



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 05:17 AM GMT

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 full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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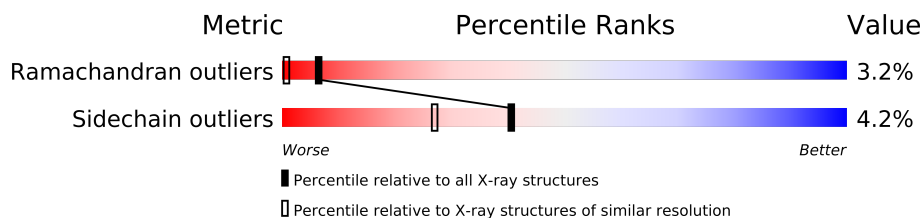
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	326	
1	10-A	326	
1	11-A	326	
1	12-A	326	
1	13-A	326	
1	14-A	326	
1	15-A	326	
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

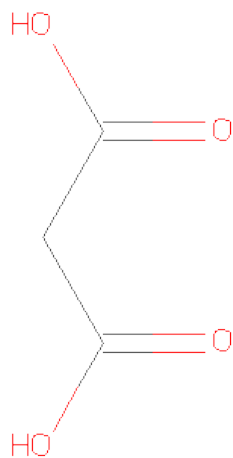
There are 3 unique types of molecules in this entry. The entry contains 40432 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

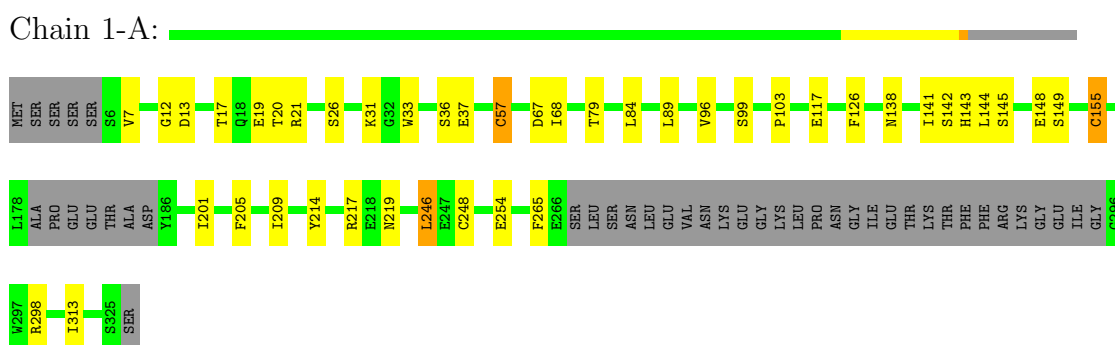
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	214	Total	O	0	0
			214	214		
3	2-A	214	Total	O	0	0
			214	214		
3	3-A	214	Total	O	0	0
			214	214		
3	4-A	214	Total	O	0	0
			214	214		
3	5-A	214	Total	O	0	0
			214	214		
3	6-A	214	Total	O	0	0
			214	214		
3	7-A	214	Total	O	0	0
			214	214		
3	8-A	214	Total	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		

### 3 Residue-property plots

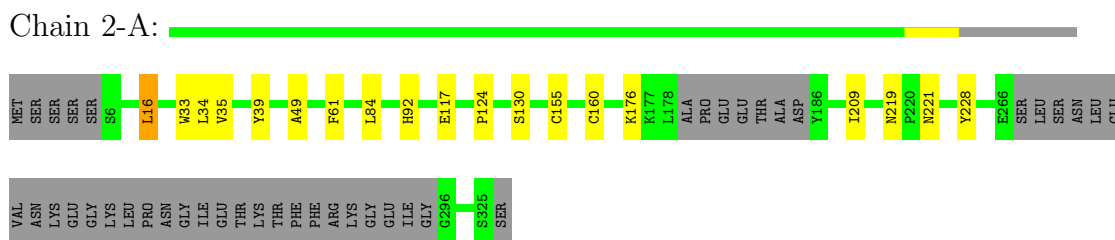
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

