



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 04:45 PM BST

PDB ID : 2Q3M
Title : Ensemble refinement of the protein crystal structure of an Arabidopsis thaliana putative steroid sulphotransferase
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

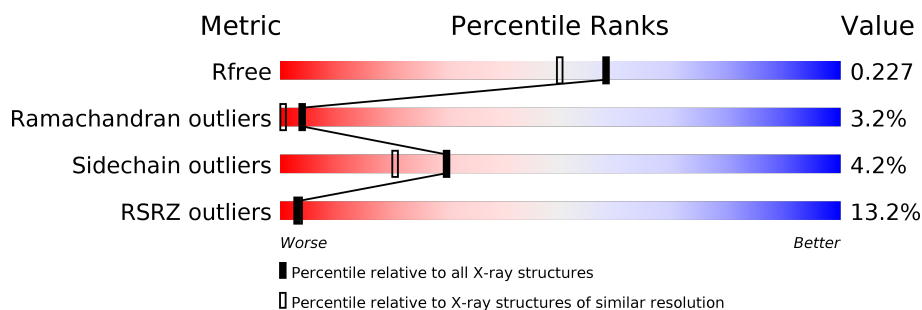
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	326	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	10-A	326	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div></div> <div>13%</div> </div> </div>
1	11-A	326	<div> <div>11%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div></div> <div>13%</div> </div> </div>
1	12-A	326	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>•</div> <div></div> <div>13%</div> </div> </div>
1	13-A	326	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	14-A	326	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div></div> <div>13%</div> </div> </div>
1	15-A	326	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div></div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	16-A	326	
1	2-A	326	
1	3-A	326	
1	4-A	326	
1	5-A	326	
1	6-A	326	
1	7-A	326	
1	8-A	326	
1	9-A	326	

2 Entry composition [i](#)

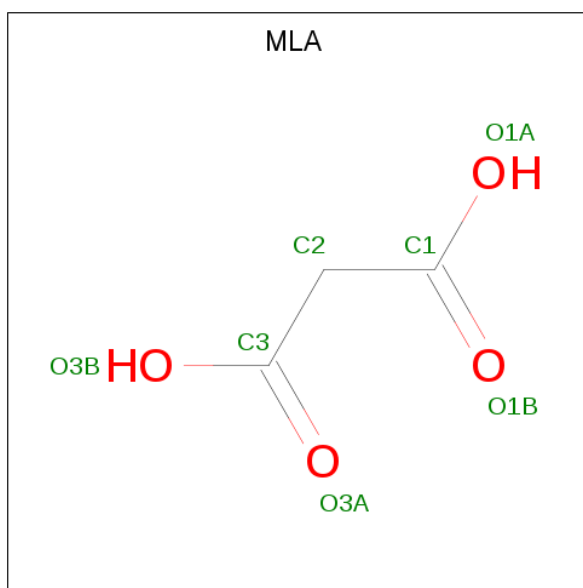
There are 3 unique types of molecules in this entry. The entry contains 40432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flavonol sulfotransferase-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	2-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	3-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	4-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	5-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	6-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	7-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	8-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	9-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	10-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	11-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	12-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	13-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	14-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	15-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	16-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	14-A	1	Total	C	O	0	0
			7	3	4		
2	15-A	1	Total	C	O	0	0
			7	3	4		
2	16-A	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	214	Total	O	0	0
			214	214		
3	2-A	214	Total	O	0	0
			214	214		
3	3-A	214	Total	O	0	0
			214	214		
3	4-A	214	Total	O	0	0
			214	214		
3	5-A	214	Total	O	0	0
			214	214		
3	6-A	214	Total	O	0	0
			214	214		
3	7-A	214	Total	O	0	0
			214	214		
3	8-A	214	Total	O	0	0
			214	214		
3	9-A	214	Total	O	0	0
			214	214		
3	10-A	214	Total	O	0	0
			214	214		
3	11-A	214	Total	O	0	0
			214	214		
3	12-A	214	Total	O	0	0
			214	214		
3	13-A	214	Total	O	0	0
			214	214		
3	14-A	214	Total	O	0	0
			214	214		
3	15-A	214	Total	O	0	0
			214	214		
3	16-A	214	Total	O	0	0
			214	214		

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.

