	-	-	X
2	SO4	4-A	1001	-	-	-	X
2	SO4	40-A	1001	-	-	-	X
2	SO4	41-A	1001	-	-	-	X
2	SO4	42-A	1001	-	-	-	X
2	SO4	43-A	1001	-	-	-	X
2	SO4	44-A	1001	-	-	-	X
2	SO4	45-A	1001	-	-	-	X
2	SO4	46-A	1001	-	-	-	X
2	SO4	47-A	1001	-	-	-	X
2	SO4	48-A	1001	-	-	-	X
2	SO4	49-A	1001	-	-	-	X
2	SO4	5-A	1001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	50-A	1001	-	-	-	X
2	SO4	51-A	1001	-	-	-	X
2	SO4	52-A	1001	-	-	-	X
2	SO4	53-A	1001	-	-	-	X
2	SO4	54-A	1001	-	-	-	X
2	SO4	55-A	1001	-	-	-	X
2	SO4	56-A	1001	-	-	-	X
2	SO4	57-A	1001	-	-	-	X
2	SO4	58-A	1001	-	-	-	X
2	SO4	59-A	1001	-	-	-	X
2	SO4	6-A	1001	-	-	-	X
2	SO4	60-A	1001	-	-	-	X
2	SO4	61-A	1001	-	-	-	X
2	SO4	62-A	1001	-	-	-	X
2	SO4	63-A	1001	-	-	-	X
2	SO4	64-A	1001	-	-	-	X
2	SO4	65-A	1001	-	-	-	X
2	SO4	66-A	1001	-	-	-	X
2	SO4	67-A	1001	-	-	-	X
2	SO4	68-A	1001	-	-	-	X
2	SO4	69-A	1001	-	-	-	X
2	SO4	7-A	1001	-	-	-	X
2	SO4	70-A	1001	-	-	-	X
2	SO4	71-A	1001	-	-	-	X
2	SO4	72-A	1001	-	-	-	X
2	SO4	73-A	1001	-	-	-	X
2	SO4	74-A	1001	-	-	-	X
2	SO4	75-A	1001	-	-	-	X
2	SO4	76-A	1001	-	-	-	X
2	SO4	77-A	1001	-	-	-	X
2	SO4	8-A	1001	-	-	-	X
2	SO4	9-A	1001	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 314292 atoms, of which 151613 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 CUTINASE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	1-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	2-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	3-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	4-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	5-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	6-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	7-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	8-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	9-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	10-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	11-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	12-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	13-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	14-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	15-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	16-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	17-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	18-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	19-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	20-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	21-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	22-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	23-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	24-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	25-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	26-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	27-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	28-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	29-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	30-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	31-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	32-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	33-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	34-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	35-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	36-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	37-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	38-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	39-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	40-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	41-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	42-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	43-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	44-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	45-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	46-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	47-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	48-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	49-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	50-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	51-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	52-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	53-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	54-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	55-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	56-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	57-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0
1	58-A	263	Total C H N O S 3980 1269 1969 352 385 5	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	59-A	263	3980	1269	1969	352	385	5	0	0	0
1	60-A	263	3980	1269	1969	352	385	5	0	0	0
1	61-A	263	3980	1269	1969	352	385	5	0	0	0
1	62-A	263	3980	1269	1969	352	385	5	0	0	0
1	63-A	263	3980	1269	1969	352	385	5	0	0	0
1	64-A	263	3980	1269	1969	352	385	5	0	0	0
1	65-A	263	3980	1269	1969	352	385	5	0	0	0
1	66-A	263	3980	1269	1969	352	385	5	0	0	0
1	67-A	263	3980	1269	1969	352	385	5	0	0	0
1	68-A	263	3980	1269	1969	352	385	5	0	0	0
1	69-A	263	3980	1269	1969	352	385	5	0	0	0
1	70-A	263	3980	1269	1969	352	385	5	0	0	0
1	71-A	263	3980	1269	1969	352	385	5	0	0	0
1	72-A	263	3980	1269	1969	352	385	5	0	0	0
1	73-A	263	3980	1269	1969	352	385	5	0	0	0
1	74-A	263	3980	1269	1969	352	385	5	0	0	0
1	75-A	263	3980	1269	1969	352	385	5	0	0	0
1	76-A	263	3980	1269	1969	352	385	5	0	0	0
1	77-A	263	3980	1269	1969	352	385	5	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	expression tag	UNP E5BBQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	LYS	-	expression tag	UNP E5BBQ3
A	-28	TYR	-	expression tag	UNP E5BBQ3
A	-27	LEU	-	expression tag	UNP E5BBQ3
A	-26	LEU	-	expression tag	UNP E5BBQ3
A	-25	PRO	-	expression tag	UNP E5BBQ3
A	-24	THR	-	expression tag	UNP E5BBQ3
A	-23	ALA	-	expression tag	UNP E5BBQ3
A	-22	ALA	-	expression tag	UNP E5BBQ3
A	-21	ALA	-	expression tag	UNP E5BBQ3
A	-20	GLY	-	expression tag	UNP E5BBQ3
A	-19	LEU	-	expression tag	UNP E5BBQ3
A	-18	LEU	-	expression tag	UNP E5BBQ3
A	-17	LEU	-	expression tag	UNP E5BBQ3
A	-16	LEU	-	expression tag	UNP E5BBQ3
A	-15	ALA	-	expression tag	UNP E5BBQ3
A	-14	ALA	-	expression tag	UNP E5BBQ3
A	-13	GLN	-	expression tag	UNP E5BBQ3
A	-12	PRO	-	expression tag	UNP E5BBQ3
A	-11	ALA	-	expression tag	UNP E5BBQ3
A	-10	MET	-	expression tag	UNP E5BBQ3
A	-9	ALA	-	expression tag	UNP E5BBQ3
A	-8	MET	-	expression tag	UNP E5BBQ3
A	-7	ASP	-	expression tag	UNP E5BBQ3
A	-6	ILE	-	expression tag	UNP E5BBQ3
A	-5	GLY	-	expression tag	UNP E5BBQ3
A	-4	ILE	-	expression tag	UNP E5BBQ3
A	-3	ASN	-	expression tag	UNP E5BBQ3
A	-2	SER	-	expression tag	UNP E5BBQ3
A	-1	ASP	-	expression tag	UNP E5BBQ3
A	0	PRO	-	expression tag	UNP E5BBQ3
A	262	TYR	-	expression tag	UNP E5BBQ3
A	263	PRO	-	expression tag	UNP E5BBQ3
A	264	ASN	-	expression tag	UNP E5BBQ3
A	265	SER	-	expression tag	UNP E5BBQ3
A	266	SER	-	expression tag	UNP E5BBQ3
A	267	SER	-	expression tag	UNP E5BBQ3
A	268	VAL	-	expression tag	UNP E5BBQ3
A	269	ASP	-	expression tag	UNP E5BBQ3
A	270	LYS	-	expression tag	UNP E5BBQ3
A	271	LEU	-	expression tag	UNP E5BBQ3
A	272	ALA	-	expression tag	UNP E5BBQ3
A	273	ALA	-	expression tag	UNP E5BBQ3

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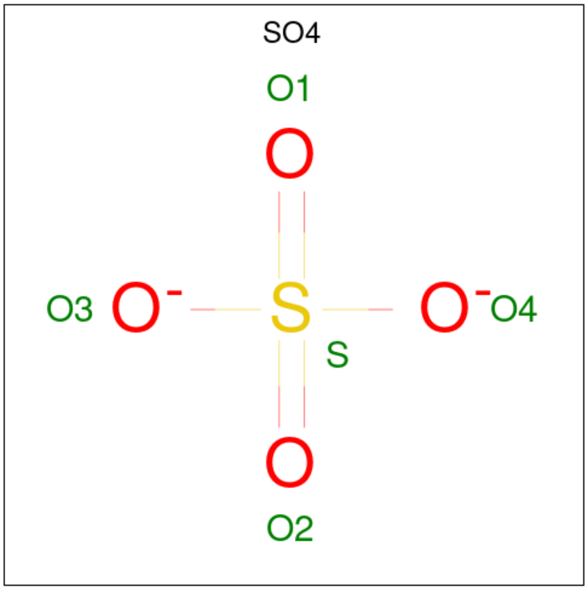
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ALA	-	expression tag	UNP E5BBQ3
A	275	LEU	-	expression tag	UNP E5BBQ3
A	276	GLU	-	expression tag	UNP E5BBQ3
A	277	HIS	-	expression tag	UNP E5BBQ3
A	278	HIS	-	expression tag	UNP E5BBQ3
A	279	HIS	-	expression tag	UNP E5BBQ3
A	280	HIS	-	expression tag	UNP E5BBQ3
A	281	HIS	-	expression tag	UNP E5BBQ3
A	282	HIS	-	expression tag	UNP E5BBQ3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total O S 5 4 1	0	0
2	2-A	1	Total O S 5 4 1	0	0
2	3-A	1	Total O S 5 4 1	0	0
2	4-A	1	Total O S 5 4 1	0	0
2	5-A	1	Total O S 5 4 1	0	0
2	6-A	1	Total O S 5 4 1	0	0
2	7-A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	8-A	1	Total O S 5 4 1	0	0
2	9-A	1	Total O S 5 4 1	0	0
2	10-A	1	Total O S 5 4 1	0	0
2	11-A	1	Total O S 5 4 1	0	0
2	12-A	1	Total O S 5 4 1	0	0
2	13-A	1	Total O S 5 4 1	0	0
2	14-A	1	Total O S 5 4 1	0	0
2	15-A	1	Total O S 5 4 1	0	0
2	16-A	1	Total O S 5 4 1	0	0
2	17-A	1	Total O S 5 4 1	0	0
2	18-A	1	Total O S 5 4 1	0	0
2	19-A	1	Total O S 5 4 1	0	0
2	20-A	1	Total O S 5 4 1	0	0
2	21-A	1	Total O S 5 4 1	0	0
2	22-A	1	Total O S 5 4 1	0	0
2	23-A	1	Total O S 5 4 1	0	0
2	24-A	1	Total O S 5 4 1	0	0
2	25-A	1	Total O S 5 4 1	0	0
2	26-A	1	Total O S 5 4 1	0	0
2	27-A	1	Total O S 5 4 1	0	0
2	28-A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	29-A	1	Total O S 5 4 1	0	0
2	30-A	1	Total O S 5 4 1	0	0
2	31-A	1	Total O S 5 4 1	0	0
2	32-A	1	Total O S 5 4 1	0	0
2	33-A	1	Total O S 5 4 1	0	0
2	34-A	1	Total O S 5 4 1	0	0
2	35-A	1	Total O S 5 4 1	0	0
2	36-A	1	Total O S 5 4 1	0	0
2	37-A	1	Total O S 5 4 1	0	0
2	38-A	1	Total O S 5 4 1	0	0
2	39-A	1	Total O S 5 4 1	0	0
2	40-A	1	Total O S 5 4 1	0	0
2	41-A	1	Total O S 5 4 1	0	0
2	42-A	1	Total O S 5 4 1	0	0
2	43-A	1	Total O S 5 4 1	0	0
2	44-A	1	Total O S 5 4 1	0	0
2	45-A	1	Total O S 5 4 1	0	0
2	46-A	1	Total O S 5 4 1	0	0
2	47-A	1	Total O S 5 4 1	0	0
2	48-A	1	Total O S 5 4 1	0	0
2	49-A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	50-A	1	Total O S 5 4 1	0	0
2	51-A	1	Total O S 5 4 1	0	0
2	52-A	1	Total O S 5 4 1	0	0
2	53-A	1	Total O S 5 4 1	0	0
2	54-A	1	Total O S 5 4 1	0	0
2	55-A	1	Total O S 5 4 1	0	0
2	56-A	1	Total O S 5 4 1	0	0
2	57-A	1	Total O S 5 4 1	0	0
2	58-A	1	Total O S 5 4 1	0	0
2	59-A	1	Total O S 5 4 1	0	0
2	60-A	1	Total O S 5 4 1	0	0
2	61-A	1	Total O S 5 4 1	0	0
2	62-A	1	Total O S 5 4 1	0	0
2	63-A	1	Total O S 5 4 1	0	0
2	64-A	1	Total O S 5 4 1	0	0
2	65-A	1	Total O S 5 4 1	0	0
2	66-A	1	Total O S 5 4 1	0	0
2	67-A	1	Total O S 5 4 1	0	0
2	68-A	1	Total O S 5 4 1	0	0
2	69-A	1	Total O S 5 4 1	0	0
2	70-A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	71-A	1	Total O S 5 4 1	0	0
2	72-A	1	Total O S 5 4 1	0	0
2	73-A	1	Total O S 5 4 1	0	0
2	74-A	1	Total O S 5 4 1	0	0
2	75-A	1	Total O S 5 4 1	0	0
2	76-A	1	Total O S 5 4 1	0	0
2	77-A	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	99	Total O 99 99	0	0
3	2-A	101	Total O 102 102	0	1
3	3-A	98	Total O 98 98	0	0
3	4-A	85	Total O 85 85	0	0
3	5-A	97	Total O 98 98	0	1
3	6-A	98	Total O 99 99	0	1
3	7-A	98	Total O 98 98	0	0
3	8-A	100	Total O 101 101	0	1
3	9-A	95	Total O 95 95	0	0
3	10-A	90	Total O 90 90	0	0
3	11-A	102	Total O 103 103	0	1
3	12-A	97	Total O 97 97	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	13-A	87	Total O 87 87	0	0
3	14-A	89	Total O 90 90	0	1
3	15-A	111	Total O 112 112	0	1
3	16-A	93	Total O 93 93	0	0
3	17-A	82	Total O 82 82	0	0
3	18-A	88	Total O 89 89	0	1
3	19-A	89	Total O 89 89	0	0
3	20-A	102	Total O 103 103	0	1
3	21-A	101	Total O 101 101	0	0
3	22-A	83	Total O 83 83	0	0
3	23-A	102	Total O 103 103	0	1
3	24-A	98	Total O 98 98	0	0
3	25-A	98	Total O 99 99	0	1
3	26-A	85	Total O 85 85	0	0
3	27-A	99	Total O 100 100	0	1
3	28-A	103	Total O 104 104	0	1
3	29-A	104	Total O 105 105	0	1
3	30-A	94	Total O 94 94	0	0
3	31-A	91	Total O 91 91	0	0
3	32-A	95	Total O 96 96	0	1
3	33-A	90	Total O 90 90	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	34-A	93	Total O 94 94	0	1
3	35-A	97	Total O 98 98	0	1
3	36-A	98	Total O 98 98	0	0
3	37-A	97	Total O 97 97	0	0
3	38-A	91	Total O 91 91	0	0
3	39-A	103	Total O 104 104	0	1
3	40-A	89	Total O 89 89	0	0
3	41-A	103	Total O 104 104	0	1
3	42-A	111	Total O 112 112	0	1
3	43-A	102	Total O 102 102	0	0
3	44-A	83	Total O 83 83	0	0
3	45-A	95	Total O 96 96	0	1
3	46-A	98	Total O 99 99	0	1
3	47-A	99	Total O 100 100	0	1
3	48-A	83	Total O 83 83	0	0
3	49-A	92	Total O 93 93	0	1
3	50-A	94	Total O 95 95	0	1
3	51-A	98	Total O 99 99	0	1
3	52-A	98	Total O 98 98	0	0
3	53-A	90	Total O 90 90	0	0
3	54-A	94	Total O 95 95	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	55-A	92	Total O 92 92	0	0
3	56-A	94	Total O 95 95	0	1
3	57-A	96	Total O 97 97	0	1
3	58-A	91	Total O 91 91	0	0
3	59-A	88	Total O 88 88	0	0
3	60-A	97	Total O 98 98	0	1
3	61-A	112	Total O 113 113	0	1
3	62-A	103	Total O 103 103	0	0
3	63-A	106	Total O 107 107	0	1
3	64-A	100	Total O 100 100	0	0
3	65-A	88	Total O 88 88	0	0
3	66-A	103	Total O 104 104	0	1
3	67-A	102	Total O 102 102	0	0
3	68-A	104	Total O 105 105	0	1
3	69-A	104	Total O 104 104	0	0
3	70-A	103	Total O 103 103	0	0
3	71-A	107	Total O 108 108	0	1
3	72-A	101	Total O 101 101	0	0
3	73-A	96	Total O 96 96	0	0
3	74-A	95	Total O 95 95	0	0
3	75-A	88	Total O 88 88	0	0

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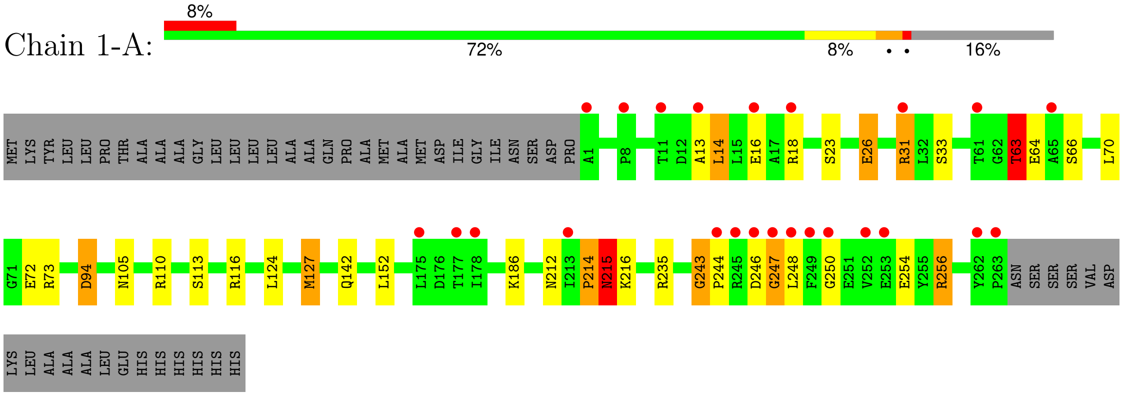
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	76-A	88	Total O 88 88	0	0
3	77-A	101	Total O 102 102	0	1

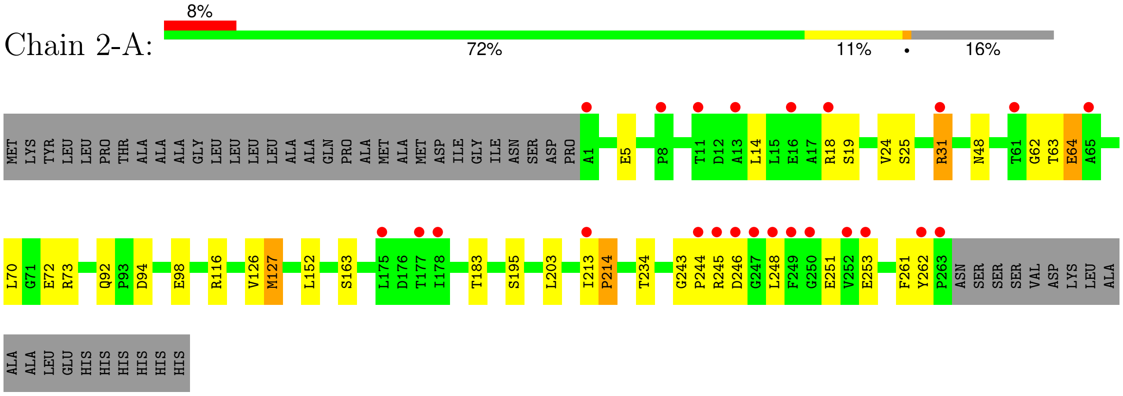
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