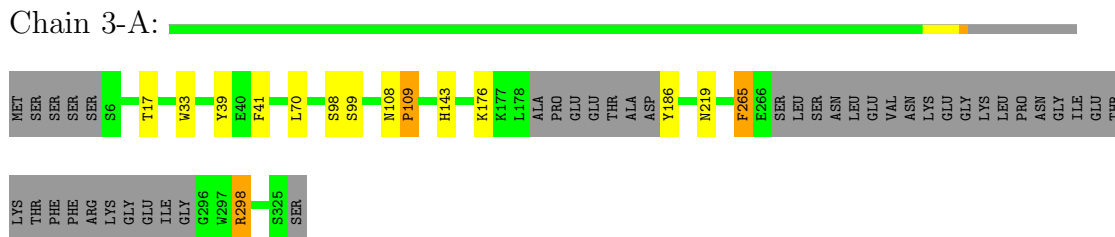
- Molecule 1: Flavonol sulfotransferase-like



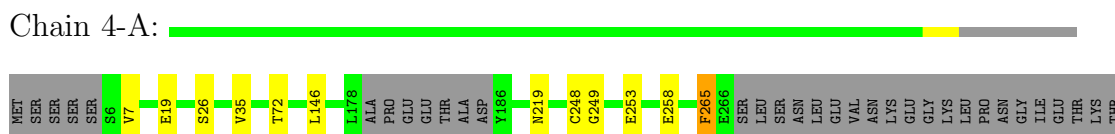
- Molecule 1: Flavonol sulfotransferase-like

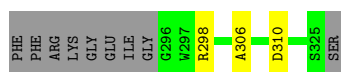


- Molecule 1: Flavonol sulfotransferase-like



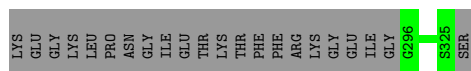
- Molecule 1: Flavonol sulfotransferase-like





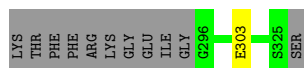
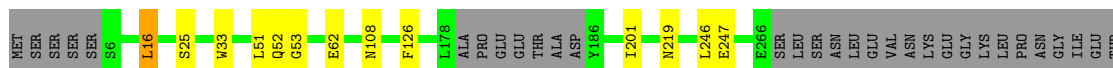
- Molecule 1: Flavonol sulfotransferase-like

Chain 5-A:



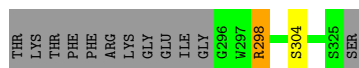
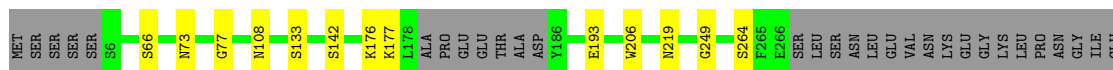
- Molecule 1: Flavonol sulfotransferase-like

Chain 6-A:



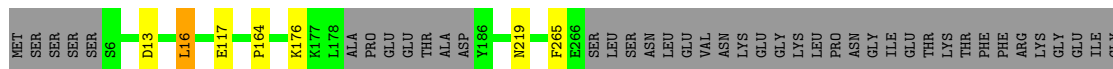
- Molecule 1: Flavonol sulfotransferase-like

Chain 7-A:



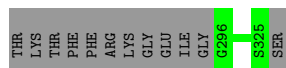
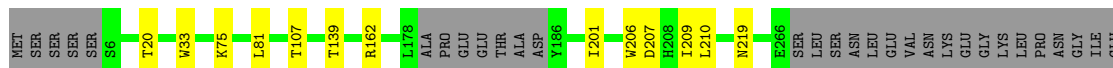
- Molecule 1: Flavonol sulfotransferase-like

Chain 8-A:



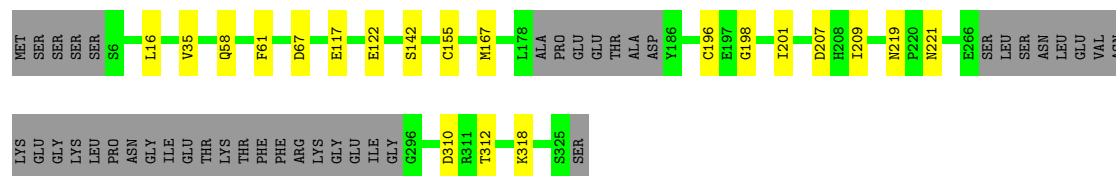
- Molecule 1: Flavonol sulfotransferase-like