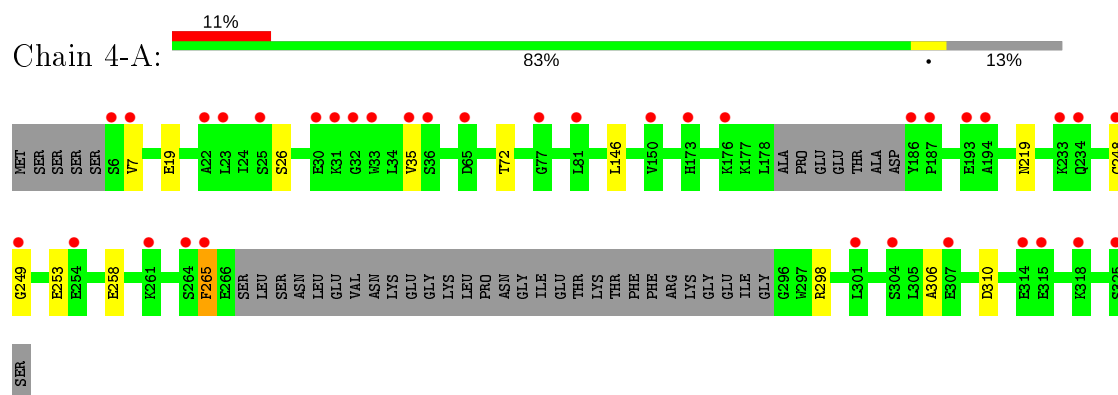
- Chain 1-A:
-
- 11% 74% 13% 13%
- MET SER SER SER SER S6 V7 G12 D13 T17 Q18 E19 T20 R21 A22 L23 I24 S25 S26 E30 K31 G32 W33 L34 V35 S36 E37 C57 D65 S66 D67 I68 G77 T78 T79 W80 L81 L84 L89 V96 S99 P103 E117 F126 M138 I141 S142 H143 L144 S145 E148 G149 V150 C155 H173 K176 K177 L178 A186 P187 E193 M194 L201 F205 L209 Y214 R217 E218 N219 R233 Q234 L246 F247 C248 G249 E254 V261 S264 F265 E266 SER LEU SER

- Chain 2-A:
-
- Sequence logo for Chain 2-A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A green bar at the top indicates the total conservation, with segments for 11%, 81%, 6%, and 13%.
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | THR | 0.00 |
| 2 | ALA | 0.00 |
| 3 | ASP | 0.00 |
| 4 | Y186 | 0.00 |
| 5 | P187 | 0.00 |
| 6 | E193 | 0.00 |
| 7 | A194 | 0.00 |
| 8 | I209 | 0.00 |
| 9 | N219 | 0.00 |
| 10 | P220 | 0.00 |
| 11 | N221 | 0.00 |
| 12 | Y228 | 0.00 |
| 13 | V233 | 0.00 |
| 14 | Q234 | 0.00 |
| 15 | C248 | 0.00 |
| 16 | Q249 | 0.00 |
| 17 | E254 | 0.00 |
| 18 | K261 | 0.00 |
| 19 | S264 | 0.00 |
| 20 | P265 | 0.00 |
| 21 | E266 | 0.00 |
| 22 | SER | 0.00 |
| 23 | LEU | 0.00 |
| 24 | SER | 0.00 |
| 25 | ASN | 0.00 |
| 26 | LEU | 0.00 |
| 27 | GLU | 0.00 |
| 28 | VAL | 0.00 |
| 29 | ASN | 0.00 |
| 30 | LYS | 0.00 |
| 31 | GLU | 0.00 |
| 32 | GLY | 0.00 |
| 33 | LYS | 0.00 |
| 34 | LEU | 0.00 |
| 35 | PRO | 0.00 |
| 36 | ASN | 0.00 |
| 37 | GLY | 0.00 |
| 38 | ILE | 0.00 |
| 39 | GLU | 0.00 |
| 40 | THR | 0.00 |
| 41 | PHE | 0.00 |
| 42 | THR | 0.00 |
| 43 | ARG | 0.00 |
| 44 | LYS | 0.00 |
| 45 | GLY | 0.00 |
| 46 | GLU | 0.00 |
| 47 | ILE | 0.00 |
| 48 | GLY | 0.00 |
| 49 | GLN | 0.00 |
| 50 | GLY | 0.00 |