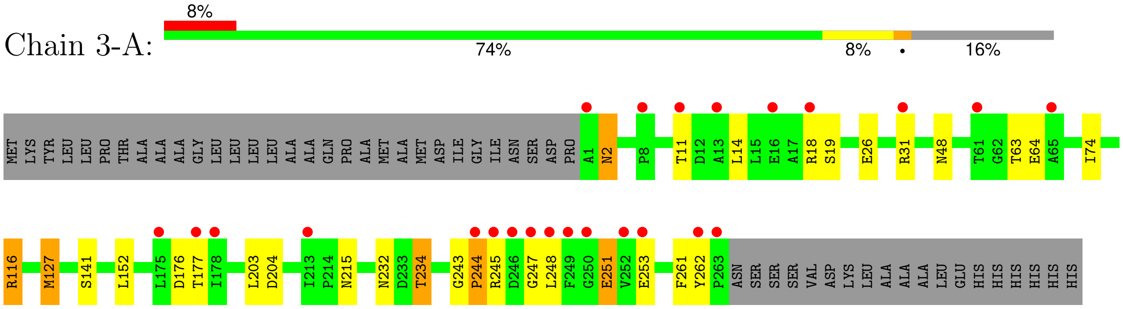
- Molecule 1: CUTINASE



- Molecule 1: CUTINASE

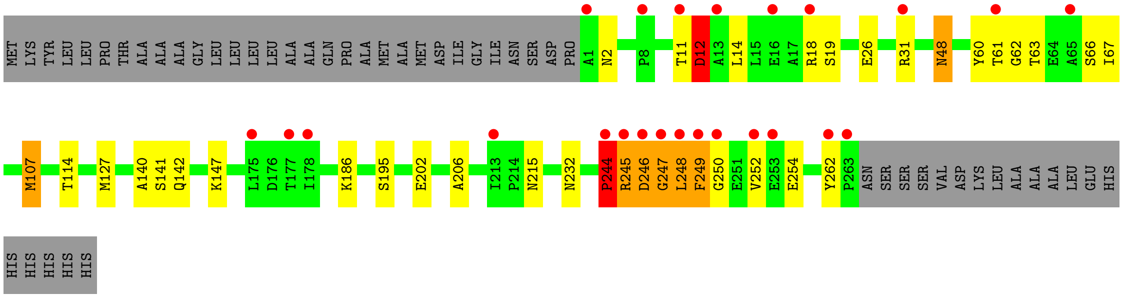


- Molecule 1: CUTINASE



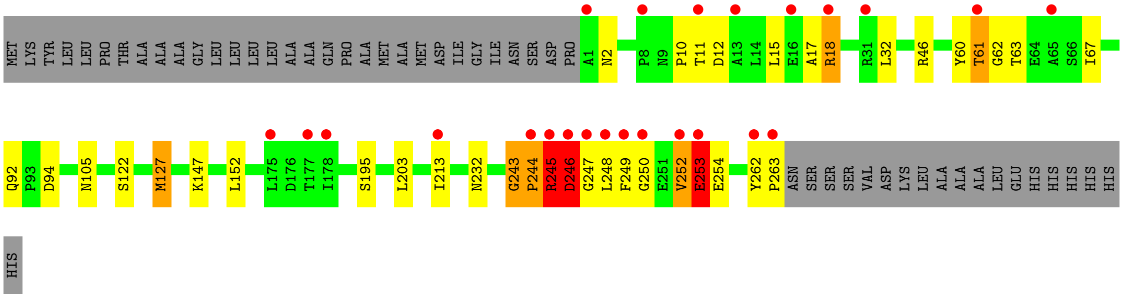
- Molecule 1: CUTINASE

Chain 4-A:



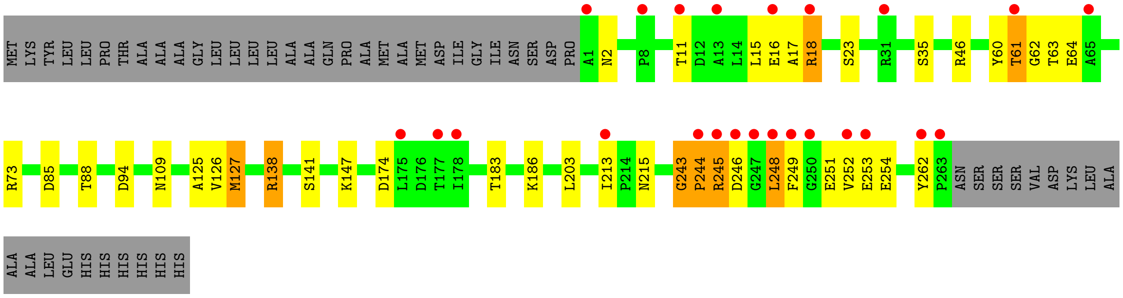
- Molecule 1: CUTINASE

Chain 5-A:



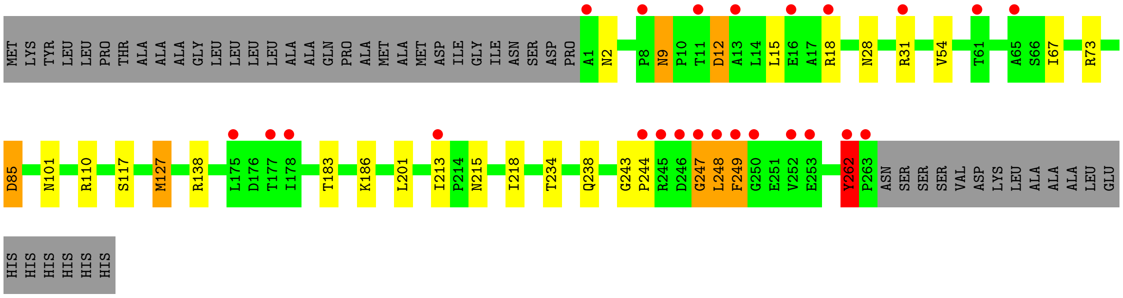
- Molecule 1: CUTINASE

Chain 6-A:



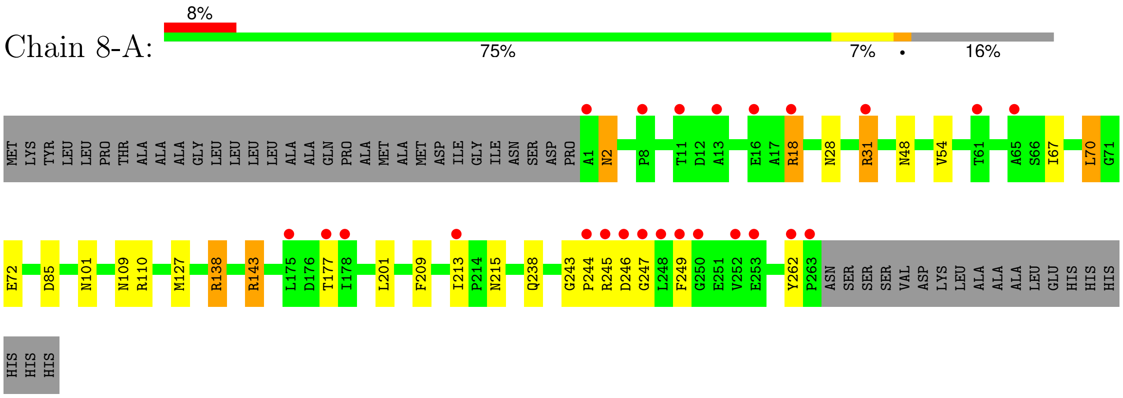
- Molecule 1: CUTINASE

Chain 7-A:



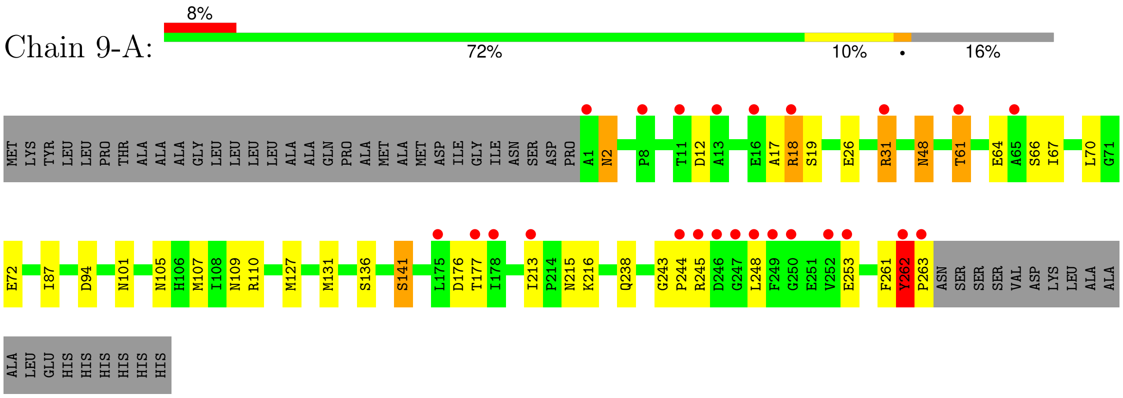
- Molecule 1: CUTINASE

Chain 8-A:



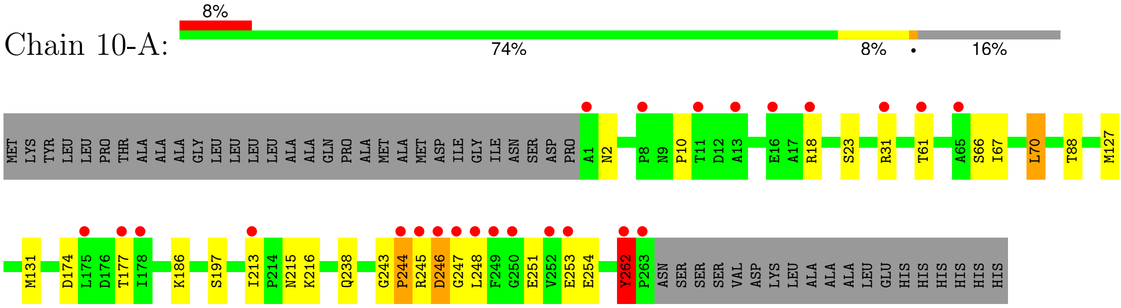
- Molecule 1: CUTINASE

Chain 9-A:



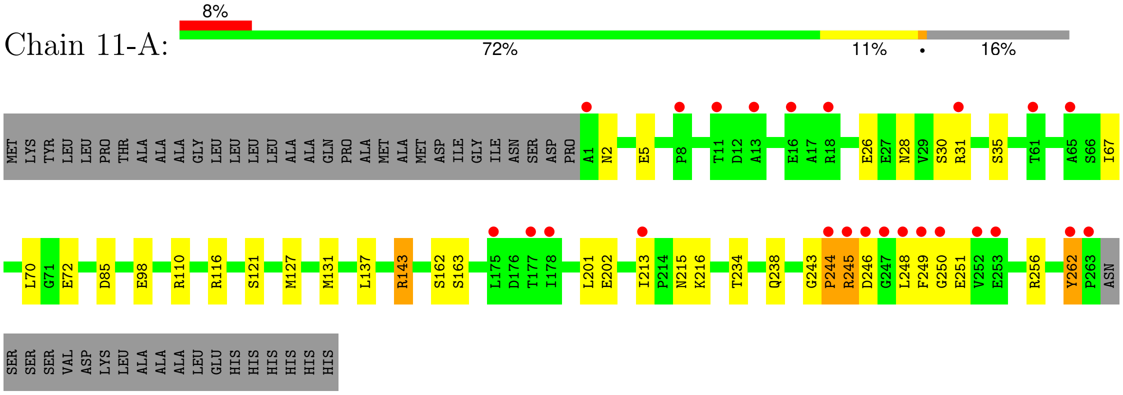
- Molecule 1: CUTINASE

Chain 10-A:

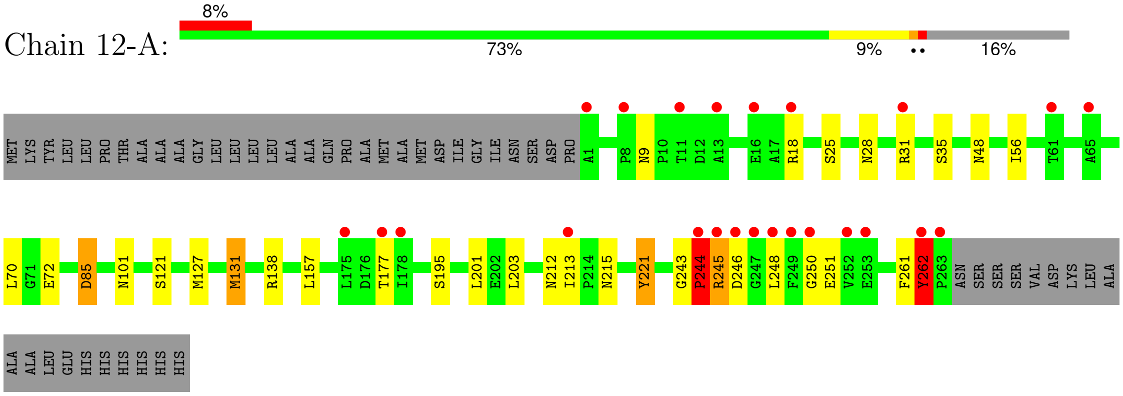


- Molecule 1: CUTINASE

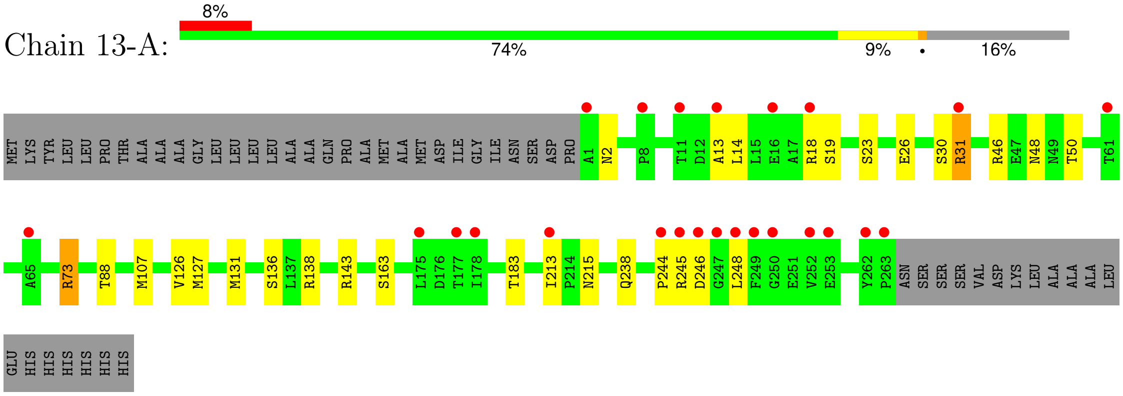
Chain 11-A:



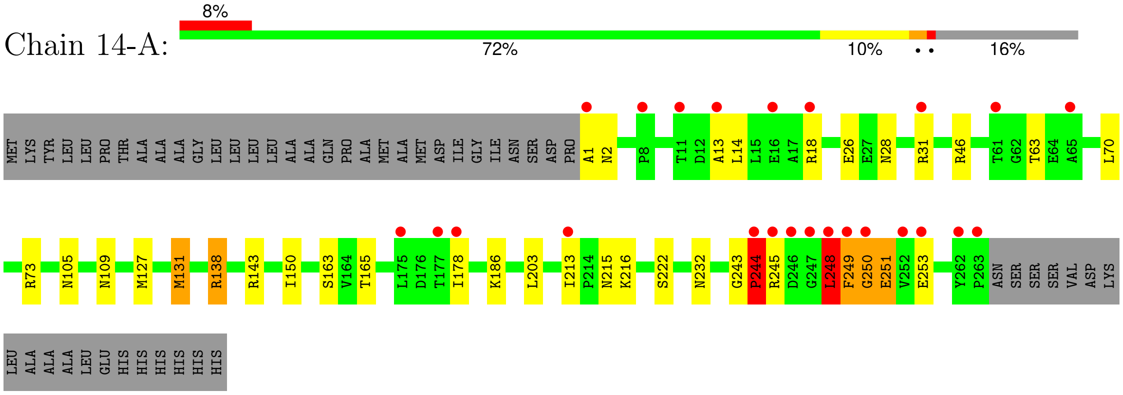
- Molecule 1: CUTINASE



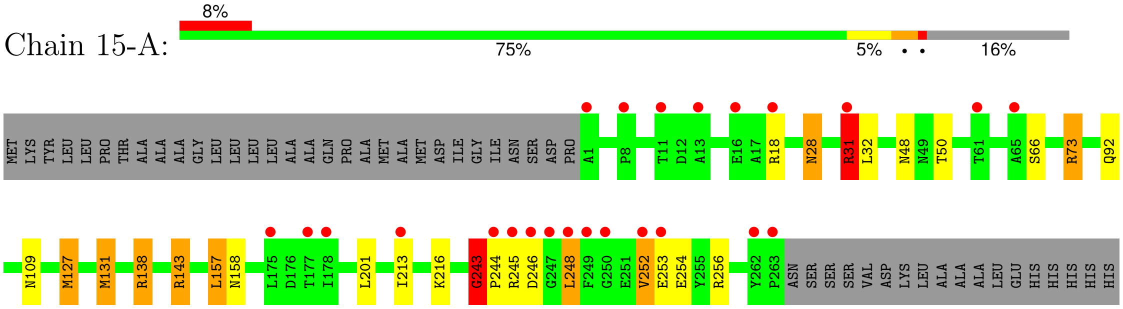
- Molecule 1: CUTINASE



- Molecule 1: CUTINASE

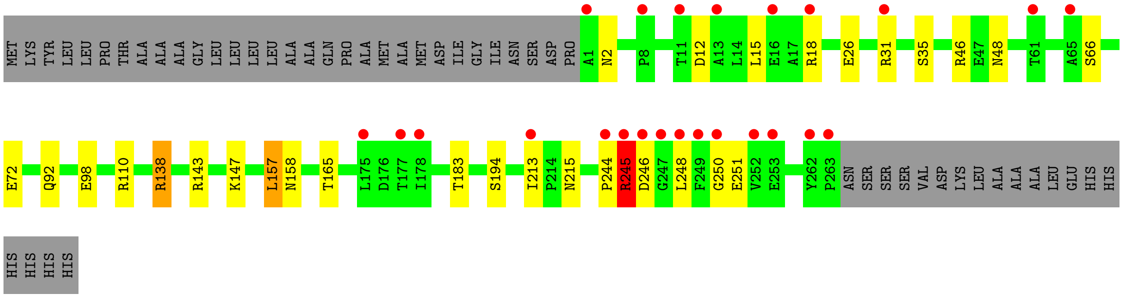


- Molecule 1: CUTINASE



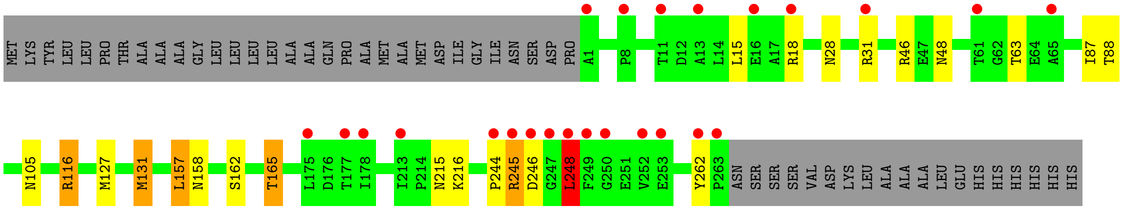
- Molecule 1: CUTINASE

Chain 16-A:



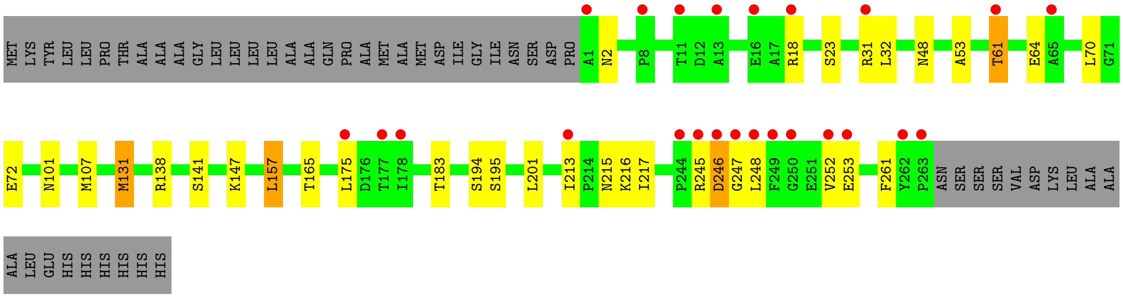
- Molecule 1: CUTINASE

Chain 17-A:



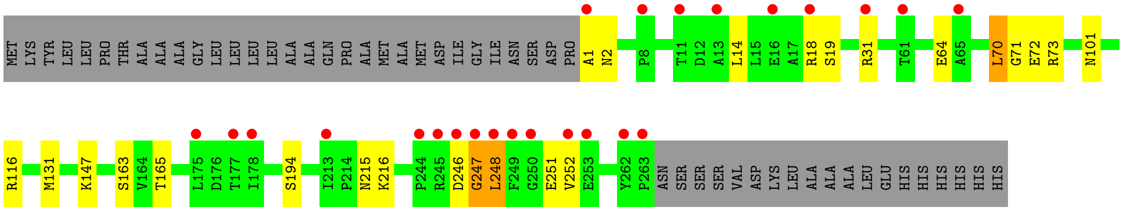
- Molecule 1: CUTINASE

Chain 18-A:

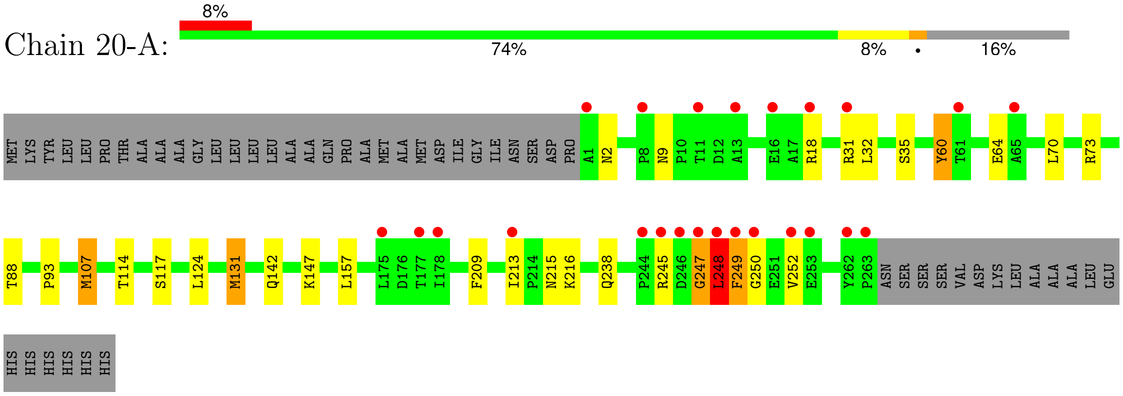


- Molecule 1: CUTINASE

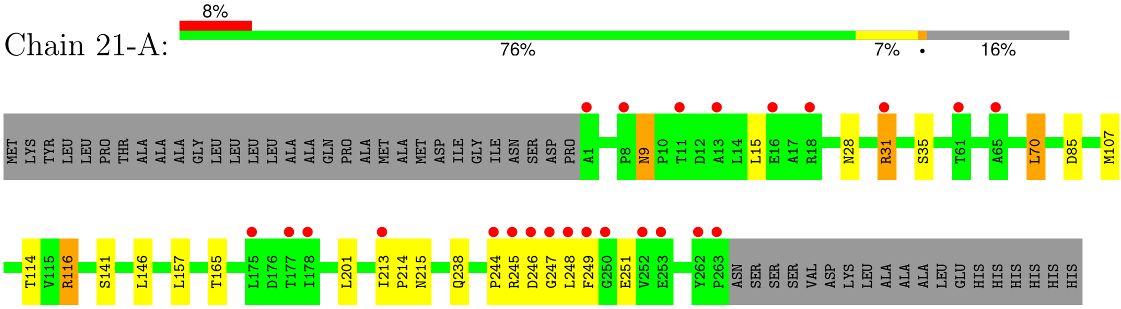
Chain 19-A:



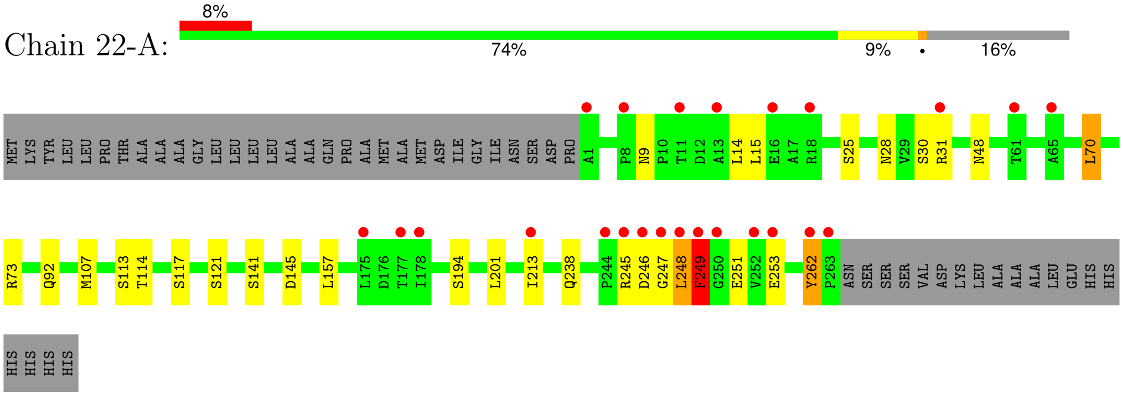
- Molecule 1: CUTINASE



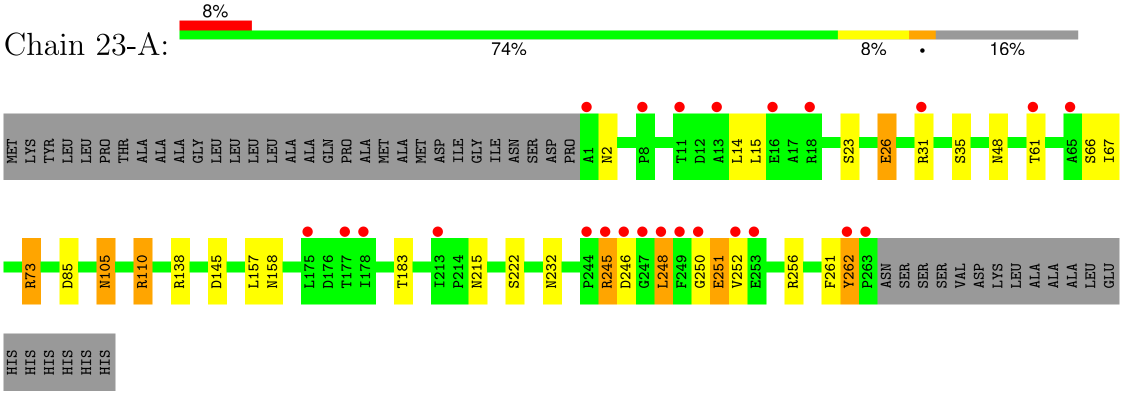
- Molecule 1: CUTINASE



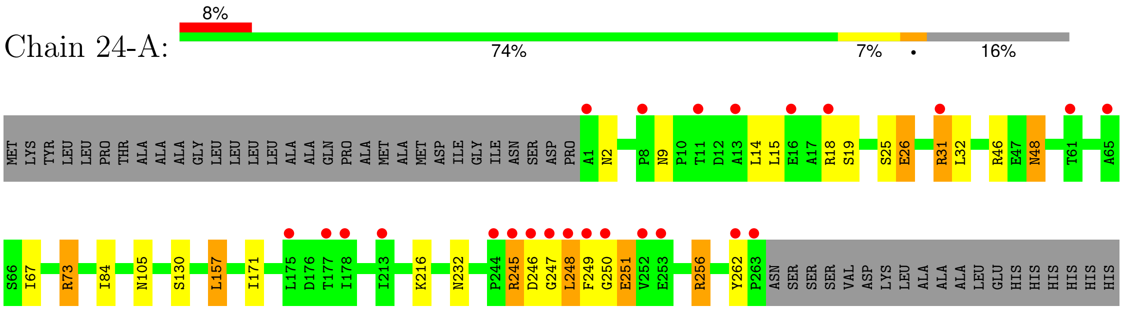
- Molecule 1: CUTINASE



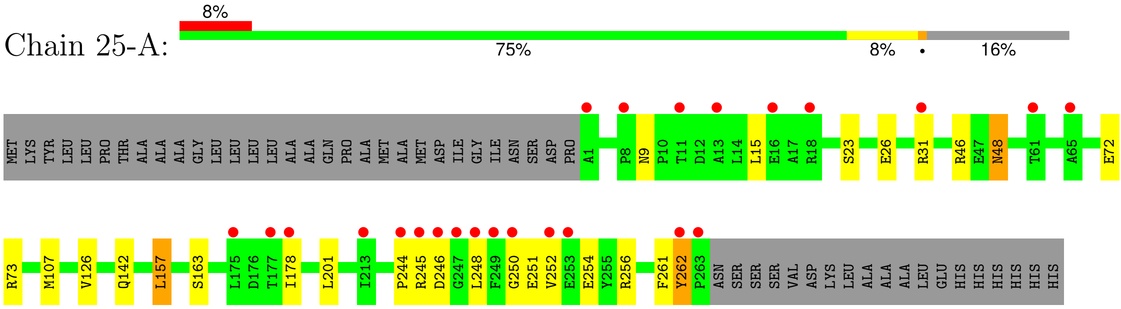
- Molecule 1: CUTINASE



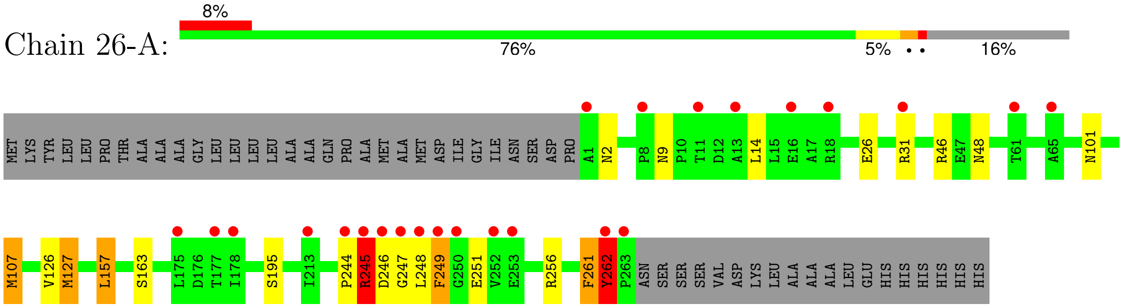
- Molecule 1: CUTINASE



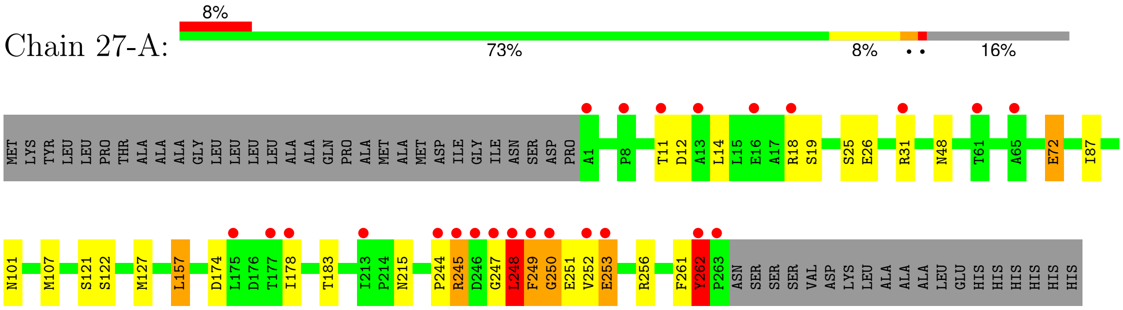
- Molecule 1: CUTINASE



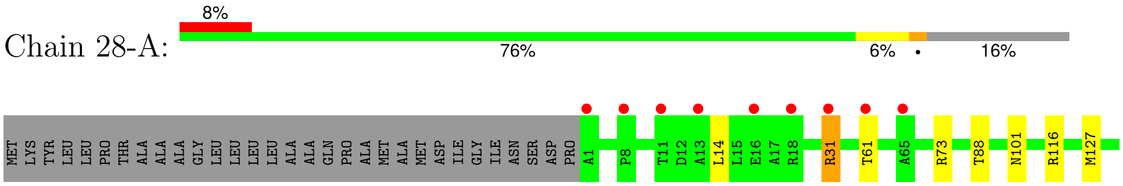
- Molecule 1: CUTINASE

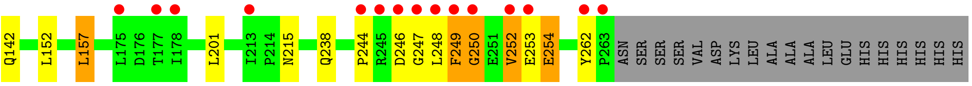


- Molecule 1: CUTINASE

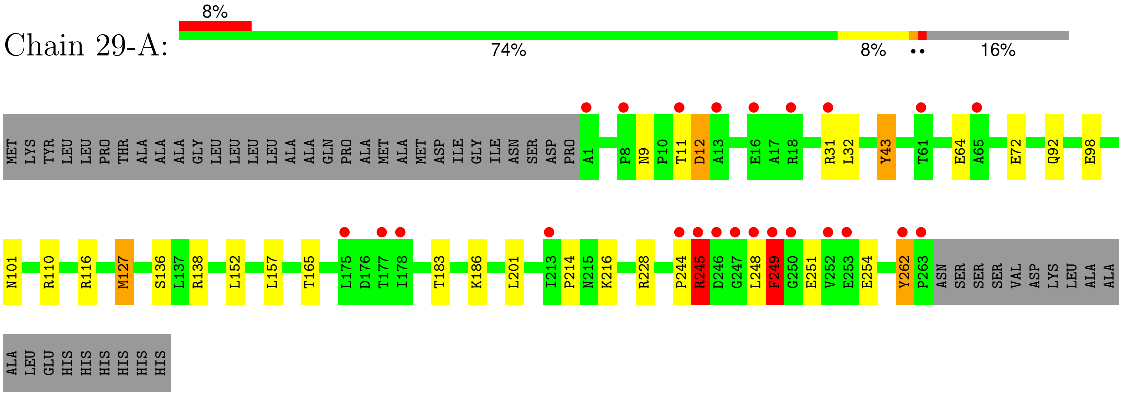


- Molecule 1: CUTINASE

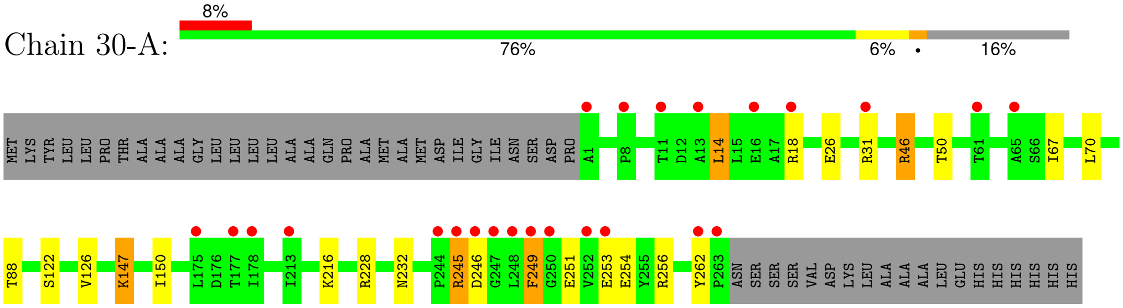




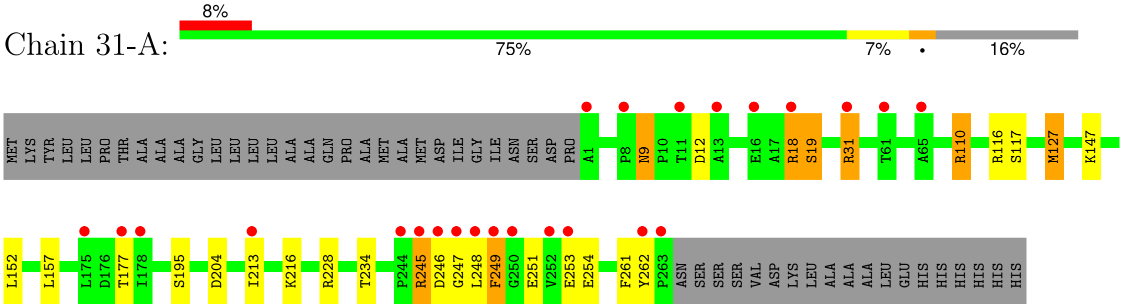
• Molecule 1: CUTINASE



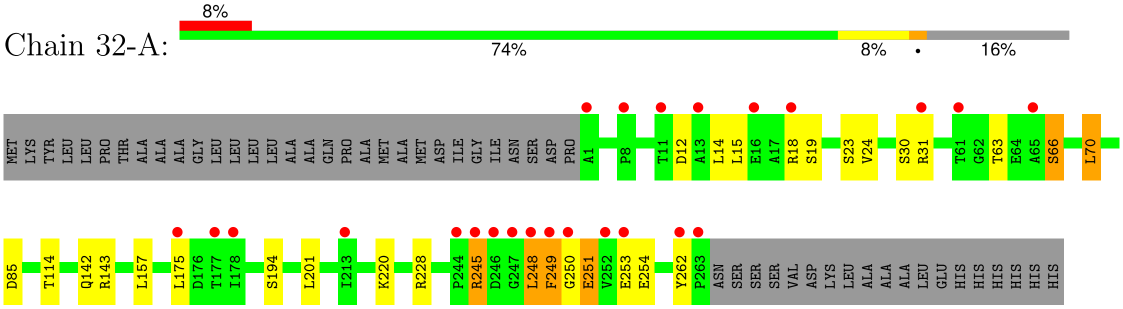
• Molecule 1: CUTINASE



• Molecule 1: CUTINASE

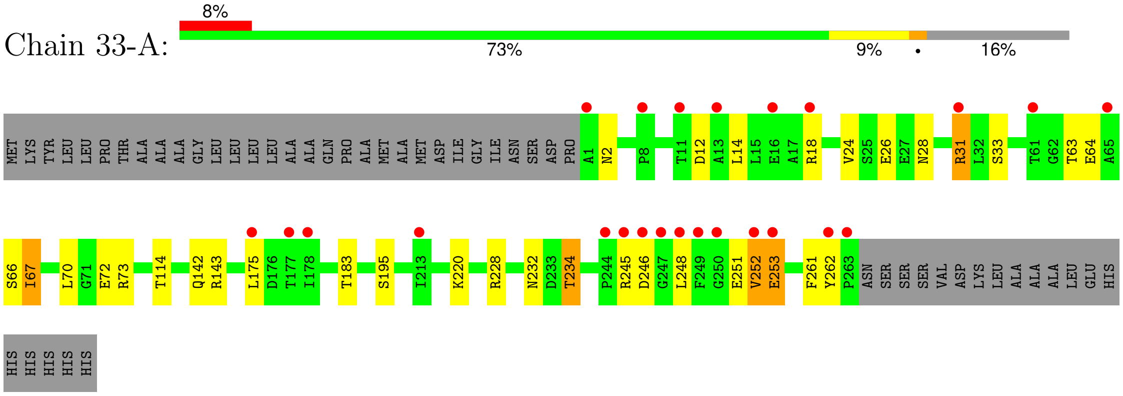


• Molecule 1: CUTINASE



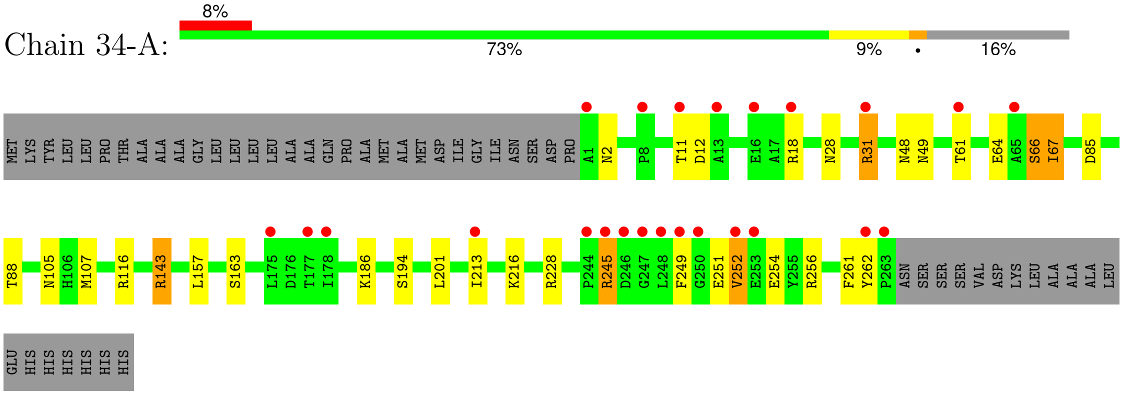
• Molecule 1: CUTINASE

Chain 33-A:



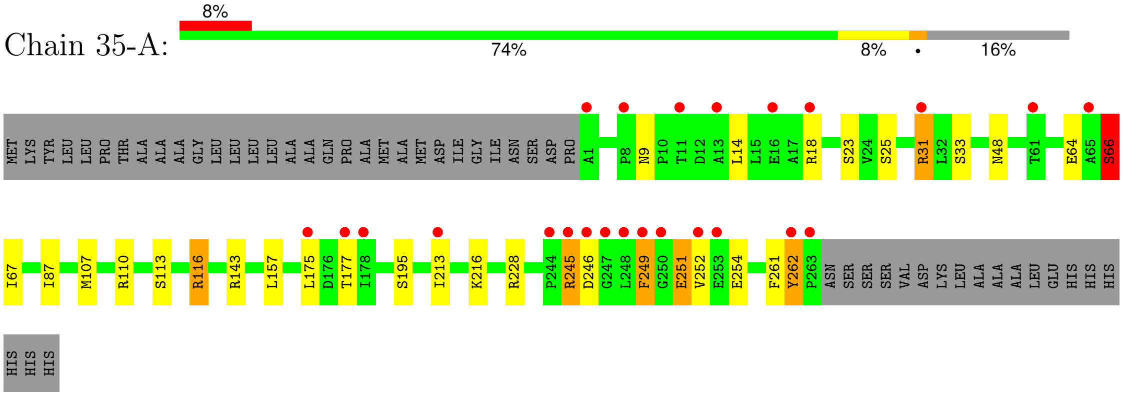
- Molecule 1: CUTINASE

Chain 34-A:



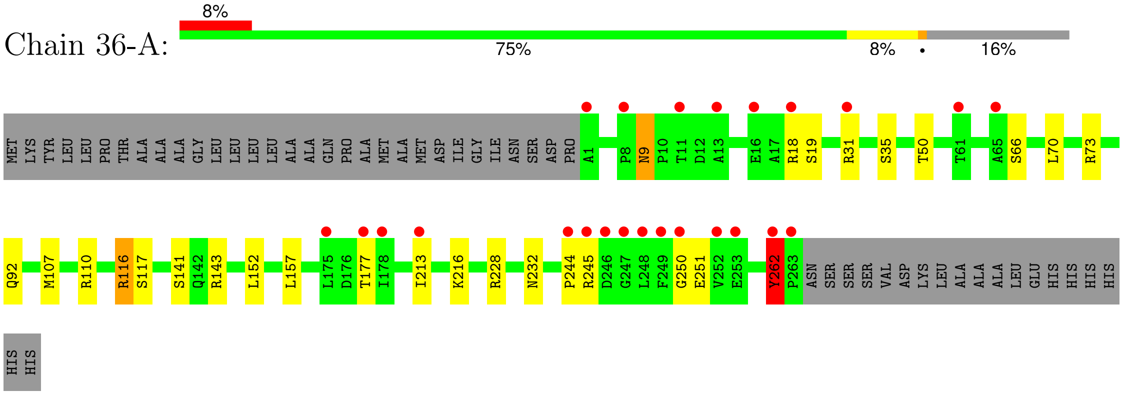
- Molecule 1: CUTINASE

Chain 35-A:

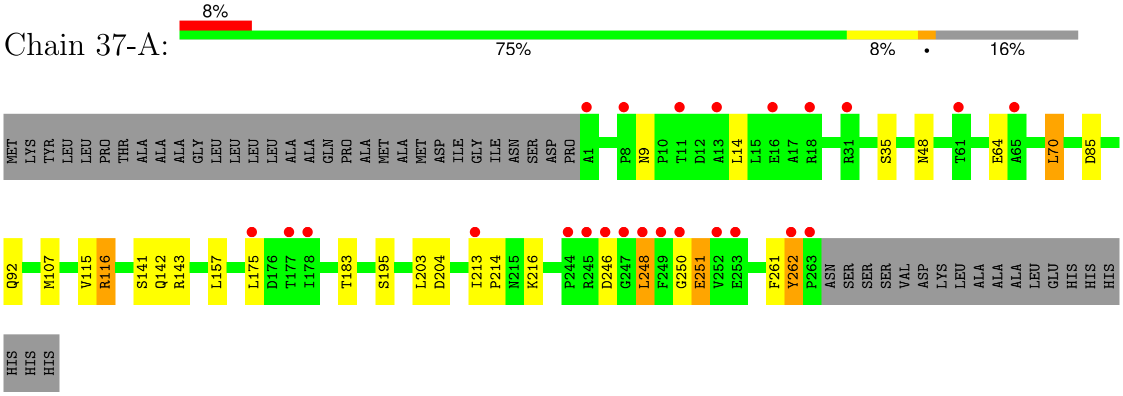


- Molecule 1: CUTINASE

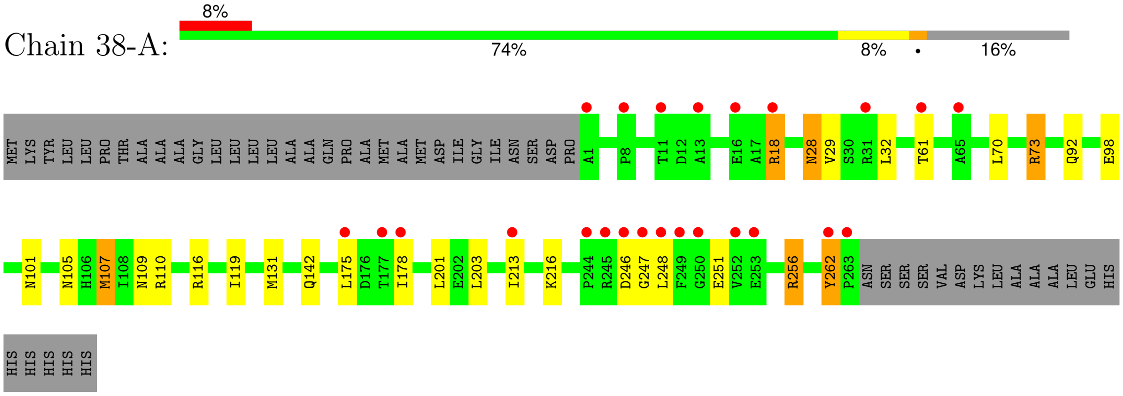
Chain 36-A:



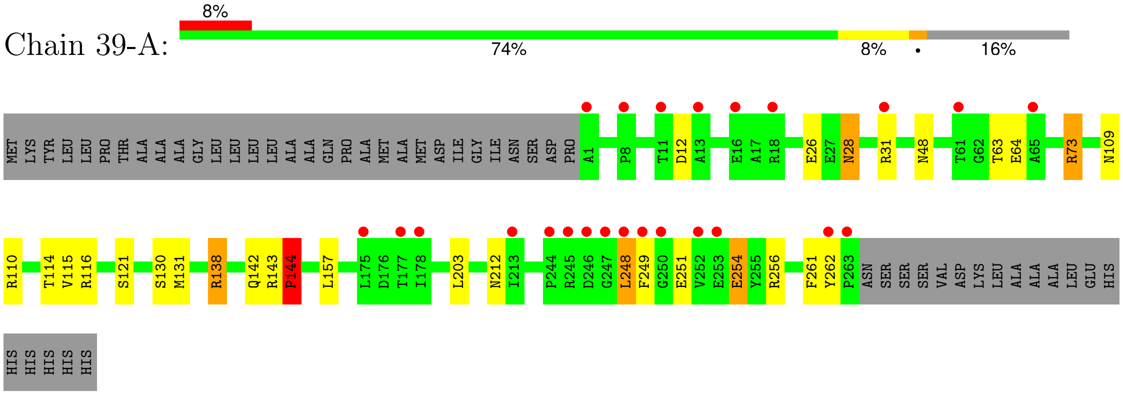
• Molecule 1: CUTINASE



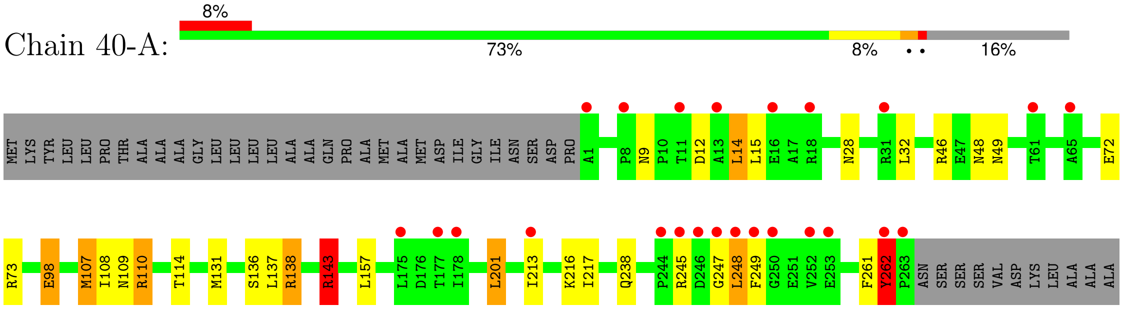
• Molecule 1: CUTINASE



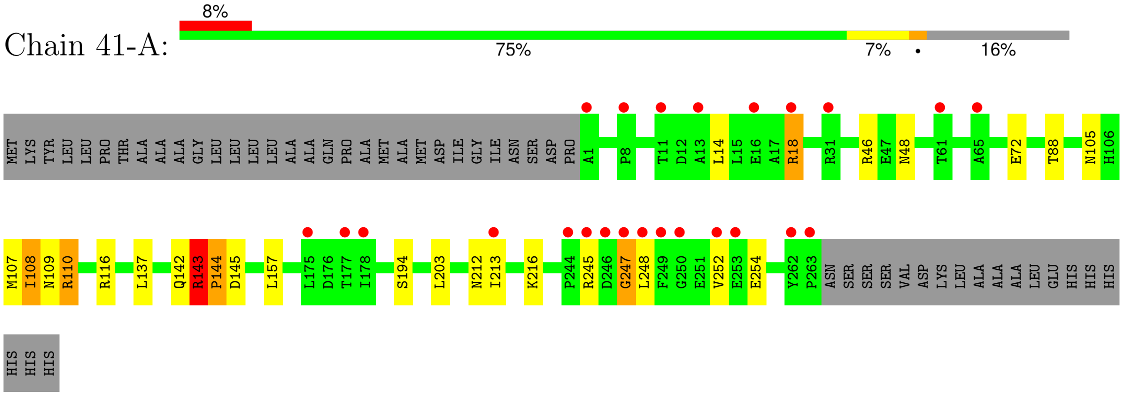
• Molecule 1: CUTINASE



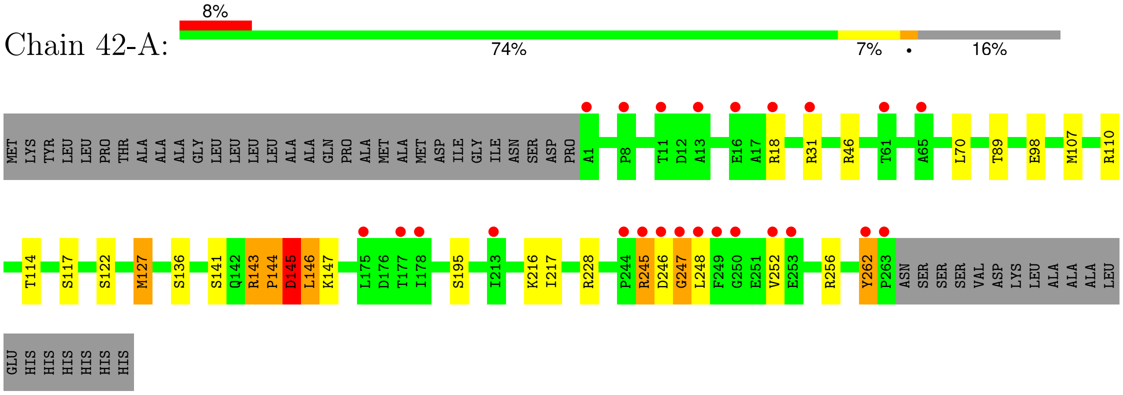
• Molecule 1: CUTINASE



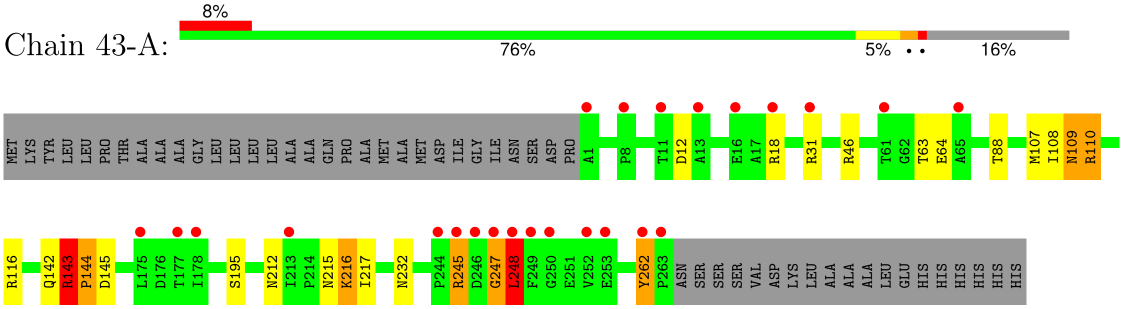
- Molecule 1: CUTINASE



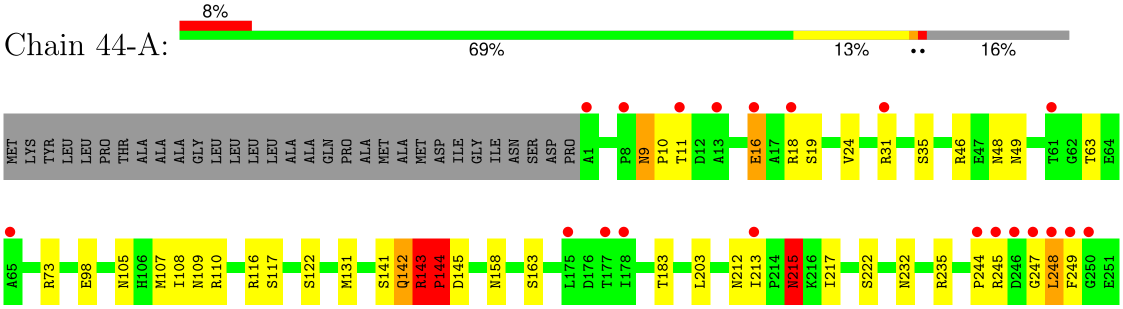
- Molecule 1: CUTINASE

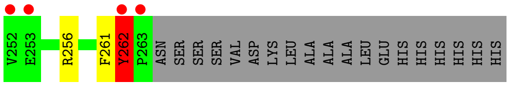


- Molecule 1: CUTINASE



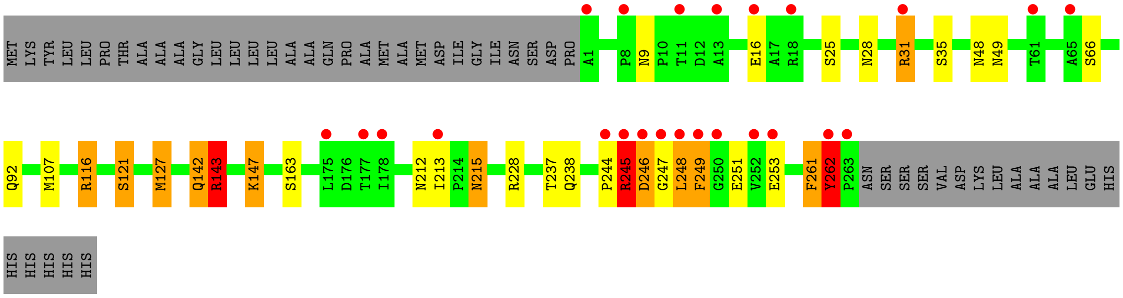
- Molecule 1: CUTINASE





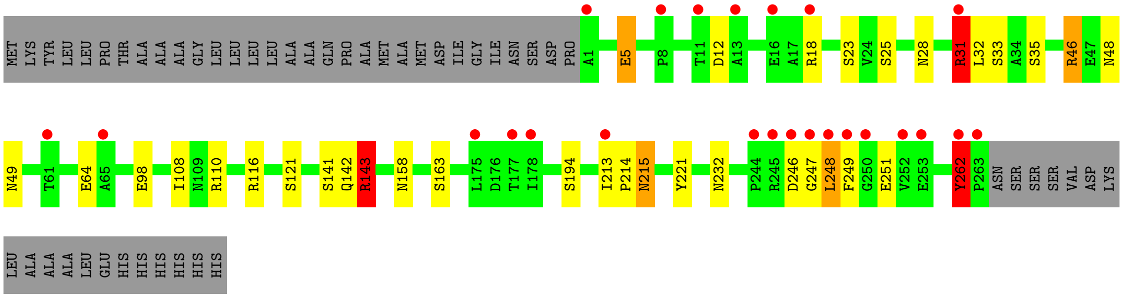
- Molecule 1: CUTINASE

Chain 45-A:



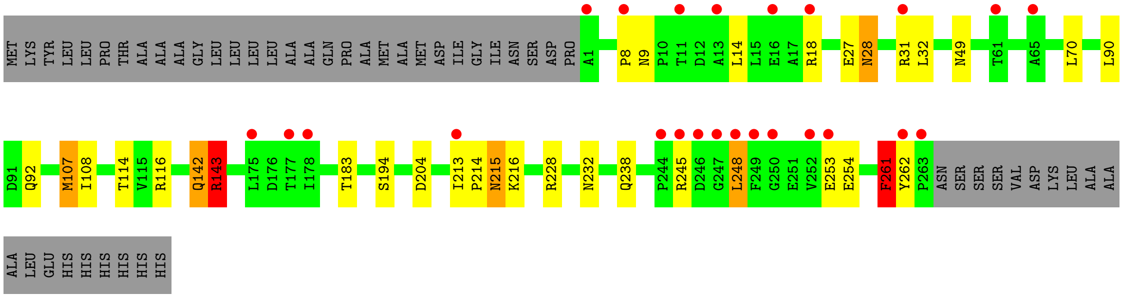
- Molecule 1: CUTINASE

Chain 46-A:



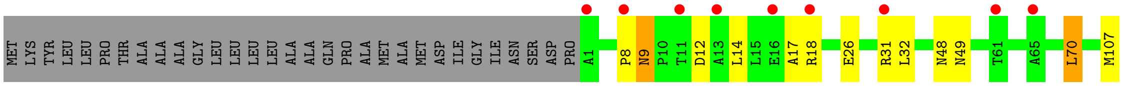
- Molecule 1: CUTINASE

Chain 47-A:



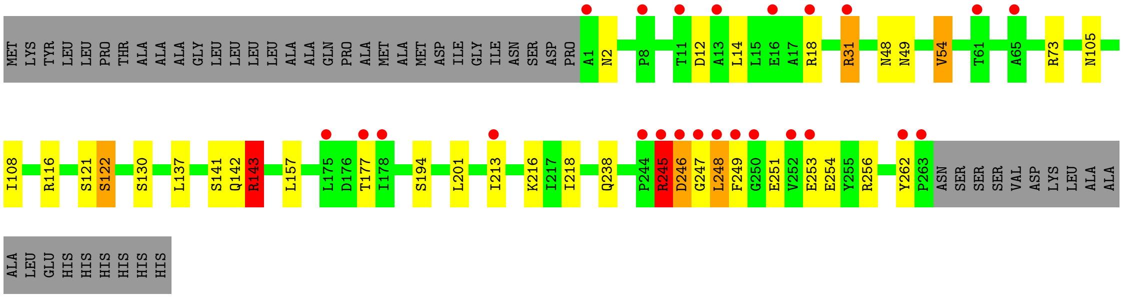
- Molecule 1: CUTINASE

Chain 48-A:



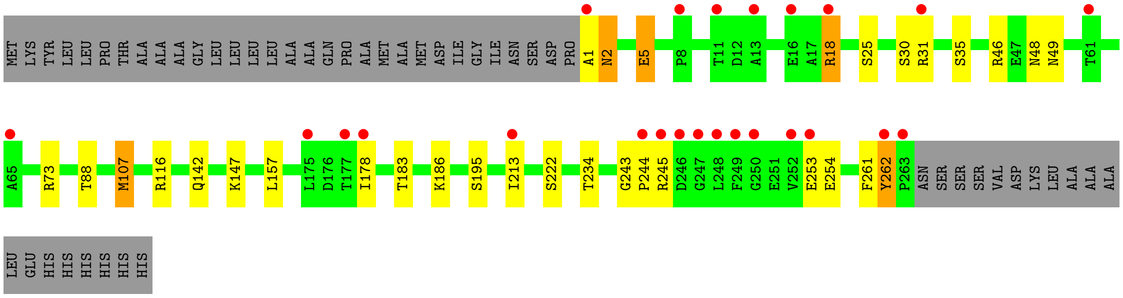
- Molecule 1: CUTINASE

Chain 49-A:



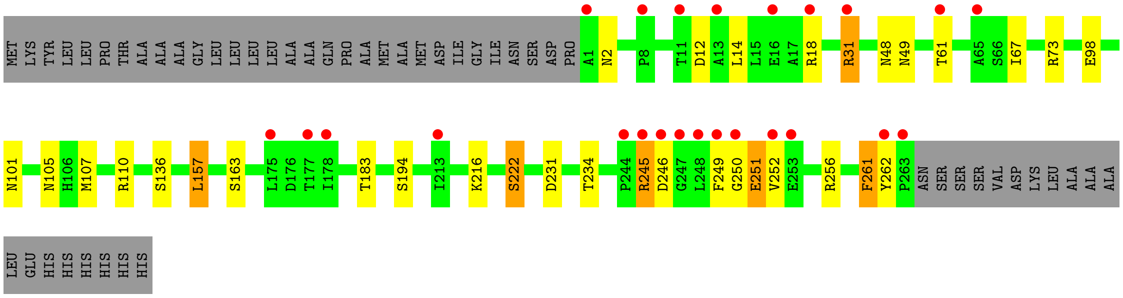
- Molecule 1: CUTINASE

Chain 50-A:



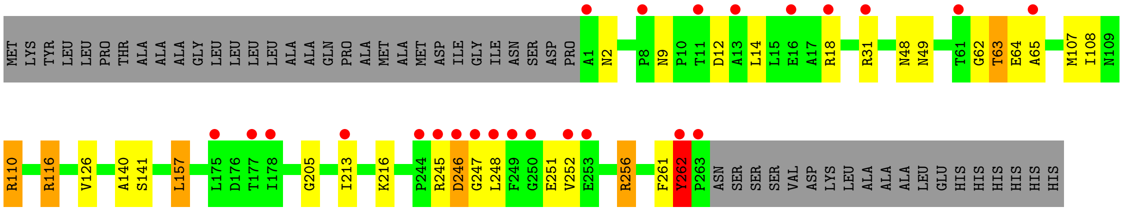
- Molecule 1: CUTINASE

Chain 51-A:



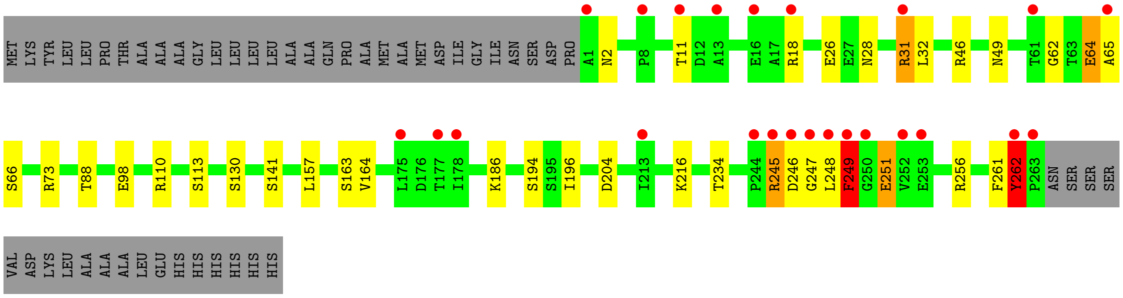
- Molecule 1: CUTINASE

Chain 52-A:



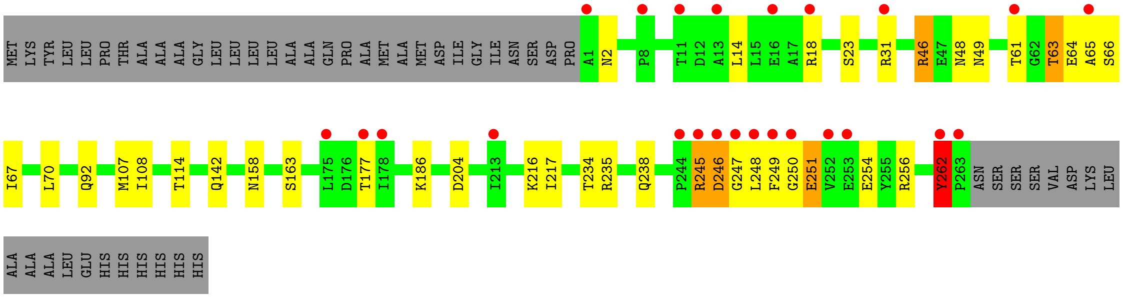
- Molecule 1: CUTINASE

Chain 53-A:



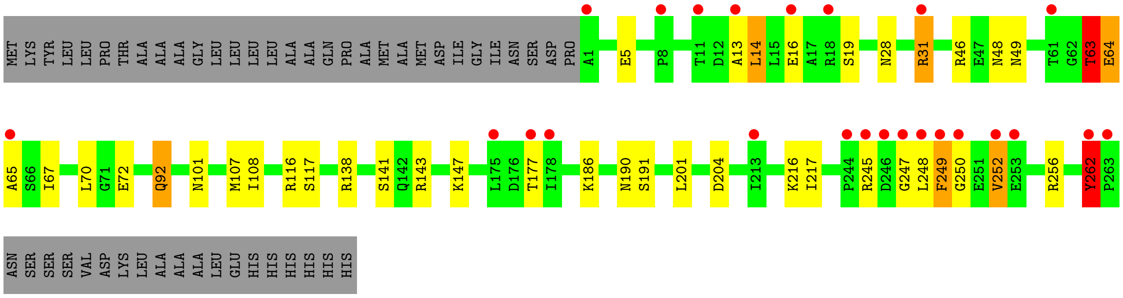
- Molecule 1: CUTINASE

Chain 54-A:



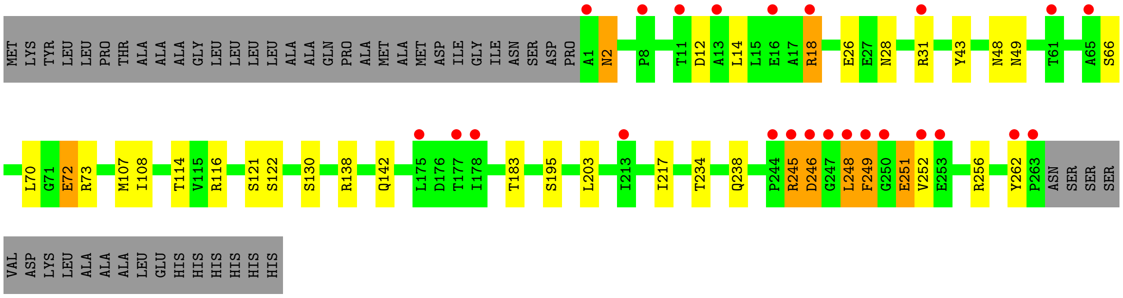
- Molecule 1: CUTINASE

Chain 55-A:



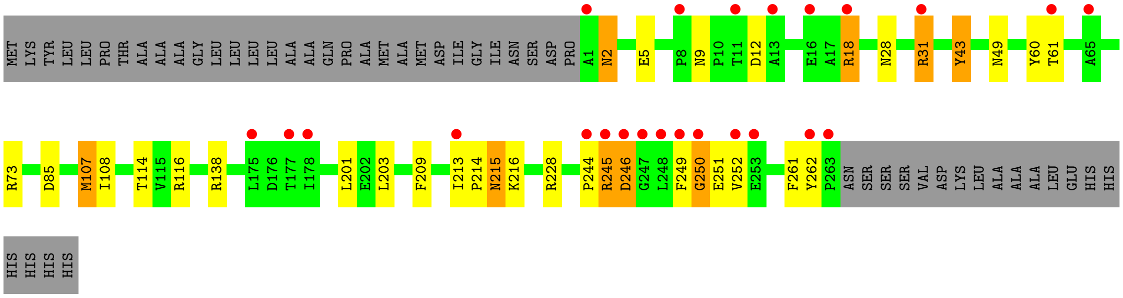
- Molecule 1: CUTINASE

Chain 56-A:



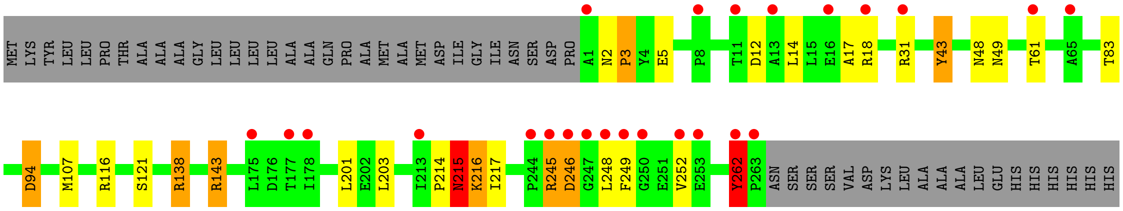
- Molecule 1: CUTINASE

Chain 57-A:



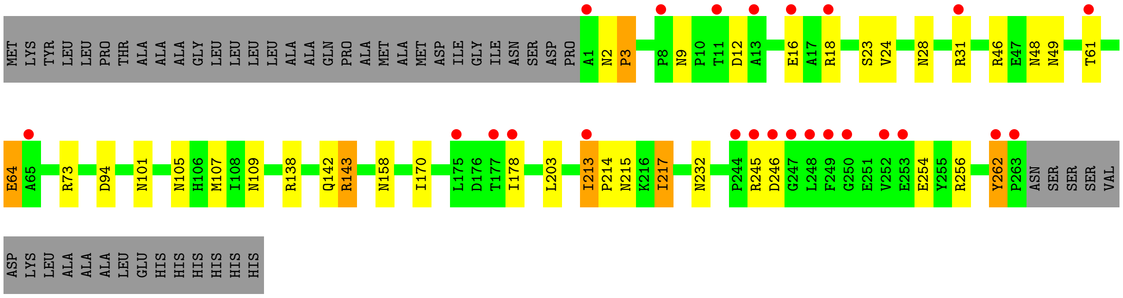
- Molecule 1: CUTINASE

Chain 58-A:



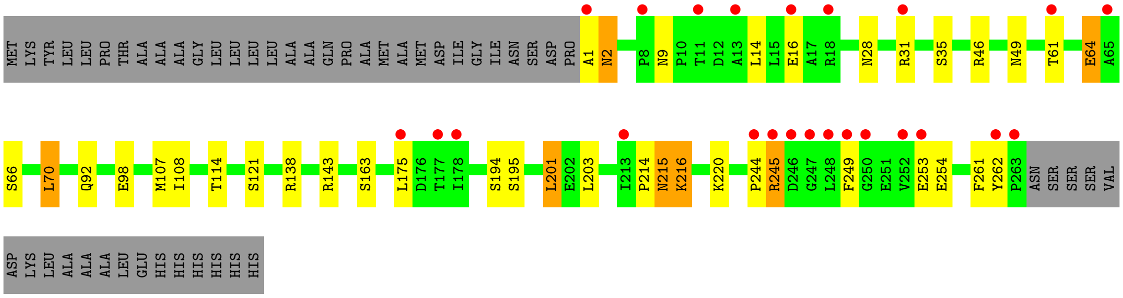
- Molecule 1: CUTINASE

Chain 59-A:



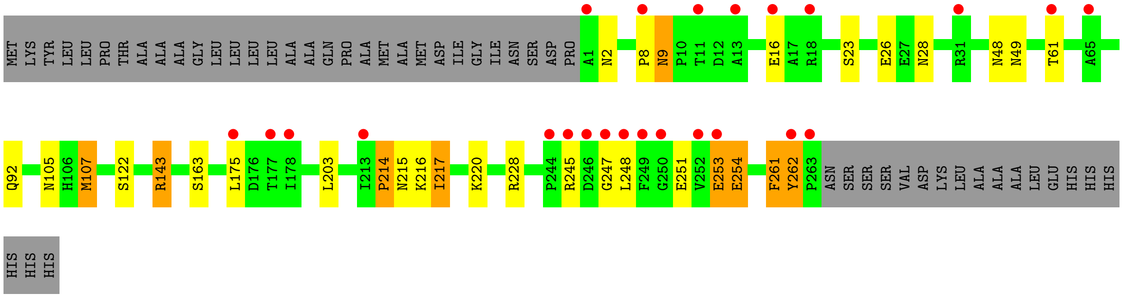
- Molecule 1: CUTINASE

Chain 60-A:



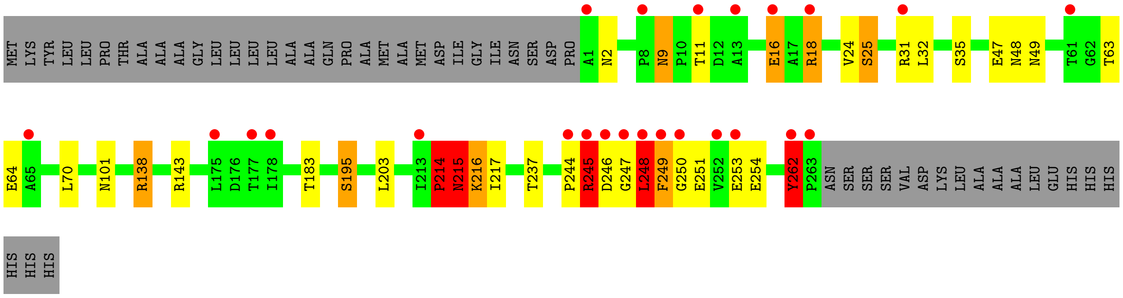
- Molecule 1: CUTINASE

Chain 61-A:



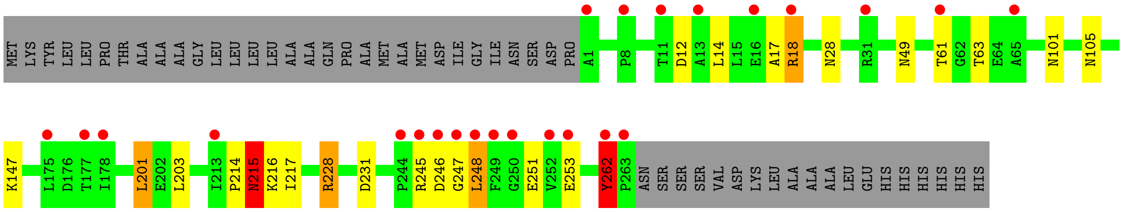
- Molecule 1: CUTINASE

Chain 62-A:



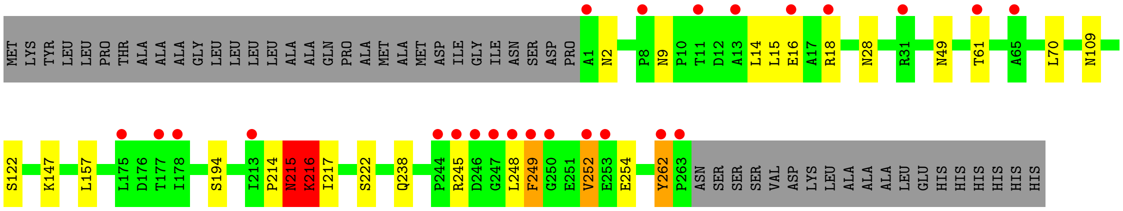
- Molecule 1: CUTINASE

Chain 63-A:



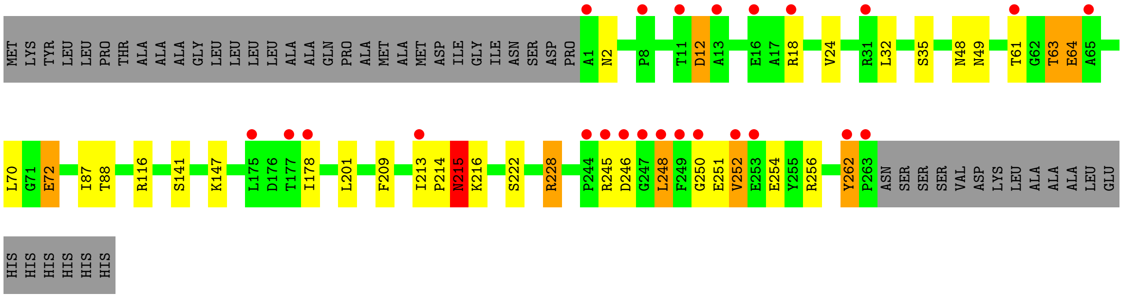
- Molecule 1: CUTINASE

Chain 64-A:



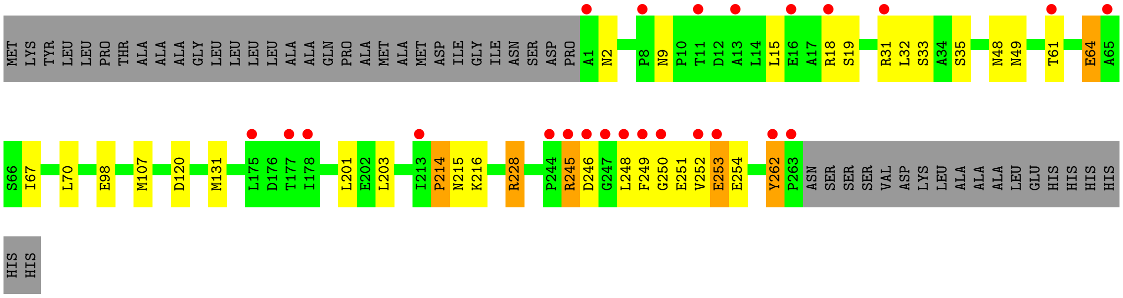
- Molecule 1: CUTINASE

Chain 65-A:



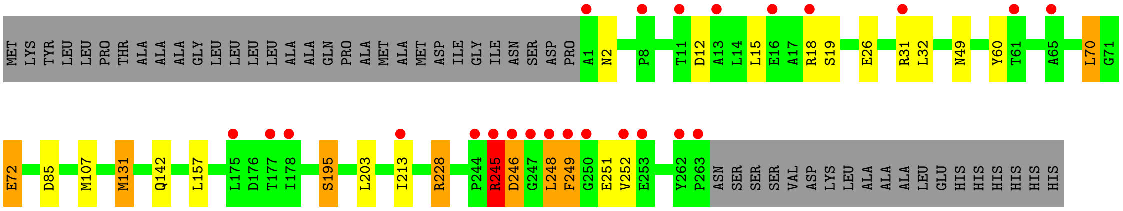
- Molecule 1: CUTINASE

Chain 66-A:



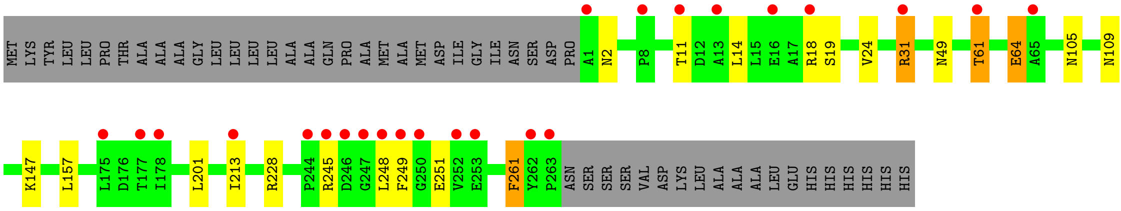
- Molecule 1: CUTINASE

Chain 67-A:



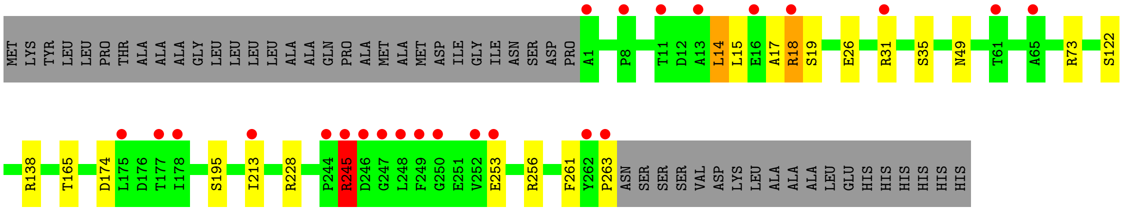
- Molecule 1: CUTINASE

Chain 68-A:



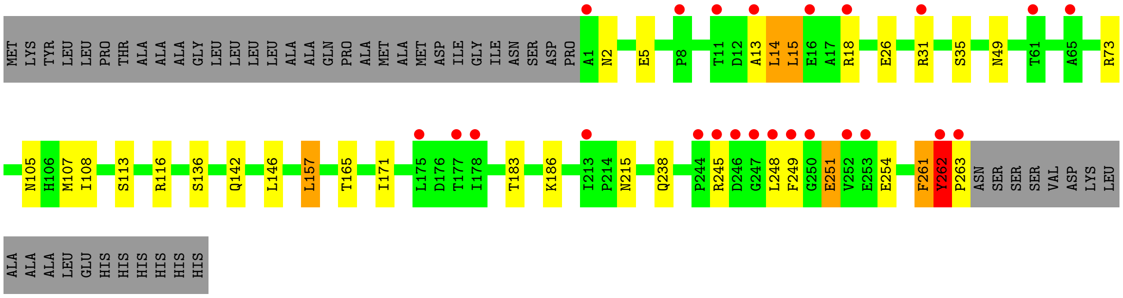
- Molecule 1: CUTINASE

Chain 69-A:



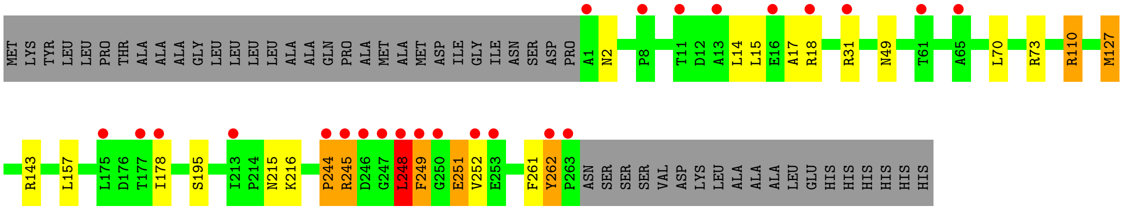
- Molecule 1: CUTINASE

Chain 70-A:



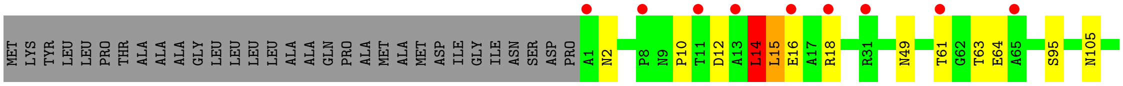
- Molecule 1: CUTINASE

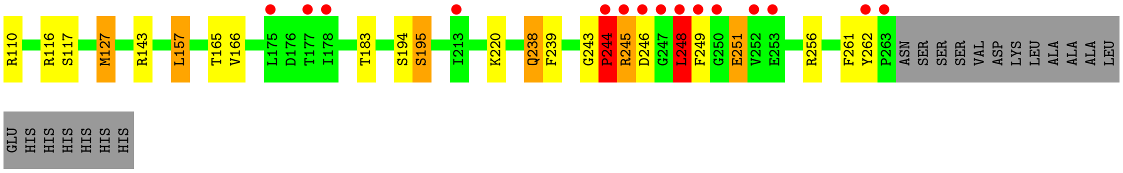
Chain 71-A:



- Molecule 1: CUTINASE

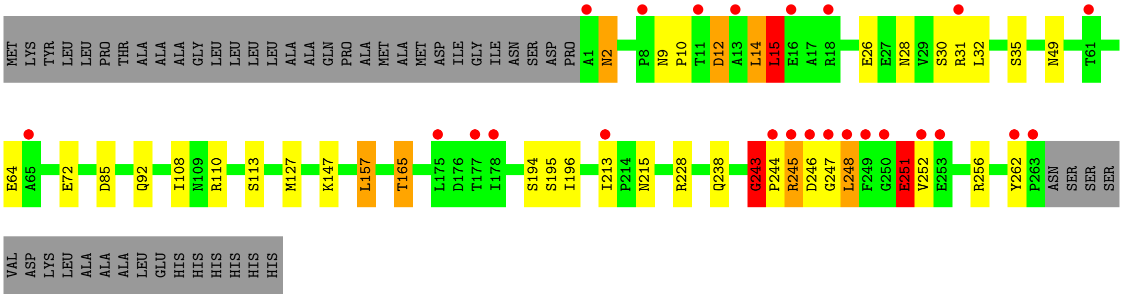
Chain 72-A:





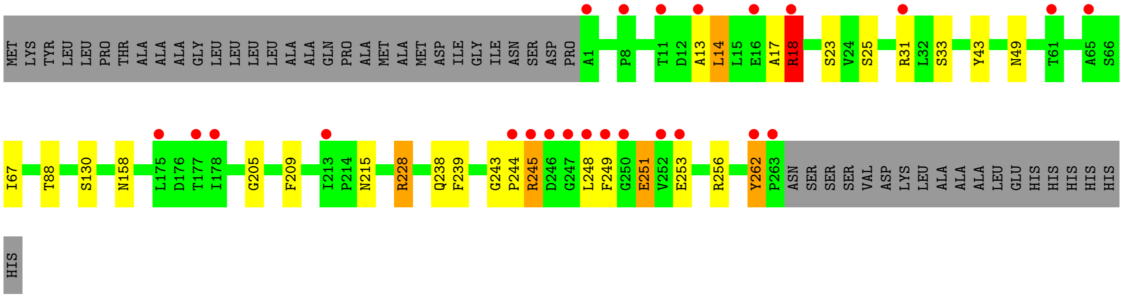
- Molecule 1: CUTINASE

Chain 73-A:



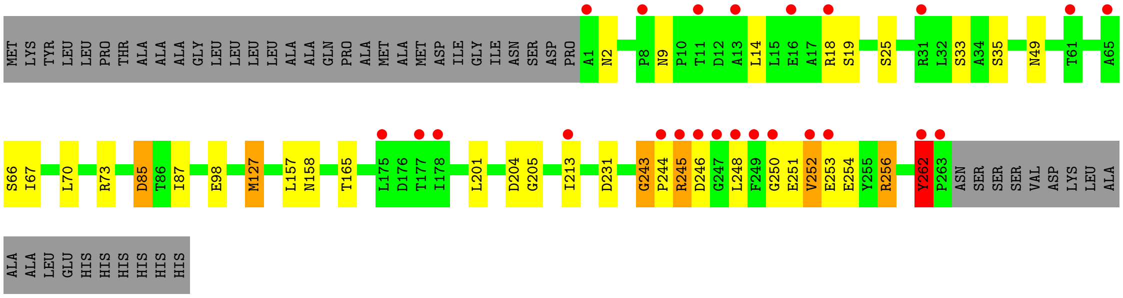
- Molecule 1: CUTINASE

Chain 74-A:



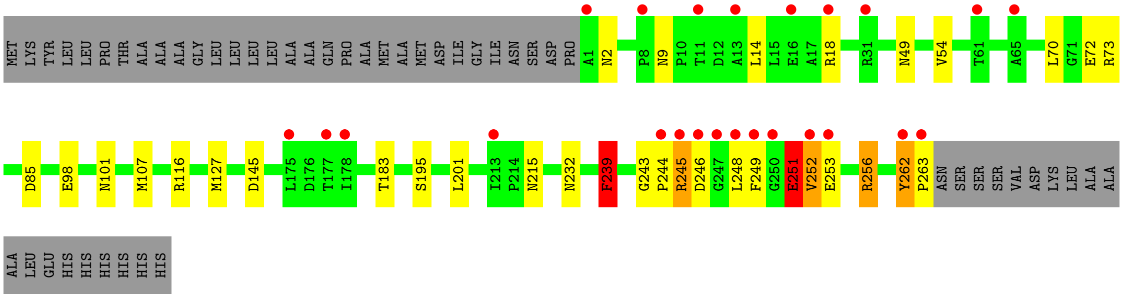
- Molecule 1: CUTINASE

Chain 75-A:



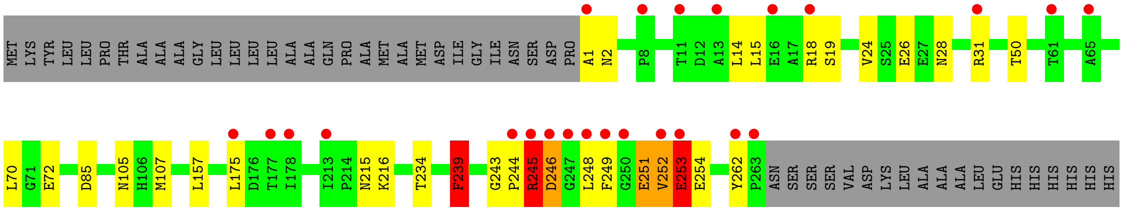
- Molecule 1: CUTINASE

Chain 76-A:



• Molecule 1: CUTINASE

Chain 77-A:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	117.90Å 117.90Å 36.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.12 – 1.55 23.12 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.12-1.55) 99.9 (23.12-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.55Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.117 , 0.149 0.130 , 0.160	Depositor DCC
R_{free} test set	3279 reflections (8.93%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 250.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	314292	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.80	1/2064 (0.0%)	1.04	12/2817 (0.4%)
1	2-A	0.88	6/2064 (0.3%)	1.04	12/2817 (0.4%)
1	3-A	0.75	3/2064 (0.1%)	0.93	3/2817 (0.1%)
1	4-A	0.79	4/2064 (0.2%)	1.09	9/2817 (0.3%)
1	5-A	0.78	2/2064 (0.1%)	1.10	12/2817 (0.4%)
1	6-A	0.79	1/2064 (0.0%)	1.13	11/2817 (0.4%)
1	7-A	0.80	6/2064 (0.3%)	0.95	9/2817 (0.3%)
1	8-A	0.75	1/2064 (0.0%)	0.95	9/2817 (0.3%)
1	9-A	0.77	1/2064 (0.0%)	0.93	5/2817 (0.2%)
1	10-A	0.78	2/2064 (0.1%)	1.03	6/2817 (0.2%)
1	11-A	0.80	4/2064 (0.2%)	0.96	9/2817 (0.3%)
1	12-A	0.76	1/2064 (0.0%)	0.98	7/2817 (0.2%)
1	13-A	0.71	0/2064	1.02	6/2817 (0.2%)
1	14-A	0.78	3/2064 (0.1%)	1.10	12/2817 (0.4%)
1	15-A	0.77	4/2064 (0.2%)	1.03	11/2817 (0.4%)
1	16-A	0.78	2/2064 (0.1%)	0.96	5/2817 (0.2%)
1	17-A	0.72	2/2064 (0.1%)	0.98	6/2817 (0.2%)
1	18-A	0.68	1/2064 (0.0%)	0.95	8/2817 (0.3%)
1	19-A	0.69	0/2064	0.90	3/2817 (0.1%)
1	20-A	0.83	4/2064 (0.2%)	0.95	5/2817 (0.2%)
1	21-A	0.73	2/2064 (0.1%)	0.89	2/2817 (0.1%)
1	22-A	0.68	0/2064	0.90	5/2817 (0.2%)
1	23-A	0.79	4/2064 (0.2%)	1.00	6/2817 (0.2%)
1	24-A	0.75	3/2064 (0.1%)	0.95	9/2817 (0.3%)
1	25-A	0.72	1/2064 (0.0%)	0.91	2/2817 (0.1%)
1	26-A	0.74	1/2064 (0.0%)	0.96	6/2817 (0.2%)
1	27-A	0.81	3/2064 (0.1%)	0.94	5/2817 (0.2%)
1	28-A	0.77	2/2064 (0.1%)	0.92	5/2817 (0.2%)
1	29-A	0.81	4/2064 (0.2%)	0.98	7/2817 (0.2%)
1	30-A	0.79	3/2064 (0.1%)	0.95	5/2817 (0.2%)
1	31-A	0.77	4/2064 (0.2%)	0.97	8/2817 (0.3%)
1	32-A	0.71	0/2064	0.89	1/2817 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	33-A	0.77	4/2064 (0.2%)	1.00	6/2817 (0.2%)
1	34-A	0.73	1/2064 (0.0%)	0.94	5/2817 (0.2%)
1	35-A	0.71	0/2064	0.99	9/2817 (0.3%)
1	36-A	0.73	1/2064 (0.0%)	0.90	6/2817 (0.2%)
1	37-A	0.74	1/2064 (0.0%)	0.94	4/2817 (0.1%)
1	38-A	0.77	1/2064 (0.0%)	0.98	6/2817 (0.2%)
1	39-A	0.80	4/2064 (0.2%)	0.92	3/2817 (0.1%)
1	40-A	0.74	2/2064 (0.1%)	0.99	8/2817 (0.3%)
1	41-A	0.78	3/2064 (0.1%)	0.95	7/2817 (0.2%)
1	42-A	0.82	3/2064 (0.1%)	0.98	8/2817 (0.3%)
1	43-A	0.81	2/2064 (0.1%)	1.00	10/2817 (0.4%)
1	44-A	0.81	2/2064 (0.1%)	1.01	9/2817 (0.3%)
1	45-A	0.82	2/2064 (0.1%)	1.05	10/2817 (0.4%)
1	46-A	0.79	4/2064 (0.2%)	1.01	6/2817 (0.2%)
1	47-A	0.80	3/2064 (0.1%)	1.04	8/2817 (0.3%)
1	48-A	0.83	4/2064 (0.2%)	1.04	12/2817 (0.4%)
1	49-A	0.83	6/2064 (0.3%)	0.98	4/2817 (0.1%)
1	50-A	0.76	1/2064 (0.0%)	0.94	6/2817 (0.2%)
1	51-A	0.75	0/2064	0.94	6/2817 (0.2%)
1	52-A	0.73	1/2064 (0.0%)	0.97	9/2817 (0.3%)
1	53-A	0.73	1/2064 (0.0%)	0.97	7/2817 (0.2%)
1	54-A	0.70	0/2064	0.96	3/2817 (0.1%)
1	55-A	0.77	2/2064 (0.1%)	1.08	17/2817 (0.6%)
1	56-A	0.76	0/2064	0.94	5/2817 (0.2%)
1	57-A	0.80	4/2064 (0.2%)	0.96	9/2817 (0.3%)
1	58-A	0.82	8/2064 (0.4%)	1.01	10/2817 (0.4%)
1	59-A	0.80	4/2064 (0.2%)	0.98	7/2817 (0.2%)
1	60-A	0.81	4/2064 (0.2%)	0.99	10/2817 (0.4%)
1	61-A	0.80	3/2064 (0.1%)	0.97	4/2817 (0.1%)
1	62-A	0.77	2/2064 (0.1%)	0.96	9/2817 (0.3%)
1	63-A	0.75	0/2064	0.96	6/2817 (0.2%)
1	64-A	0.74	2/2064 (0.1%)	0.91	4/2817 (0.1%)
1	65-A	0.74	2/2064 (0.1%)	0.94	8/2817 (0.3%)
1	66-A	0.73	2/2064 (0.1%)	0.93	5/2817 (0.2%)
1	67-A	0.74	2/2064 (0.1%)	0.98	7/2817 (0.2%)
1	68-A	0.71	1/2064 (0.0%)	0.92	5/2817 (0.2%)
1	69-A	0.71	0/2064	1.04	8/2817 (0.3%)
1	70-A	0.76	2/2064 (0.1%)	0.96	5/2817 (0.2%)
1	71-A	0.73	0/2064	0.89	4/2817 (0.1%)
1	72-A	0.73	1/2064 (0.0%)	1.00	10/2817 (0.4%)
1	73-A	0.84	6/2064 (0.3%)	1.05	12/2817 (0.4%)
1	74-A	0.79	5/2064 (0.2%)	0.96	5/2817 (0.2%)
1	75-A	0.74	1/2064 (0.0%)	0.95	9/2817 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	76-A	0.78	2/2064 (0.1%)	1.01	9/2817 (0.3%)
1	77-A	0.72	2/2064 (0.1%)	0.92	2/2817 (0.1%)
All	All	0.77	176/158928 (0.1%)	0.98	543/216909 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	5
1	2-A	0	3
1	3-A	0	5
1	4-A	0	5
1	5-A	0	9
1	6-A	0	9
1	7-A	0	3
1	8-A	0	2
1	9-A	0	3
1	10-A	0	2
1	11-A	0	2
1	12-A	0	5
1	14-A	0	3
1	15-A	0	2
1	16-A	0	1
1	17-A	0	1
1	18-A	0	1
1	19-A	0	4
1	20-A	0	2
1	21-A	0	1
1	22-A	0	1
1	23-A	0	4
1	24-A	0	4
1	25-A	0	3
1	26-A	0	4
1	27-A	0	3
1	28-A	0	4
1	29-A	0	5
1	31-A	0	1
1	32-A	0	2
1	34-A	0	2
1	35-A	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	36-A	0	2
1	37-A	0	3
1	38-A	0	1
1	39-A	0	2
1	40-A	0	2
1	41-A	0	2
1	42-A	0	3
1	43-A	0	5
1	44-A	0	9
1	45-A	0	8
1	46-A	0	4
1	47-A	0	4
1	48-A	0	4
1	49-A	0	1
1	50-A	0	3
1	51-A	0	1
1	52-A	0	3
1	53-A	0	8
1	54-A	0	3
1	55-A	0	4
1	56-A	0	2
1	57-A	0	4
1	58-A	0	2
1	59-A	0	3
1	60-A	0	2
1	61-A	0	3
1	62-A	0	5
1	63-A	0	4
1	64-A	0	4
1	65-A	0	3
1	66-A	0	2
1	67-A	0	3
1	68-A	0	2
1	69-A	0	4
1	70-A	0	4
1	71-A	0	1
1	72-A	0	2
1	73-A	0	6
1	74-A	0	4
1	75-A	0	6
1	76-A	0	2
1	77-A	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	249

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	20-A	131	MET	CB-CG	15.09	1.99	1.51
1	14-A	131	MET	CB-CG	11.82	1.89	1.51
1	70-A	5	GLU	CB-CG	10.43	1.72	1.52
1	57-A	43	TYR	CB-CG	-9.79	1.36	1.51
1	59-A	64	GLU	CB-CG	9.10	1.69	1.52

The worst 5 of 543 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6-A	243	GLY	C-N-CD	-22.23	71.71	120.60
1	5-A	243	GLY	C-N-CD	-20.43	75.65	120.60
1	10-A	243	GLY	C-N-CD	-19.10	78.58	120.60
1	4-A	127	MET	CG-SD-CE	-16.77	73.37	100.20
1	14-A	127	MET	CG-SD-CE	-16.75	73.39	100.20

There are no chirality outliers.