Chain 9-A:



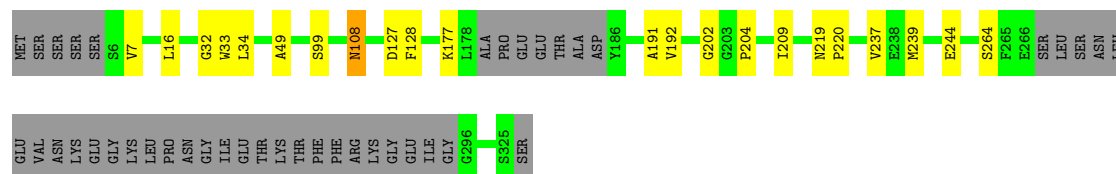
- Molecule 1: Flavonol sulfotransferase-like

Chain 10-A:



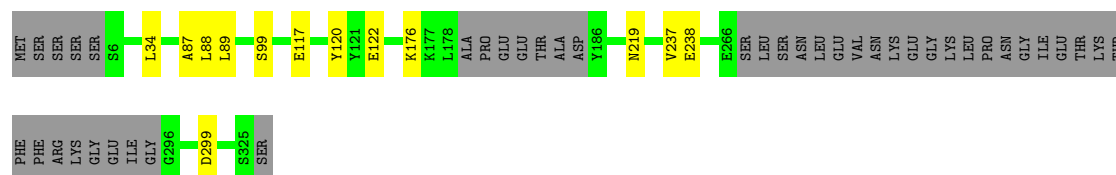
- Molecule 1: Flavonol sulfotransferase-like

Chain 11-A:



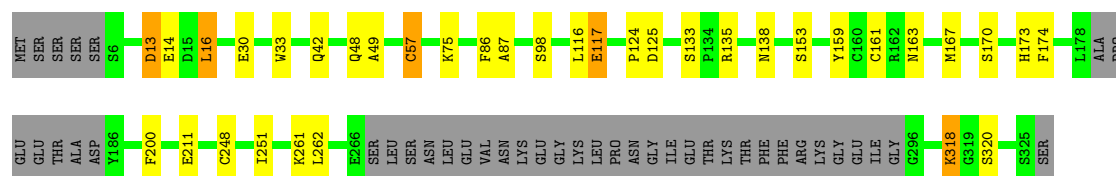
- Molecule 1: Flavonol sulfotransferase-like

Chain 12-A:



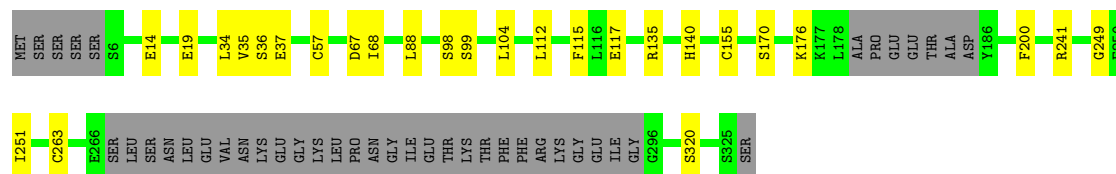
- Molecule 1: Flavonol sulfotransferase-like

Chain 13-A:



- Molecule 1: Flavonol sulfotransferase-like

Chain 14-A:



- Molecule 1: Flavonol sulfotransferase-like

Chain 15-A:

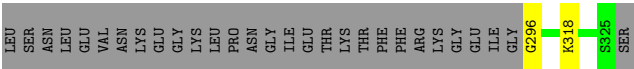
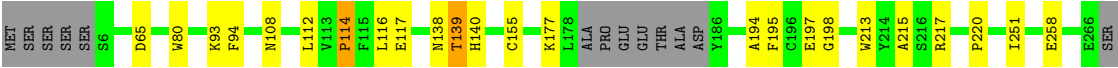






● Molecule 1: Flavonol sulfotransferase-like

Chain 16-A:



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.48Å 120.90Å 74.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 1.90	Depositor
% Data completeness (in resolution range)	99.3 (19.79-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.157 , 0.217	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.121	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 32629 reflections	Xtriage
Total number of atoms	40432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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