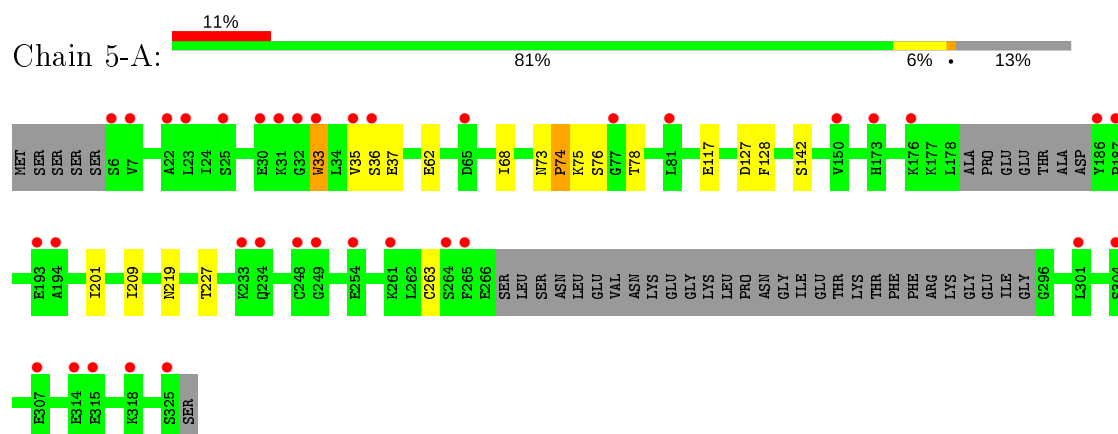
- Chain 3-A:
-
- 11%
- 83%
- 13%
- MET SER SER SER SER S6 V7 T17 A22 L23 L24 S25 E30 K31 G32 W33 L34 V35 S36 Y39 E40 F41 D65 L70 G77 L81 S98 S99 N108 P109 H143 V150 H173 K176 A177 L178 ALA PRO GLU GLU THR ALA ASP Y186 P187
- E193 A194 N219 K233 Q234 C248 G249 E254 K261 S264 F265 E286 SER LEU LEU ASN LEU VAL E40 ASN LYS GLU GLY LYS LEU PRO PRG ASN GLY ILE GLU THR THR PHE ARG LYS GLY GLU ILE G286 G297 R298 L301 S304 E307 E314 E315



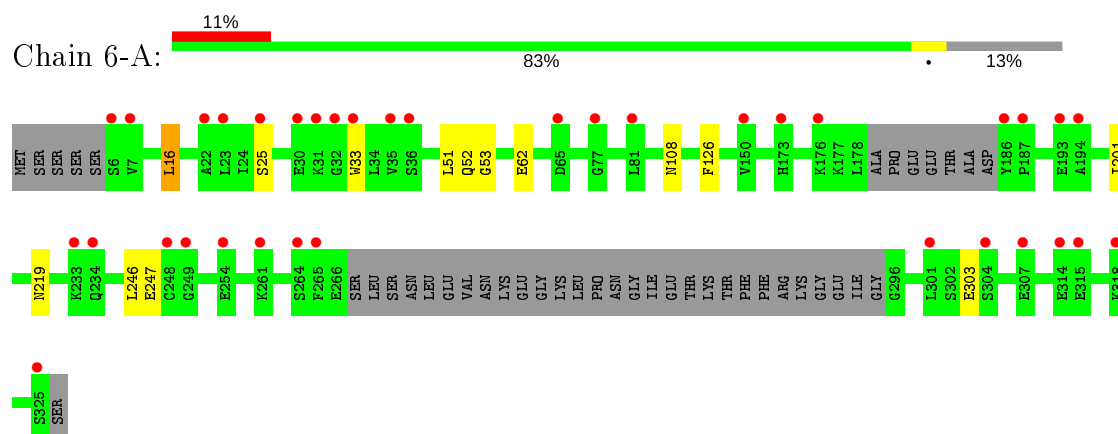
- Molecule 1: Flavonol sulfotransferase-like



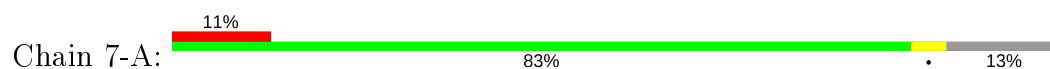
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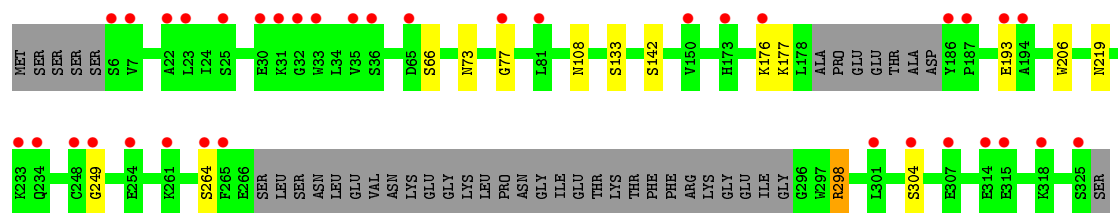