5 of 249 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	13	ALA	Peptide
1	1-A	214	PRO	Peptide
1	1-A	247	GLY	Peptide
1	1-A	250	GLY	Peptide
1	1-A	63	THR	Peptide

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	2011	1969	1963	0	0
1	2-A	2011	1969	1963	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-A	2011	1969	1963	0	0
1	4-A	2011	1969	1963	0	0
1	5-A	2011	1969	1963	0	0
1	6-A	2011	1969	1963	0	0
1	7-A	2011	1969	1963	0	0
1	8-A	2011	1969	1963	0	0
1	9-A	2011	1969	1963	0	0
1	10-A	2011	1969	1963	0	0
1	11-A	2011	1969	1963	0	0
1	12-A	2011	1969	1963	0	0
1	13-A	2011	1969	1963	0	0
1	14-A	2011	1969	1963	0	0
1	15-A	2011	1969	1963	0	0
1	16-A	2011	1969	1963	0	0
1	17-A	2011	1969	1963	0	0
1	18-A	2011	1969	1963	0	0
1	19-A	2011	1969	1963	0	0
1	20-A	2011	1969	1963	0	0
1	21-A	2011	1969	1963	0	0
1	22-A	2011	1969	1963	0	0
1	23-A	2011	1969	1963	0	0
1	24-A	2011	1969	1963	0	0
1	25-A	2011	1969	1963	0	0
1	26-A	2011	1969	1963	0	0
1	27-A	2011	1969	1963	0	0
1	28-A	2011	1969	1963	0	0
1	29-A	2011	1969	1963	0	0
1	30-A	2011	1969	1963	0	0
1	31-A	2011	1969	1963	0	0
1	32-A	2011	1969	1963	0	0
1	33-A	2011	1969	1963	0	0
1	34-A	2011	1969	1963	0	0
1	35-A	2011	1969	1963	0	0
1	36-A	2011	1969	1963	0	0
1	37-A	2011	1969	1963	0	0
1	38-A	2011	1969	1963	0	0
1	39-A	2011	1969	1963	0	0
1	40-A	2011	1969	1963	0	0
1	41-A	2011	1969	1963	0	0
1	42-A	2011	1969	1963	0	0
1	43-A	2011	1969	1963	0	0
1	44-A	2011	1969	1963	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	45-A	2011	1969	1963	0	0
1	46-A	2011	1969	1963	0	0
1	47-A	2011	1969	1963	0	0
1	48-A	2011	1969	1963	0	0
1	49-A	2011	1969	1963	0	0
1	50-A	2011	1969	1963	0	0
1	51-A	2011	1969	1963	0	0
1	52-A	2011	1969	1963	0	0
1	53-A	2011	1969	1963	0	0
1	54-A	2011	1969	1963	0	0
1	55-A	2011	1969	1963	0	0
1	56-A	2011	1969	1963	0	0
1	57-A	2011	1969	1963	0	0
1	58-A	2011	1969	1963	0	0
1	59-A	2011	1969	1963	0	0
1	60-A	2011	1969	1963	0	0
1	61-A	2011	1969	1963	0	0
1	62-A	2011	1969	1963	0	0
1	63-A	2011	1969	1963	0	0
1	64-A	2011	1969	1963	0	0
1	65-A	2011	1969	1963	0	0
1	66-A	2011	1969	1963	0	0
1	67-A	2011	1969	1963	0	0
1	68-A	2011	1969	1963	0	0
1	69-A	2011	1969	1963	0	0
1	70-A	2011	1969	1963	0	0
1	71-A	2011	1969	1963	0	0
1	72-A	2011	1969	1963	0	0
1	73-A	2011	1969	1963	0	0
1	74-A	2011	1969	1963	0	0
1	75-A	2011	1969	1963	0	0
1	76-A	2011	1969	1963	0	0
1	77-A	2011	1969	1963	0	0
2	1-A	5	0	0	0	0
2	2-A	5	0	0	0	0
2	3-A	5	0	0	0	0
2	4-A	5	0	0	0	0
2	5-A	5	0	0	0	0
2	6-A	5	0	0	0	0
2	7-A	5	0	0	0	0
2	8-A	5	0	0	0	0
2	9-A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	10-A	5	0	0	0	0
2	11-A	5	0	0	0	0
2	12-A	5	0	0	0	0
2	13-A	5	0	0	0	0
2	14-A	5	0	0	0	0
2	15-A	5	0	0	0	0
2	16-A	5	0	0	0	0
2	17-A	5	0	0	0	0
2	18-A	5	0	0	0	0
2	19-A	5	0	0	0	0
2	20-A	5	0	0	0	0
2	21-A	5	0	0	0	0
2	22-A	5	0	0	0	0
2	23-A	5	0	0	0	0
2	24-A	5	0	0	0	0
2	25-A	5	0	0	0	0
2	26-A	5	0	0	0	0
2	27-A	5	0	0	0	0
2	28-A	5	0	0	0	0
2	29-A	5	0	0	0	0
2	30-A	5	0	0	0	0
2	31-A	5	0	0	0	0
2	32-A	5	0	0	0	0
2	33-A	5	0	0	0	0
2	34-A	5	0	0	0	0
2	35-A	5	0	0	0	0
2	36-A	5	0	0	0	0
2	37-A	5	0	0	0	0
2	38-A	5	0	0	0	0
2	39-A	5	0	0	0	0
2	40-A	5	0	0	0	0
2	41-A	5	0	0	0	0
2	42-A	5	0	0	0	0
2	43-A	5	0	0	0	0
2	44-A	5	0	0	0	0
2	45-A	5	0	0	0	0
2	46-A	5	0	0	0	0
2	47-A	5	0	0	0	0
2	48-A	5	0	0	0	0
2	49-A	5	0	0	0	0
2	50-A	5	0	0	0	0
2	51-A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	52-A	5	0	0	0	0
2	53-A	5	0	0	0	0
2	54-A	5	0	0	0	0
2	55-A	5	0	0	0	0
2	56-A	5	0	0	0	0
2	57-A	5	0	0	0	0
2	58-A	5	0	0	0	0
2	59-A	5	0	0	0	0
2	60-A	5	0	0	0	0
2	61-A	5	0	0	0	0
2	62-A	5	0	0	0	0
2	63-A	5	0	0	0	0
2	64-A	5	0	0	0	0
2	65-A	5	0	0	0	0
2	66-A	5	0	0	0	0
2	67-A	5	0	0	0	0
2	68-A	5	0	0	0	0
2	69-A	5	0	0	0	0
2	70-A	5	0	0	0	0
2	71-A	5	0	0	0	0
2	72-A	5	0	0	0	0
2	73-A	5	0	0	0	0
2	74-A	5	0	0	0	0
2	75-A	5	0	0	0	0
2	76-A	5	0	0	0	0
2	77-A	5	0	0	0	0
3	1-A	99	0	0	0	0
3	2-A	102	0	0	0	0
3	3-A	98	0	0	0	0
3	4-A	85	0	0	0	0
3	5-A	98	0	0	0	0
3	6-A	99	0	0	0	0
3	7-A	98	0	0	0	0
3	8-A	101	0	0	0	0
3	9-A	95	0	0	0	0
3	10-A	90	0	0	0	0
3	11-A	103	0	0	0	0
3	12-A	97	0	0	0	0
3	13-A	87	0	0	0	0
3	14-A	90	0	0	0	0
3	15-A	112	0	0	0	0
3	16-A	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	17-A	82	0	0	0	0
3	18-A	89	0	0	0	0
3	19-A	89	0	0	0	0
3	20-A	103	0	0	0	0
3	21-A	101	0	0	0	0
3	22-A	83	0	0	0	0
3	23-A	103	0	0	0	0
3	24-A	98	0	0	0	0
3	25-A	99	0	0	0	0
3	26-A	85	0	0	0	0
3	27-A	100	0	0	0	0
3	28-A	104	0	0	0	0
3	29-A	105	0	0	0	0
3	30-A	94	0	0	0	0
3	31-A	91	0	0	0	0
3	32-A	96	0	0	0	0
3	33-A	90	0	0	0	0
3	34-A	94	0	0	0	0
3	35-A	98	0	0	0	0
3	36-A	98	0	0	0	0
3	37-A	97	0	0	0	0
3	38-A	91	0	0	0	0
3	39-A	104	0	0	0	0
3	40-A	89	0	0	0	0
3	41-A	104	0	0	0	0
3	42-A	112	0	0	0	0
3	43-A	102	0	0	0	0
3	44-A	83	0	0	0	0
3	45-A	96	0	0	0	0
3	46-A	99	0	0	0	0
3	47-A	100	0	0	0	0
3	48-A	83	0	0	0	0
3	49-A	93	0	0	0	0
3	50-A	95	0	0	0	0
3	51-A	99	0	0	0	0
3	52-A	98	0	0	0	0
3	53-A	90	0	0	0	0
3	54-A	95	0	0	0	0
3	55-A	92	0	0	0	0
3	56-A	95	0	0	0	0
3	57-A	97	0	0	0	0
3	58-A	91	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	59-A	88	0	0	0	0
3	60-A	98	0	0	0	0
3	61-A	113	0	0	0	0
3	62-A	103	0	0	0	0
3	63-A	107	0	0	0	0
3	64-A	100	0	0	0	0
3	65-A	88	0	0	0	0
3	66-A	104	0	0	0	0
3	67-A	102	0	0	0	0
3	68-A	105	0	0	0	0
3	69-A	104	0	0	0	0
3	70-A	103	0	0	0	0
3	71-A	108	0	0	0	0
3	72-A	101	0	0	0	0
3	73-A	96	0	0	0	0
3	74-A	95	0	0	0	0
3	75-A	88	0	0	0	0
3	76-A	88	0	0	0	0
3	77-A	102	0	0	0	0
All	All	162679	151613	151151	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	261/313 (83%)	242 (93%)	11 (4%)	8 (3%)	4	0
1	2-A	261/313 (83%)	239 (92%)	18 (7%)	4 (2%)	10	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-A	261/313 (83%)	238 (91%)	17 (6%)	6 (2%)	6	0
1	4-A	261/313 (83%)	237 (91%)	12 (5%)	12 (5%)	2	0
1	5-A	261/313 (83%)	233 (89%)	16 (6%)	12 (5%)	2	0
1	6-A	261/313 (83%)	239 (92%)	16 (6%)	6 (2%)	6	0
1	7-A	261/313 (83%)	247 (95%)	7 (3%)	7 (3%)	5	0
1	8-A	261/313 (83%)	243 (93%)	14 (5%)	4 (2%)	10	1
1	9-A	261/313 (83%)	240 (92%)	13 (5%)	8 (3%)	4	0
1	10-A	261/313 (83%)	248 (95%)	10 (4%)	3 (1%)	14	2
1	11-A	261/313 (83%)	242 (93%)	14 (5%)	5 (2%)	8	1
1	12-A	261/313 (83%)	243 (93%)	14 (5%)	4 (2%)	10	1
1	13-A	261/313 (83%)	243 (93%)	13 (5%)	5 (2%)	8	1
1	14-A	261/313 (83%)	244 (94%)	12 (5%)	5 (2%)	8	1
1	15-A	261/313 (83%)	244 (94%)	13 (5%)	4 (2%)	10	1
1	16-A	261/313 (83%)	240 (92%)	18 (7%)	3 (1%)	14	2
1	17-A	261/313 (83%)	244 (94%)	13 (5%)	4 (2%)	10	1
1	18-A	261/313 (83%)	238 (91%)	16 (6%)	7 (3%)	5	0
1	19-A	261/313 (83%)	243 (93%)	15 (6%)	3 (1%)	14	2
1	20-A	261/313 (83%)	240 (92%)	18 (7%)	3 (1%)	14	2
1	21-A	261/313 (83%)	244 (94%)	13 (5%)	4 (2%)	10	1
1	22-A	261/313 (83%)	244 (94%)	14 (5%)	3 (1%)	14	2
1	23-A	261/313 (83%)	245 (94%)	10 (4%)	6 (2%)	6	0
1	24-A	261/313 (83%)	248 (95%)	9 (3%)	4 (2%)	10	1
1	25-A	261/313 (83%)	245 (94%)	13 (5%)	3 (1%)	14	2
1	26-A	261/313 (83%)	243 (93%)	14 (5%)	4 (2%)	10	1
1	27-A	261/313 (83%)	243 (93%)	11 (4%)	7 (3%)	5	0
1	28-A	261/313 (83%)	242 (93%)	13 (5%)	6 (2%)	6	0
1	29-A	261/313 (83%)	241 (92%)	18 (7%)	2 (1%)	19	4
1	30-A	261/313 (83%)	249 (95%)	6 (2%)	6 (2%)	6	0
1	31-A	261/313 (83%)	242 (93%)	9 (3%)	10 (4%)	3	0
1	32-A	261/313 (83%)	245 (94%)	10 (4%)	6 (2%)	6	0
1	33-A	261/313 (83%)	241 (92%)	12 (5%)	8 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	34-A	261/313 (83%)	242 (93%)	11 (4%)	8 (3%)	4	0
1	35-A	261/313 (83%)	237 (91%)	19 (7%)	5 (2%)	8	1
1	36-A	261/313 (83%)	241 (92%)	15 (6%)	5 (2%)	8	1
1	37-A	261/313 (83%)	244 (94%)	11 (4%)	6 (2%)	6	0
1	38-A	261/313 (83%)	240 (92%)	15 (6%)	6 (2%)	6	0
1	39-A	261/313 (83%)	244 (94%)	12 (5%)	5 (2%)	8	1
1	40-A	261/313 (83%)	238 (91%)	16 (6%)	7 (3%)	5	0
1	41-A	261/313 (83%)	242 (93%)	13 (5%)	6 (2%)	6	0
1	42-A	261/313 (83%)	242 (93%)	12 (5%)	7 (3%)	5	0
1	43-A	261/313 (83%)	239 (92%)	13 (5%)	9 (3%)	3	0
1	44-A	261/313 (83%)	236 (90%)	14 (5%)	11 (4%)	3	0
1	45-A	261/313 (83%)	235 (90%)	16 (6%)	10 (4%)	3	0
1	46-A	261/313 (83%)	241 (92%)	13 (5%)	7 (3%)	5	0
1	47-A	261/313 (83%)	241 (92%)	13 (5%)	7 (3%)	5	0
1	48-A	261/313 (83%)	239 (92%)	14 (5%)	8 (3%)	4	0
1	49-A	261/313 (83%)	238 (91%)	13 (5%)	10 (4%)	3	0
1	50-A	261/313 (83%)	241 (92%)	13 (5%)	7 (3%)	5	0
1	51-A	261/313 (83%)	243 (93%)	12 (5%)	6 (2%)	6	0
1	52-A	261/313 (83%)	235 (90%)	14 (5%)	12 (5%)	2	0
1	53-A	261/313 (83%)	241 (92%)	10 (4%)	10 (4%)	3	0
1	54-A	261/313 (83%)	239 (92%)	11 (4%)	11 (4%)	3	0
1	55-A	261/313 (83%)	240 (92%)	12 (5%)	9 (3%)	3	0
1	56-A	261/313 (83%)	242 (93%)	8 (3%)	11 (4%)	3	0
1	57-A	261/313 (83%)	243 (93%)	8 (3%)	10 (4%)	3	0
1	58-A	261/313 (83%)	241 (92%)	11 (4%)	9 (3%)	3	0
1	59-A	261/313 (83%)	239 (92%)	16 (6%)	6 (2%)	6	0
1	60-A	261/313 (83%)	242 (93%)	11 (4%)	8 (3%)	4	0
1	61-A	261/313 (83%)	236 (90%)	17 (6%)	8 (3%)	4	0
1	62-A	261/313 (83%)	240 (92%)	11 (4%)	10 (4%)	3	0
1	63-A	261/313 (83%)	243 (93%)	13 (5%)	5 (2%)	8	1
1	64-A	261/313 (83%)	239 (92%)	15 (6%)	7 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	65-A	261/313 (83%)	240 (92%)	11 (4%)	10 (4%)	3	0
1	66-A	261/313 (83%)	240 (92%)	13 (5%)	8 (3%)	4	0
1	67-A	261/313 (83%)	247 (95%)	9 (3%)	5 (2%)	8	1
1	68-A	261/313 (83%)	241 (92%)	17 (6%)	3 (1%)	14	2
1	69-A	261/313 (83%)	245 (94%)	14 (5%)	2 (1%)	19	4
1	70-A	261/313 (83%)	243 (93%)	11 (4%)	7 (3%)	5	0
1	71-A	261/313 (83%)	241 (92%)	12 (5%)	8 (3%)	4	0
1	72-A	261/313 (83%)	229 (88%)	19 (7%)	13 (5%)	2	0
1	73-A	261/313 (83%)	235 (90%)	14 (5%)	12 (5%)	2	0
1	74-A	261/313 (83%)	235 (90%)	17 (6%)	9 (3%)	3	0
1	75-A	261/313 (83%)	243 (93%)	12 (5%)	6 (2%)	6	0
1	76-A	261/313 (83%)	241 (92%)	12 (5%)	8 (3%)	4	0
1	77-A	261/313 (83%)	243 (93%)	12 (5%)	6 (2%)	6	0
All	All	20097/24101 (83%)	18565 (92%)	1007 (5%)	525 (3%)	5	0