All (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
1	2-A	160	CYS	CB-SG	5.72	1.92	1.82
1	13-A	57	CYS	CB-SG	-5.53	1.72	1.81
1	8-A	117	GLU	CB-CG	-5.23	1.42	1.52
1	13-A	117	GLU	CB-CG	-5.18	1.42	1.52

All (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
1	2-A	16	LEU	CA-CB-CG	-6.65	100.00	115.30
1	14-A	112	LEU	CA-CB-CG	6.37	129.95	115.30
1	1-A	57	CYS	CA-CB-SG	6.27	125.29	114.00
1	14-A	67	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	13-A	133	SER	N-CA-C	-6.14	94.42	111.00
1	10-A	67	ASP	CB-CG-OD1	6.07	123.77	118.30
1	10-A	16	LEU	CA-CB-CG	-5.72	102.13	115.30
1	5-A	75	LYS	N-CA-C	5.67	126.30	111.00
1	10-A	196	CYS	CA-CB-SG	-5.63	103.87	114.00
1	13-A	163	ASN	N-CA-C	-5.59	95.90	111.00
1	1-A	246	LEU	CA-CB-CG	5.47	127.89	115.30
1	14-A	104	LEU	CA-CB-CG	-5.47	102.72	115.30
1	13-A	75	LYS	N-CA-C	5.47	125.76	111.00
1	13-A	116	LEU	N-CA-C	5.45	125.70	111.00
1	6-A	16	LEU	CA-CB-CG	-5.44	102.80	115.30
1	15-A	217	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	15-A	75	LYS	N-CA-C	5.36	125.48	111.00
1	14-A	320	SER	N-CA-C	5.31	125.35	111.00
1	15-A	133	SER	N-CA-C	-5.31	96.67	111.00
1	11-A	202	GLY	N-CA-C	5.26	126.26	113.10
1	9-A	162	ARG	N-CA-C	-5.16	97.06	111.00
1	16-A	296	GLY	N-CA-C	-5.11	100.32	113.10

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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
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	1
1	14-A	2306	0	2277	0	1
1	15-A	2306	0	2277	0	1
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1
3	14-A	214	0	0	0	1
3	15-A	214	0	0	0	1
3	16-A	214	0	0	0	0
All	All	40432	0	36465	0	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:GLU:OE2	3:A:1095:HOH:O[6_654]	1.97	0.23
1:A:14:GLU:OE2	3:A:1086:HOH:O[3_655]	2.04	0.16
1:A:125:ASP:OD2	3:A:980:HOH:O[3_655]	2.16	0.04

## 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%)	5	0
1	3-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	10	2
1	4-A	278/326 (85%)	258 (93%)	14 (5%)	6 (2%)	10	2
1	5-A	278/326 (85%)	244 (88%)	25 (9%)	9 (3%)	6	1
1	6-A	278/326 (85%)	256 (92%)	15 (5%)	7 (2%)	9	1
1	7-A	278/326 (85%)	252 (91%)	17 (6%)	9 (3%)	6	1
1	8-A	278/326 (85%)	263 (95%)	14 (5%)	1 (0%)	43	29
1	9-A	278/326 (85%)	245 (88%)	28 (10%)	5 (2%)	13	3
1	10-A	278/326 (85%)	239 (86%)	33 (12%)	6 (2%)	10	2
1	11-A	278/326 (85%)	239 (86%)	26 (9%)	13 (5%)	4	0
1	12-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	10	2
1	13-A	278/326 (85%)	238 (86%)	25 (9%)	15 (5%)	3	0
1	14-A	278/326 (85%)	240 (86%)	32 (12%)	6 (2%)	10	2
1	15-A	278/326 (85%)	236 (85%)	34 (12%)	8 (3%)	7	1
1	16-A	278/326 (85%)	240 (86%)	24 (9%)	14 (5%)	3	0
All	All	4448/5216 (85%)	3915 (88%)	390 (9%)	143 (3%)	6	1

All (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
1	1-A	141	ILE
1	1-A	144	LEU
1	1-A	155	CYS