- Molecule 1: Flavonol sulfotransferase-like

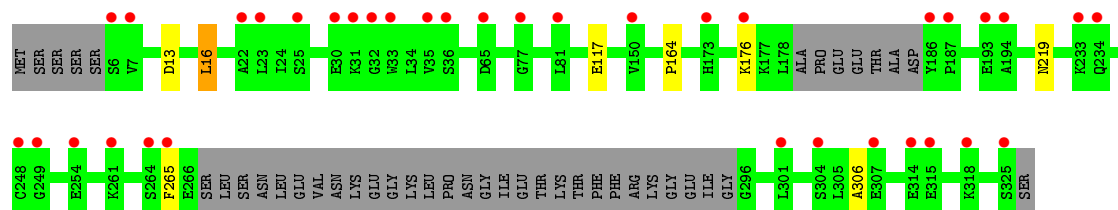
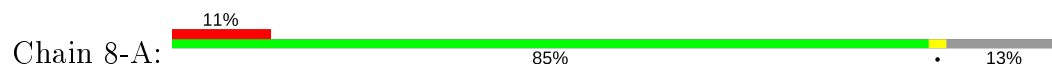


- Molecule 1: Flavonol sulfotransferase-like

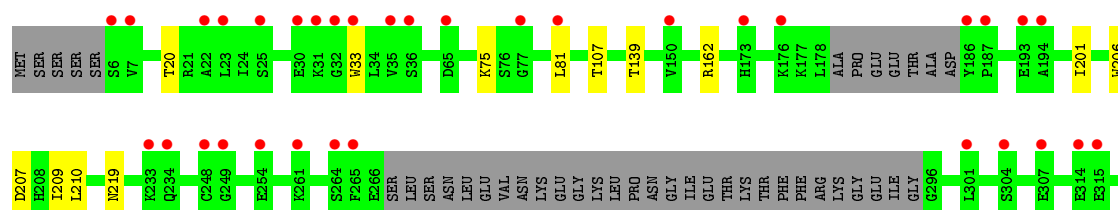
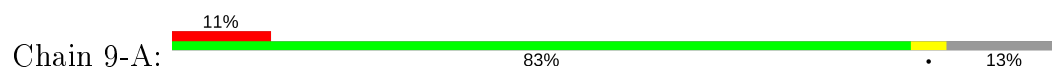




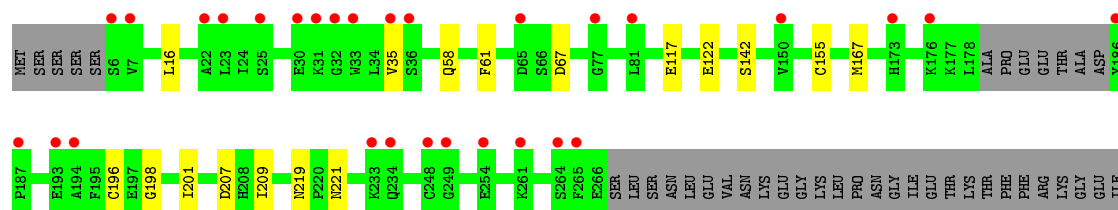
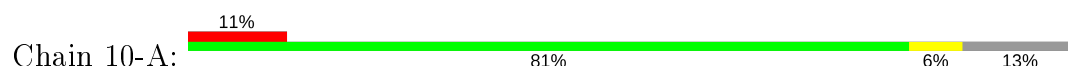
• Molecule 1: Flavonol sulfotransferase-like



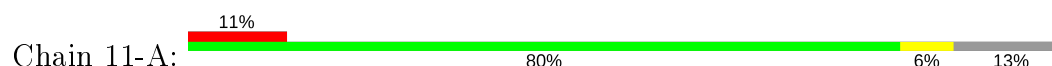
• Molecule 1: Flavonol sulfotransferase-like