5 of 525 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	215	ASN
1	1-A	244	PRO
1	1-A	248	LEU
1	3-A	2	ASN
1	3-A	244	PRO

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	216/254 (85%)	190 (88%)	26 (12%)	5	0
1	2-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	3-A	216/254 (85%)	195 (90%)	21 (10%)	8	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	5-A	216/254 (85%)	197 (91%)	19 (9%)	10	1
1	6-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	7-A	216/254 (85%)	197 (91%)	19 (9%)	10	1
1	8-A	216/254 (85%)	196 (91%)	20 (9%)	9	0
1	9-A	216/254 (85%)	186 (86%)	30 (14%)	3	0
1	10-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	11-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	12-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	13-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	14-A	216/254 (85%)	186 (86%)	30 (14%)	3	0
1	15-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	16-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	17-A	216/254 (85%)	196 (91%)	20 (9%)	9	0
1	18-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	19-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	20-A	216/254 (85%)	188 (87%)	28 (13%)	4	0
1	21-A	216/254 (85%)	194 (90%)	22 (10%)	7	0
1	22-A	216/254 (85%)	187 (87%)	29 (13%)	4	0
1	23-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	24-A	216/254 (85%)	193 (89%)	23 (11%)	6	0
1	25-A	216/254 (85%)	195 (90%)	21 (10%)	8	0
1	26-A	216/254 (85%)	196 (91%)	20 (9%)	9	0
1	27-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	28-A	216/254 (85%)	200 (93%)	16 (7%)	13	1
1	29-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	30-A	216/254 (85%)	200 (93%)	16 (7%)	13	1
1	31-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	32-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	33-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	34-A	216/254 (85%)	190 (88%)	26 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	35-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	36-A	216/254 (85%)	197 (91%)	19 (9%)	10	1
1	37-A	216/254 (85%)	196 (91%)	20 (9%)	9	0
1	38-A	216/254 (85%)	193 (89%)	23 (11%)	6	0
1	39-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	40-A	216/254 (85%)	188 (87%)	28 (13%)	4	0
1	41-A	216/254 (85%)	197 (91%)	19 (9%)	10	1
1	42-A	216/254 (85%)	194 (90%)	22 (10%)	7	0
1	43-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	44-A	216/254 (85%)	184 (85%)	32 (15%)	3	0
1	45-A	216/254 (85%)	190 (88%)	26 (12%)	5	0
1	46-A	216/254 (85%)	185 (86%)	31 (14%)	3	0
1	47-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	48-A	216/254 (85%)	193 (89%)	23 (11%)	6	0
1	49-A	216/254 (85%)	188 (87%)	28 (13%)	4	0
1	50-A	216/254 (85%)	195 (90%)	21 (10%)	8	0
1	51-A	216/254 (85%)	190 (88%)	26 (12%)	5	0
1	52-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	53-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	54-A	216/254 (85%)	186 (86%)	30 (14%)	3	0
1	55-A	216/254 (85%)	187 (87%)	29 (13%)	4	0
1	56-A	216/254 (85%)	187 (87%)	29 (13%)	4	0
1	57-A	216/254 (85%)	194 (90%)	22 (10%)	7	0
1	58-A	216/254 (85%)	193 (89%)	23 (11%)	6	0
1	59-A	216/254 (85%)	187 (87%)	29 (13%)	4	0
1	60-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	61-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	62-A	216/254 (85%)	184 (85%)	32 (15%)	3	0
1	63-A	216/254 (85%)	196 (91%)	20 (9%)	9	0
1	64-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	65-A	216/254 (85%)	191 (88%)	25 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	66-A	216/254 (85%)	190 (88%)	26 (12%)	5	0
1	67-A	216/254 (85%)	194 (90%)	22 (10%)	7	0
1	68-A	216/254 (85%)	200 (93%)	16 (7%)	13	1
1	69-A	216/254 (85%)	200 (93%)	16 (7%)	13	1
1	70-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	71-A	216/254 (85%)	195 (90%)	21 (10%)	8	0
1	72-A	216/254 (85%)	189 (88%)	27 (12%)	4	0
1	73-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	74-A	216/254 (85%)	198 (92%)	18 (8%)	11	1
1	75-A	216/254 (85%)	191 (88%)	25 (12%)	5	0
1	76-A	216/254 (85%)	192 (89%)	24 (11%)	6	0
1	77-A	216/254 (85%)	188 (87%)	28 (13%)	4	0
All	All	16632/19558 (85%)	14796 (89%)	1836 (11%)	6	0

5 of 1836 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	40-A	108	ILE
1	75-A	98	GLU
1	49-A	108	ILE
1	74-A	238	GLN
1	67-A	72	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

77 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	SO4	34-A	1001	-	4,4,4	0.40	0	6,6,6	0.53	0
2	SO4	20-A	1001	-	4,4,4	0.30	0	6,6,6	0.46	0
2	SO4	5-A	1001	-	4,4,4	0.28	0	6,6,6	0.34	0
2	SO4	71-A	1001	-	4,4,4	0.32	0	6,6,6	0.43	0
2	SO4	24-A	1001	-	4,4,4	0.16	0	6,6,6	0.55	0
2	SO4	38-A	1001	-	4,4,4	0.24	0	6,6,6	0.70	0
2	SO4	72-A	1001	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	42-A	1001	-	4,4,4	0.38	0	6,6,6	0.53	0
2	SO4	63-A	1001	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	7-A	1001	-	4,4,4	0.37	0	6,6,6	0.36	0
2	SO4	28-A	1001	-	4,4,4	0.39	0	6,6,6	0.39	0
2	SO4	32-A	1001	-	4,4,4	0.31	0	6,6,6	0.54	0
2	SO4	46-A	1001	-	4,4,4	0.40	0	6,6,6	0.65	0
2	SO4	11-A	1001	-	4,4,4	0.52	0	6,6,6	0.43	0
2	SO4	73-A	1001	-	4,4,4	0.29	0	6,6,6	0.53	0
2	SO4	54-A	1001	-	4,4,4	0.24	0	6,6,6	0.64	0
2	SO4	64-A	1001	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	50-A	1001	-	4,4,4	0.37	0	6,6,6	0.47	0
2	SO4	39-A	1001	-	4,4,4	0.24	0	6,6,6	0.52	0
2	SO4	56-A	1001	-	4,4,4	0.28	0	6,6,6	0.69	0
2	SO4	52-A	1001	-	4,4,4	0.18	0	6,6,6	0.79	0
2	SO4	13-A	1001	-	4,4,4	0.22	0	6,6,6	0.30	0
2	SO4	59-A	1001	-	4,4,4	0.23	0	6,6,6	0.52	0
2	SO4	47-A	1001	-	4,4,4	0.37	0	6,6,6	0.62	0
2	SO4	41-A	1001	-	4,4,4	0.27	0	6,6,6	0.79	0
2	SO4	16-A	1001	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	17-A	1001	-	4,4,4	0.25	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	SO4	2-A	1001	-	4,4,4	0.40	0	6,6,6	0.30	0
2	SO4	27-A	1001	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	35-A	1001	-	4,4,4	0.42	0	6,6,6	0.65	0
2	SO4	51-A	1001	-	4,4,4	0.44	0	6,6,6	0.74	0
2	SO4	36-A	1001	-	4,4,4	0.37	0	6,6,6	0.18	0
2	SO4	48-A	1001	-	4,4,4	0.29	0	6,6,6	0.61	0
2	SO4	67-A	1001	-	4,4,4	0.36	0	6,6,6	0.39	0
2	SO4	15-A	1001	-	4,4,4	0.32	0	6,6,6	0.67	0
2	SO4	3-A	1001	-	4,4,4	0.50	0	6,6,6	0.74	0
2	SO4	70-A	1001	-	4,4,4	0.37	0	6,6,6	0.44	0
2	SO4	74-A	1001	-	4,4,4	0.36	0	6,6,6	0.66	0
2	SO4	14-A	1001	-	4,4,4	0.38	0	6,6,6	0.41	0
2	SO4	10-A	1001	-	4,4,4	0.25	0	6,6,6	0.31	0
2	SO4	40-A	1001	-	4,4,4	0.39	0	6,6,6	0.50	0
2	SO4	37-A	1001	-	4,4,4	0.45	0	6,6,6	0.15	0
2	SO4	55-A	1001	-	4,4,4	0.25	0	6,6,6	0.48	0
2	SO4	23-A	1001	-	4,4,4	0.09	0	6,6,6	0.57	0
2	SO4	43-A	1001	-	4,4,4	0.40	0	6,6,6	0.63	0
2	SO4	31-A	1001	-	4,4,4	0.20	0	6,6,6	0.53	0
2	SO4	53-A	1001	-	4,4,4	0.18	0	6,6,6	0.42	0
2	SO4	4-A	1001	-	4,4,4	0.51	0	6,6,6	0.62	0
2	SO4	18-A	1001	-	4,4,4	0.31	0	6,6,6	0.74	0
2	SO4	29-A	1001	-	4,4,4	0.33	0	6,6,6	0.56	0
2	SO4	22-A	1001	-	4,4,4	0.25	0	6,6,6	0.63	0
2	SO4	8-A	1001	-	4,4,4	0.20	0	6,6,6	0.53	0
2	SO4	58-A	1001	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	75-A	1001	-	4,4,4	0.39	0	6,6,6	0.50	0
2	SO4	25-A	1001	-	4,4,4	0.40	0	6,6,6	0.36	0
2	SO4	12-A	1001	-	4,4,4	0.33	0	6,6,6	0.64	0
2	SO4	19-A	1001	-	4,4,4	0.30	0	6,6,6	0.40	0
2	SO4	45-A	1001	-	4,4,4	0.22	0	6,6,6	0.51	0
2	SO4	65-A	1001	-	4,4,4	0.18	0	6,6,6	0.46	0
2	SO4	62-A	1001	-	4,4,4	0.32	0	6,6,6	0.59	0
2	SO4	1-A	1001	-	4,4,4	0.29	0	6,6,6	0.67	0
2	SO4	49-A	1001	-	4,4,4	0.35	0	6,6,6	0.79	0
2	SO4	9-A	1001	-	4,4,4	0.37	0	6,6,6	0.40	0
2	SO4	60-A	1001	-	4,4,4	0.28	0	6,6,6	0.38	0
2	SO4	30-A	1001	-	4,4,4	0.44	0	6,6,6	0.48	0
2	SO4	26-A	1001	-	4,4,4	0.31	0	6,6,6	0.76	0
2	SO4	21-A	1001	-	4,4,4	0.29	0	6,6,6	0.35	0
2	SO4	33-A	1001	-	4,4,4	0.25	0	6,6,6	0.50	0
2	SO4	77-A	1001	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	66-A	1001	-	4,4,4	0.41	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	6-A	1001	-	4,4,4	0.40	0	6,6,6	0.47	0
2	SO4	76-A	1001	-	4,4,4	0.31	0	6,6,6	0.36	0
2	SO4	57-A	1001	-	4,4,4	0.30	0	6,6,6	0.47	0
2	SO4	69-A	1001	-	4,4,4	0.22	0	6,6,6	0.61	0
2	SO4	44-A	1001	-	4,4,4	0.32	0	6,6,6	1.00	1 (16%)
2	SO4	61-A	1001	-	4,4,4	0.36	0	6,6,6	0.38	0
2	SO4	68-A	1001	-	4,4,4	0.25	0	6,6,6	0.60	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	44-A	1001	SO4	O4-S-O1	-2.01	99.03	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	2-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	3-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	4-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	5-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	6-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	7-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	8-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	9-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	10-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	11-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	12-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	13-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	14-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	15-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	16-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	17-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	18-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	19-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	20-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	21-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	22-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	23-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	24-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	25-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	26-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	27-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	28-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	29-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	30-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	31-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	32-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	33-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	34-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	35-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	36-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	37-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	38-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	39-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	40-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	41-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	42-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	43-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	44-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	45-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	46-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	47-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	48-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	49-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	50-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	51-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	52-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	53-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	54-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)
1	55-A	263/313 (84%)	0.31	24 (9%) 9 10	9, 14, 19, 25	263 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	56-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	57-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	58-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	59-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	60-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	61-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	62-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	63-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	64-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	65-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	66-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	67-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	68-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	69-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	70-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	71-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	72-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	73-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	74-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	75-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	76-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
1	77-A	263/313 (84%)	0.31	24 (9%)	9	10	9, 14, 19, 25	263 (100%)
All	All	20251/24101 (84%)	0.31	1848 (9%)	11	10	9, 14, 19, 25	20251 (100%)

The worst 5 of 1848 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	248	LEU	23.6
1	2-A	248	LEU	23.6
1	3-A	248	LEU	23.6
1	4-A	248	LEU	23.6
1	5-A	248	LEU	23.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	SO4	1-A	1001	5/5	0.12	0.70	24,24,24,26	5
2	SO4	2-A	1001	5/5	0.12	0.70	22,22,23,24	5
2	SO4	3-A	1001	5/5	0.12	0.70	24,25,25,26	5
2	SO4	4-A	1001	5/5	0.12	0.70	26,26,28,28	5
2	SO4	5-A	1001	5/5	0.12	0.70	27,28,29,30	5
2	SO4	6-A	1001	5/5	0.12	0.70	25,26,27,27	5
2	SO4	7-A	1001	5/5	0.12	0.70	24,24,26,26	5
2	SO4	8-A	1001	5/5	0.12	0.70	24,24,25,26	5
2	SO4	9-A	1001	5/5	0.12	0.70	20,22,22,23	5
2	SO4	10-A	1001	5/5	0.12	0.70	21,21,23,23	5
2	SO4	11-A	1001	5/5	0.12	0.70	21,22,23,24	5
2	SO4	12-A	1001	5/5	0.12	0.70	20,21,21,22	5
2	SO4	13-A	1001	5/5	0.12	0.70	22,23,23,24	5
2	SO4	14-A	1001	5/5	0.12	0.70	23,24,25,25	5
2	SO4	15-A	1001	5/5	0.12	0.70	21,23,23,23	5
2	SO4	16-A	1001	5/5	0.12	0.70	21,22,22,23	5
2	SO4	17-A	1001	5/5	0.12	0.70	21,21,22,23	5
2	SO4	18-A	1001	5/5	0.12	0.70	21,21,22,23	5
2	SO4	19-A	1001	5/5	0.12	0.70	20,20,22,22	5
2	SO4	20-A	1001	5/5	0.12	0.70	18,19,19,21	5
2	SO4	21-A	1001	5/5	0.12	0.70	18,19,19,20	5
2	SO4	22-A	1001	5/5	0.12	0.70	19,21,21,21	5
2	SO4	23-A	1001	5/5	0.12	0.70	23,23,24,25	5
2	SO4	24-A	1001	5/5	0.12	0.70	23,24,25,26	5
2	SO4	25-A	1001	5/5	0.12	0.70	21,22,22,23	5
2	SO4	26-A	1001	5/5	0.12	0.70	20,21,21,23	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	27-A	1001	5/5	0.12	0.70	22,22,23,24	5
2	SO4	28-A	1001	5/5	0.12	0.70	23,24,24,25	5
2	SO4	29-A	1001	5/5	0.12	0.70	24,25,26,26	5
2	SO4	30-A	1001	5/5	0.12	0.70	25,26,27,27	5
2	SO4	31-A	1001	5/5	0.12	0.70	26,28,28,29	5
2	SO4	32-A	1001	5/5	0.12	0.70	27,27,29,29	5
2	SO4	33-A	1001	5/5	0.12	0.70	27,28,29,29	5
2	SO4	34-A	1001	5/5	0.12	0.70	25,25,27,27	5
2	SO4	35-A	1001	5/5	0.12	0.70	24,24,24,26	5
2	SO4	36-A	1001	5/5	0.12	0.70	24,24,26,26	5
2	SO4	37-A	1001	5/5	0.12	0.70	23,24,24,25	5
2	SO4	38-A	1001	5/5	0.12	0.70	24,25,25,26	5
2	SO4	39-A	1001	5/5	0.12	0.70	25,27,27,28	5
2	SO4	40-A	1001	5/5	0.12	0.70	27,28,29,30	5
2	SO4	41-A	1001	5/5	0.12	0.70	26,27,28,28	5
2	SO4	42-A	1001	5/5	0.12	0.70	24,25,26,27	5
2	SO4	43-A	1001	5/5	0.12	0.70	23,24,25,25	5
2	SO4	44-A	1001	5/5	0.12	0.70	24,25,26,27	5
2	SO4	45-A	1001	5/5	0.12	0.70	24,24,25,26	5
2	SO4	46-A	1001	5/5	0.12	0.70	23,24,24,25	5
2	SO4	47-A	1001	5/5	0.12	0.70	21,21,22,23	5
2	SO4	48-A	1001	5/5	0.12	0.70	22,23,23,24	5
2	SO4	49-A	1001	5/5	0.12	0.70	22,23,24,24	5
2	SO4	50-A	1001	5/5	0.12	0.70	20,20,22,22	5
2	SO4	51-A	1001	5/5	0.12	0.70	18,19,19,20	5
2	SO4	52-A	1001	5/5	0.12	0.70	20,21,21,22	5
2	SO4	53-A	1001	5/5	0.12	0.70	20,21,21,22	5
2	SO4	54-A	1001	5/5	0.12	0.70	21,22,22,23	5
2	SO4	55-A	1001	5/5	0.12	0.70	22,22,23,24	5
2	SO4	56-A	1001	5/5	0.12	0.70	25,25,26,27	5
2	SO4	57-A	1001	5/5	0.12	0.70	25,26,26,28	5
2	SO4	58-A	1001	5/5	0.12	0.70	27,27,28,29	5
2	SO4	59-A	1001	5/5	0.12	0.70	29,30,31,32	5
2	SO4	60-A	1001	5/5	0.12	0.70	30,30,30,32	5
2	SO4	61-A	1001	5/5	0.12	0.70	28,28,29,30	5
2	SO4	62-A	1001	5/5	0.12	0.70	27,27,29,30	5
2	SO4	63-A	1001	5/5	0.12	0.70	26,27,27,28	5
2	SO4	64-A	1001	5/5	0.12	0.70	25,25,26,27	5
2	SO4	65-A	1001	5/5	0.12	0.70	24,24,25,26	5
2	SO4	66-A	1001	5/5	0.12	0.70	23,24,25,25	5
2	SO4	67-A	1001	5/5	0.12	0.70	26,26,26,28	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	68-A	1001	5/5	0.12	0.70	27,28,29,29	5
2	SO4	69-A	1001	5/5	0.12	0.70	31,31,32,33	5
2	SO4	70-A	1001	5/5	0.12	0.70	29,31,31,32	5
2	SO4	71-A	1001	5/5	0.12	0.70	29,31,31,32	5
2	SO4	72-A	1001	5/5	0.12	0.70	27,28,29,30	5
2	SO4	73-A	1001	5/5	0.12	0.70	25,27,28,28	5
2	SO4	74-A	1001	5/5	0.12	0.70	24,25,26,27	5
2	SO4	75-A	1001	5/5	0.12	0.70	23,24,25,25	5
2	SO4	76-A	1001	5/5	0.12	0.70	25,26,27,27	5
2	SO4	77-A	1001	5/5	0.12	0.70	26,26,28,28	5

6.5 Other polymers

There are no such residues in this entry.