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Mol	Chain	Res	Type
1	1-A	201	ILE
1	1-A	209	ILE
1	2-A	34	LEU
1	2-A	61	PHE
1	2-A	124	PRO
1	2-A	228	TYR
1	3-A	99	SER
1	4-A	306	ALA
1	5-A	37	GLU
1	6-A	51	LEU
1	6-A	247	GLU
1	9-A	210	LEU
1	10-A	61	PHE
1	11-A	99	SER
1	12-A	87	ALA
1	12-A	88	LEU
1	13-A	48	GLN
1	13-A	211	GLU
1	13-A	318	LYS
1	14-A	34	LEU
1	14-A	99	SER
1	14-A	249	GLY
1	14-A	263	CYS
1	15-A	49	ALA
1	15-A	99	SER
1	15-A	132	PRO
1	16-A	155	CYS
1	16-A	195	PHE
1	16-A	215	ALA
1	16-A	220	PRO
1	1-A	12	GLY
1	1-A	21	ARG
1	1-A	99	SER
1	1-A	143	HIS
1	1-A	298	ARG
1	2-A	49	ALA
1	2-A	130	SER
1	2-A	221	ASN
1	3-A	298	ARG
1	4-A	19	GLU
1	4-A	248	CYS
1	4-A	265	PHE

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Mol	Chain	Res	Type
1	5-A	127	ASP
1	5-A	263	CYS
1	6-A	108	ASN
1	7-A	193	GLU
1	7-A	249	GLY
1	9-A	20	THR
1	9-A	201	ILE
1	11-A	33	TRP
1	11-A	127	ASP
1	11-A	264	SER
1	12-A	34	LEU
1	12-A	237	VAL
1	13-A	87	ALA
1	13-A	153	SER
1	13-A	261	LYS
1	13-A	262	LEU
1	14-A	135	ARG
1	14-A	176	LYS
1	15-A	177	LYS
1	1-A	31	LYS
1	1-A	36	SER
1	1-A	57	CYS
1	1-A	313	ILE
1	2-A	155	CYS
1	3-A	109	PRO
1	6-A	53	GLY
1	6-A	246	LEU
1	7-A	142	SER
1	7-A	264	SER
1	8-A	306	ALA
1	9-A	206	TRP
1	9-A	209	ILE
1	10-A	58	GLN
1	10-A	207	ASP
1	11-A	32	GLY
1	11-A	177	LYS
1	11-A	191	ALA
1	11-A	237	VAL
1	12-A	99	SER
1	12-A	238	GLU
1	13-A	13	ASP
1	16-A	116	LEU

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Mol	Chain	Res	Type
1	16-A	213	TRP
1	16-A	318	LYS
1	1-A	26	SER
1	2-A	84	LEU
1	3-A	17	THR
1	3-A	143	HIS
1	3-A	265	PHE
1	5-A	33	TRP
1	6-A	25	SER
1	7-A	177	LYS
1	7-A	206	TRP
1	7-A	298	ARG
1	11-A	49	ALA
1	11-A	108	ASN
1	13-A	86	PHE
1	13-A	124	PRO
1	13-A	320	SER
1	15-A	88	LEU
1	15-A	95	PRO
1	16-A	139	THR
1	16-A	177	LYS
1	16-A	197	GLU
1	1-A	68	ILE
1	1-A	205	PHE
1	5-A	35	VAL
1	5-A	74	PRO
1	6-A	52	GLN
1	10-A	318	LYS
1	13-A	167	MET
1	16-A	112	LEU
1	16-A	194	ALA
1	5-A	36	SER
1	5-A	201	ILE
1	7-A	77	GLY
1	7-A	108	ASN
1	11-A	192	VAL
1	13-A	14	GLU
1	13-A	42	GLN
1	13-A	49	ALA
1	15-A	77	GLY
1	4-A	249	GLY
1	10-A	201	ILE