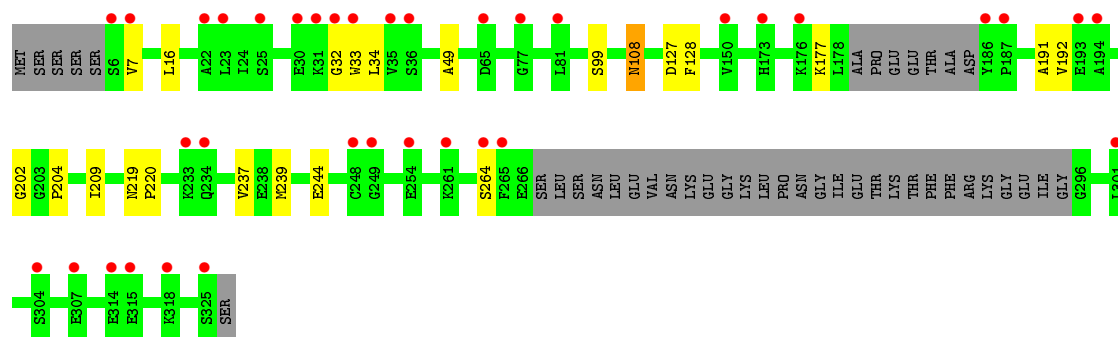


• Molecule 1: Flavonol sulfotransferase-like

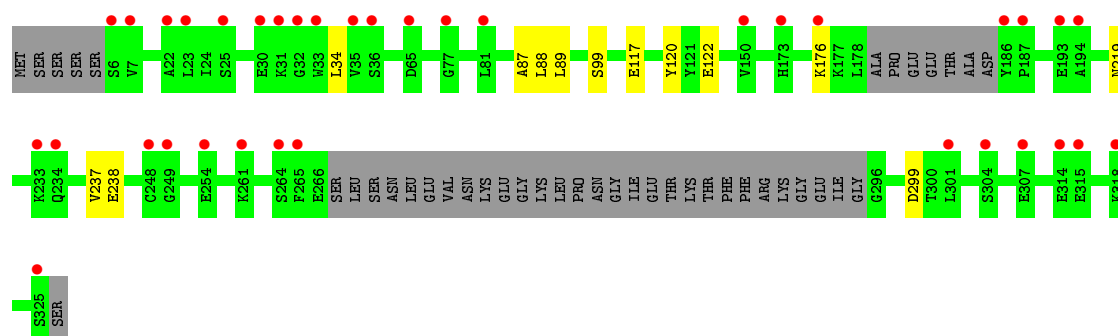
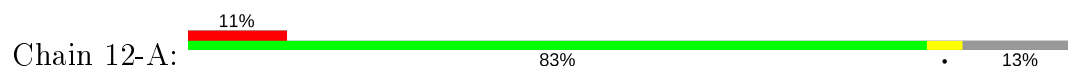


• Molecule 1: Flavonol sulfotransferase-like

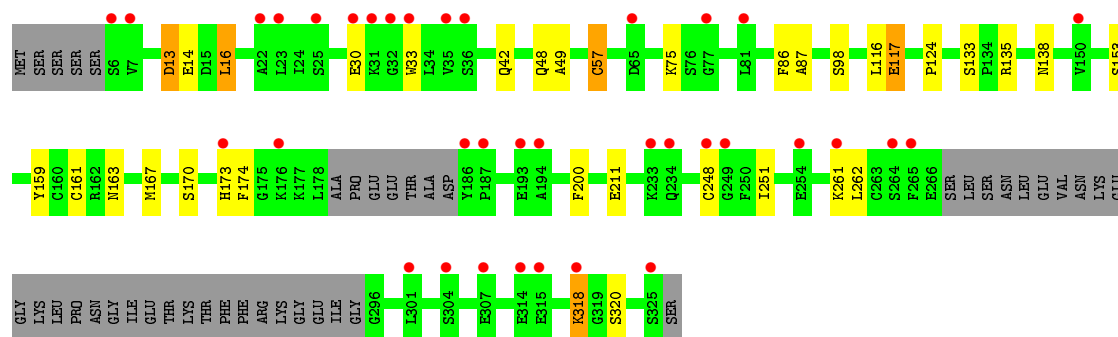
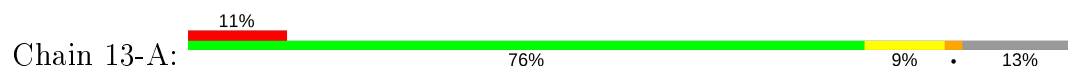




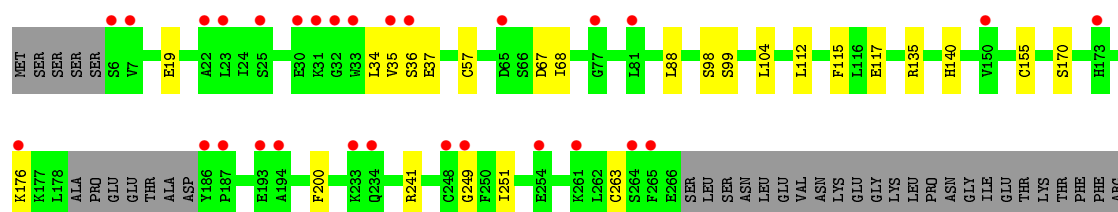
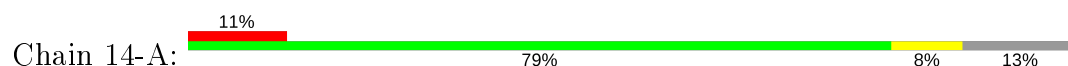
- Molecule 1: Flavonol sulfotransferase-like

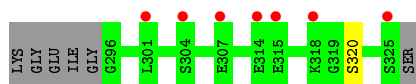


- Molecule 1: Flavonol sulfotransferase-like

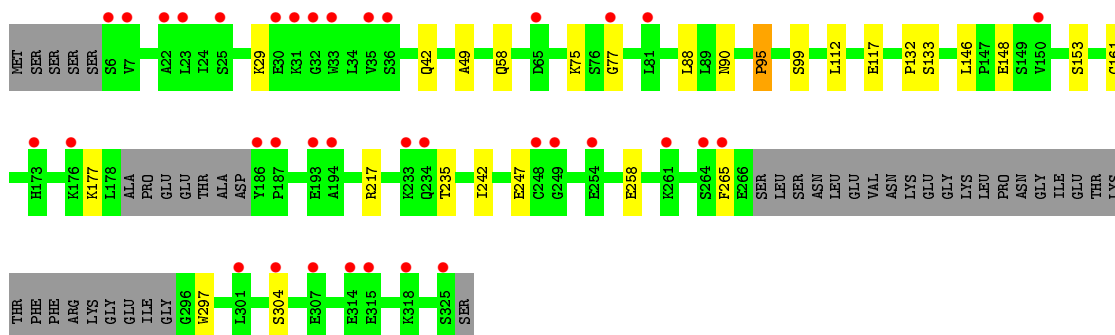
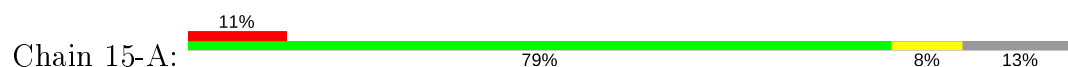


- Molecule 1: Flavonol sulfotransferase-like

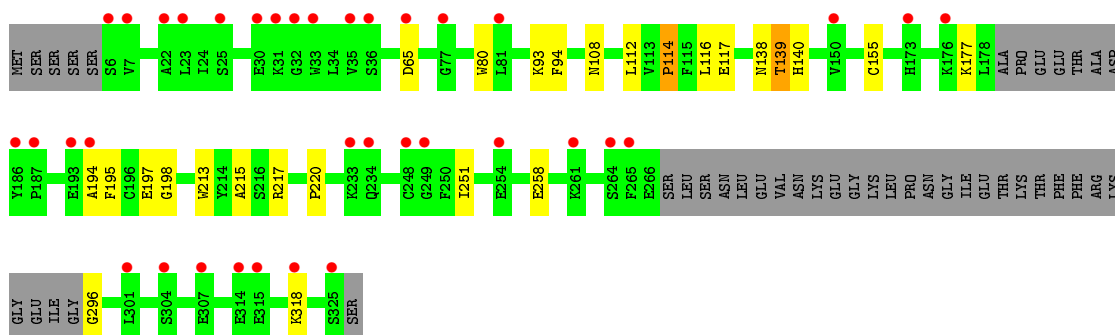
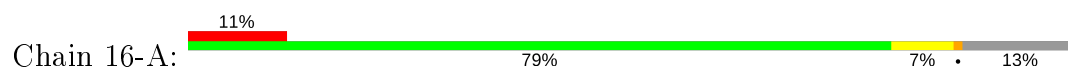




- Molecule 1: Flavonol sulfotransferase-like



- Molecule 1: Flavonol sulfotransferase-like



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.48 Å 120.90 Å 74.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 1.90 19.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.79-1.90) 99.3 (19.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 1.90 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.217 0.169 , 0.227	Depositor DCC
R_{free} test set	1654 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	40432	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2/2367 (0.1%)	0.85	2/3201 (0.1%)
1	2-A	0.75	1/2367 (0.0%)	0.79	1/3201 (0.0%)
1	3-A	0.75	0/2367	0.79	0/3201
1	4-A	0.76	0/2367	0.78	0/3201
1	5-A	0.75	0/2367	0.78	1/3201 (0.0%)
1	6-A	0.76	0/2367	0.79	1/3201 (0.0%)
1	7-A	0.72	0/2367	0.76	0/3201
1	8-A	0.74	1/2367 (0.0%)	0.80	1/3201 (0.0%)
1	9-A	0.73	0/2367	0.79	1/3201 (0.0%)
1	10-A	0.77	0/2367	0.84	3/3201 (0.1%)
1	11-A	0.76	0/2367	0.80	2/3201 (0.1%)
1	12-A	0.74	0/2367	0.77	0/3201
1	13-A	0.91	2/2367 (0.1%)	0.97	5/3201 (0.2%)
1	14-A	0.90	0/2367	0.97	4/3201 (0.1%)
1	15-A	0.94	2/2367 (0.1%)	0.96	3/3201 (0.1%)
1	16-A	0.91	1/2367 (0.0%)	0.92	3/3201 (0.1%)
All	All	0.80	9/37872 (0.0%)	0.84	27/51216 (0.1%)

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	1
1	2-A	0	1
1	3-A	0	1
1	12-A	0	1
1	13-A	0	1
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	117	GLU	CB-CG	-9.26	1.34	1.52
1	15-A	58	GLN	CG-CD	6.42	1.65	1.51
1	1-A	248	CYS	CB-SG	5.88	1.92	1.82
1	1-A	57	CYS	CB-SG	5.76	1.92	1.82
1	16-A	65	ASP	CB-CG	5.72	1.63	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	16	LEU	CA-CB-CG	-7.15	98.86	115.30
1	13-A	16	LEU	CA-CB-CG	-7.13	98.90	115.30
1	16-A	65	ASP	CB-CG-OD1	7.01	124.61	118.30
1	8-A	16	LEU	CA-CB-CG	-6.77	99.74	115.30
1	16-A	94	PHE	N-CA-C	-6.75	92.77	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	214	TYR	Sidechain
1	12-A	120	TYR	Sidechain
1	13-A	159	TYR	Sidechain
1	2-A	39	TYR	Sidechain
1	3-A	39	TYR	Sidechain

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	2306	0	2277	0	0
1	2-A	2306	0	2277	0	0
1	3-A	2306	0	2277	0	0
1	4-A	2306	0	2277	0	0
1	5-A	2306	0	2277	0	0
1	6-A	2306	0	2277	0	0
1	7-A	2306	0	2277	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8-A	2306	0	2277	0	0
1	9-A	2306	0	2277	0	0
1	10-A	2306	0	2277	0	0
1	11-A	2306	0	2277	0	0
1	12-A	2306	0	2277	0	0
1	13-A	2306	0	2277	0	0
1	14-A	2306	0	2277	0	0
1	15-A	2306	0	2277	0	0
1	16-A	2306	0	2277	0	0
2	1-A	7	0	2	0	0
2	2-A	7	0	2	0	0
2	3-A	7	0	2	0	0
2	4-A	7	0	2	0	0
2	5-A	7	0	2	0	0
2	6-A	7	0	2	0	0
2	7-A	7	0	2	0	0
2	8-A	7	0	2	0	0
2	9-A	7	0	2	0	0
2	10-A	7	0	2	0	0
2	11-A	7	0	3	0	0
2	12-A	7	0	2	0	0
2	13-A	7	0	2	0	0
2	14-A	7	0	2	0	0
2	15-A	7	0	2	0	0
2	16-A	7	0	2	0	0
3	1-A	214	0	0	0	0
3	2-A	214	0	0	0	0
3	3-A	214	0	0	0	0
3	4-A	214	0	0	0	0
3	5-A	214	0	0	0	0
3	6-A	214	0	0	0	0
3	7-A	214	0	0	0	0
3	8-A	214	0	0	0	0
3	9-A	214	0	0	0	0
3	10-A	214	0	0	0	0
3	11-A	214	0	0	0	0
3	12-A	214	0	0	0	0
3	13-A	214	0	0	0	0
3	14-A	214	0	0	0	0
3	15-A	214	0	0	0	0
3	16-A	214	0	0	0	0
All	All	40432	0	36465	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	278/326 (85%)	217 (78%)	39 (14%)	22 (8%)	1	0
1	2-A	278/326 (85%)	242 (87%)	26 (9%)	10 (4%)	3	0
1	3-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	6	1
1	4-A	278/326 (85%)	258 (93%)	14 (5%)	6 (2%)	6	1
1	5-A	278/326 (85%)	244 (88%)	25 (9%)	9 (3%)	4	0
1	6-A	278/326 (85%)	256 (92%)	15 (5%)	7 (2%)	5	1
1	7-A	278/326 (85%)	252 (91%)	17 (6%)	9 (3%)	4	0
1	8-A	278/326 (85%)	263 (95%)	14 (5%)	1 (0%)	34	24
1	9-A	278/326 (85%)	245 (88%)	28 (10%)	5 (2%)	8	2
1	10-A	278/326 (85%)	239 (86%)	33 (12%)	6 (2%)	6	1
1	11-A	278/326 (85%)	239 (86%)	26 (9%)	13 (5%)	2	0
1	12-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	6	1
1	13-A	278/326 (85%)	238 (86%)	25 (9%)	15 (5%)	2	0
1	14-A	278/326 (85%)	240 (86%)	32 (12%)	6 (2%)	6	1
1	15-A	278/326 (85%)	236 (85%)	34 (12%)	8 (3%)	4	1
1	16-A	278/326 (85%)	240 (86%)	24 (9%)	14 (5%)	2	0
All	All	4448/5216 (85%)	3915 (88%)	390 (9%)	143 (3%)	4	0

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	13	ASP
1	1-A	33	TRP
1	1-A	67	ASP
1	1-A	79	THR
1	1-A	84	LEU

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	258/294 (88%)	237 (92%)	21 (8%)	11	4
1	2-A	258/294 (88%)	251 (97%)	7 (3%)	44	38
1	3-A	258/294 (88%)	247 (96%)	11 (4%)	29	19
1	4-A	258/294 (88%)	248 (96%)	10 (4%)	32	23
1	5-A	258/294 (88%)	246 (95%)	12 (5%)	26	16
1	6-A	258/294 (88%)	251 (97%)	7 (3%)	44	38
1	7-A	258/294 (88%)	251 (97%)	7 (3%)	44	38
1	8-A	258/294 (88%)	252 (98%)	6 (2%)	50	45
1	9-A	258/294 (88%)	251 (97%)	7 (3%)	44	38
1	10-A	258/294 (88%)	247 (96%)	11 (4%)	29	19
1	11-A	258/294 (88%)	250 (97%)	8 (3%)	40	32
1	12-A	258/294 (88%)	252 (98%)	6 (2%)	50	45
1	13-A	258/294 (88%)	241 (93%)	17 (7%)	16	8
1	14-A	258/294 (88%)	242 (94%)	16 (6%)	18	9
1	15-A	258/294 (88%)	243 (94%)	15 (6%)	20	10
1	16-A	258/294 (88%)	247 (96%)	11 (4%)	29	19
All	All	4128/4704 (88%)	3956 (96%)	172 (4%)	30	20

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8-A	164	PRO

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Mol	Chain	Res	Type
1	10-A	221	ASN
1	15-A	265	PHE
1	8-A	265	PHE
1	9-A	219	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-A	110	HIS
1	10-A	52	GLN
1	15-A	140	HIS
1	8-A	219	ASN
1	9-A	110	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	MLA	6-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	3-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	14-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	2-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	10-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	5-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	1-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	16-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	13-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	4-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	9-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	12-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	15-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	11-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	7-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	8-A	901	-	0,6,6	0.00	-	0,7,7	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLA	6-A	901	-	-	0/0/4/4	-
2	MLA	3-A	901	-	-	0/0/4/4	-
2	MLA	14-A	901	-	-	0/0/4/4	-
2	MLA	2-A	901	-	-	0/0/4/4	-
2	MLA	10-A	901	-	-	0/0/4/4	-
2	MLA	5-A	901	-	-	0/0/4/4	-
2	MLA	1-A	901	-	-	0/0/4/4	-
2	MLA	16-A	901	-	-	0/0/4/4	-
2	MLA	13-A	901	-	-	0/0/4/4	-
2	MLA	4-A	901	-	-	0/0/4/4	-
2	MLA	9-A	901	-	-	0/0/4/4	-
2	MLA	12-A	901	-	-	0/0/4/4	-
2	MLA	15-A	901	-	-	0/0/4/4	-
2	MLA	11-A	901	-	-	0/0/4/4	-
2	MLA	7-A	901	-	-	0/0/4/4	-
2	MLA	8-A	901	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

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	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	2-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	3-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	4-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	5-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	6-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	7-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	8-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	9-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	10-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	11-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	12-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	13-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	14-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	15-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
1	16-A	284/326 (87%)	0.74	36 (12%) 3 4	12, 25, 50, 67	284 (100%)
All	All	4544/5216 (87%)	0.74	576 (12%) 3 4	12, 25, 51, 67	4544 (100%)

The worst 5 of 576 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	33	TRP	14.9
1	2-A	33	TRP	14.9
1	3-A	33	TRP	14.9
1	4-A	33	TRP	14.9
1	5-A	33	TRP	14.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLA	6-A	901	7/7	0.95	0.14	19,24,24,28	7
2	MLA	3-A	901	7/7	0.95	0.14	15,21,27,30	7
2	MLA	14-A	901	7/7	0.95	0.14	8,15,24,27	7
2	MLA	2-A	901	7/7	0.95	0.14	15,20,25,27	7
2	MLA	10-A	901	7/7	0.95	0.14	0,11,25,28	7
2	MLA	5-A	901	7/7	0.95	0.14	22,25,25,28	7
2	MLA	1-A	901	7/7	0.95	0.14	0,10,27,29	7
2	MLA	16-A	901	7/7	0.95	0.14	12,18,24,26	7
2	MLA	13-A	901	7/7	0.95	0.14	17,21,22,24	7
2	MLA	4-A	901	7/7	0.95	0.14	17,20,25,28	7
2	MLA	9-A	901	7/7	0.95	0.14	23,26,27,28	7
2	MLA	12-A	901	7/7	0.95	0.14	0,11,29,31	7
2	MLA	15-A	901	7/7	0.95	0.14	20,21,25,25	7
2	MLA	11-A	901	7/7	0.95	0.14	2,10,19,22	7
2	MLA	7-A	901	7/7	0.95	0.14	20,23,25,26	7
2	MLA	8-A	901	7/7	0.95	0.14	22,24,25,27	7

6.5 Other polymers [i](#)

There are no such residues in this entry.