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Mol	Chain	Res	Type
1	15-A	146	LEU
1	2-A	209	ILE
1	4-A	146	LEU
1	5-A	209	ILE
1	11-A	220	PRO
1	16-A	198	GLY
1	10-A	198	GLY
1	16-A	114	PRO
1	11-A	204	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	258/294 (88%)	237 (92%)	21 (8%)	17	6
1	2-A	258/294 (88%)	251 (97%)	7 (3%)	57	47
1	3-A	258/294 (88%)	247 (96%)	11 (4%)	40	26
1	4-A	258/294 (88%)	248 (96%)	10 (4%)	43	30
1	5-A	258/294 (88%)	246 (95%)	12 (5%)	36	22
1	6-A	258/294 (88%)	251 (97%)	7 (3%)	57	47
1	7-A	258/294 (88%)	251 (97%)	7 (3%)	57	47
1	8-A	258/294 (88%)	252 (98%)	6 (2%)	63	55
1	9-A	258/294 (88%)	251 (97%)	7 (3%)	57	47
1	10-A	258/294 (88%)	247 (96%)	11 (4%)	40	26
1	11-A	258/294 (88%)	250 (97%)	8 (3%)	52	41
1	12-A	258/294 (88%)	252 (98%)	6 (2%)	63	55
1	13-A	258/294 (88%)	241 (93%)	17 (7%)	24	11
1	14-A	258/294 (88%)	242 (94%)	16 (6%)	26	12
1	15-A	258/294 (88%)	243 (94%)	15 (6%)	28	15
1	16-A	258/294 (88%)	247 (96%)	11 (4%)	40	26
All	All	4128/4704 (88%)	3956 (96%)	172 (4%)	40	27

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	7	VAL
1	1-A	17	THR
1	1-A	19	GLU
1	1-A	20	THR
1	1-A	37	GLU
1	1-A	89	LEU
1	1-A	96	VAL
1	1-A	103	PRO
1	1-A	117	GLU
1	1-A	126	PHE
1	1-A	138	ASN
1	1-A	142	SER
1	1-A	145	SER
1	1-A	148	GLU
1	1-A	149	SER
1	1-A	155	CYS
1	1-A	217	ARG
1	1-A	219	ASN
1	1-A	246	LEU
1	1-A	254	GLU
1	1-A	265	PHE
1	2-A	16	LEU
1	2-A	33	TRP
1	2-A	35	VAL
1	2-A	92	HIS
1	2-A	117	GLU
1	2-A	176	LYS
1	2-A	219	ASN
1	3-A	33	TRP
1	3-A	41	PHE
1	3-A	70	LEU
1	3-A	98	SER
1	3-A	108	ASN
1	3-A	109	PRO
1	3-A	176	LYS
1	3-A	186	TYR
1	3-A	219	ASN
1	3-A	265	PHE
1	3-A	298	ARG
1	4-A	7	VAL
1	4-A	26	SER
1	4-A	35	VAL

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Mol	Chain	Res	Type
1	4-A	72	THR
1	4-A	219	ASN
1	4-A	253	GLU
1	4-A	258	GLU
1	4-A	265	PHE
1	4-A	298	ARG
1	4-A	310	ASP
1	5-A	33	TRP
1	5-A	62	GLU
1	5-A	68	ILE
1	5-A	73	ASN
1	5-A	74	PRO
1	5-A	76	SER
1	5-A	78	THR
1	5-A	117	GLU
1	5-A	128	PHE
1	5-A	142	SER
1	5-A	219	ASN
1	5-A	227	THR
1	6-A	16	LEU
1	6-A	33	TRP
1	6-A	62	GLU
1	6-A	126	PHE
1	6-A	201	ILE
1	6-A	219	ASN
1	6-A	303	GLU
1	7-A	66	SER
1	7-A	73	ASN
1	7-A	133	SER
1	7-A	176	LYS
1	7-A	219	ASN
1	7-A	298	ARG
1	7-A	304	SER
1	8-A	13	ASP
1	8-A	16	LEU
1	8-A	164	PRO
1	8-A	176	LYS
1	8-A	219	ASN
1	8-A	265	PHE
1	9-A	33	TRP
1	9-A	75	LYS
1	9-A	81	LEU

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Mol	Chain	Res	Type
1	9-A	107	THR
1	9-A	139	THR
1	9-A	207	ASP
1	9-A	219	ASN
1	10-A	35	VAL
1	10-A	117	GLU
1	10-A	122	GLU
1	10-A	142	SER
1	10-A	155	CYS
1	10-A	167	MET
1	10-A	209	ILE
1	10-A	219	ASN
1	10-A	221	ASN
1	10-A	310	ASP
1	10-A	312	THR
1	11-A	7	VAL
1	11-A	34	LEU
1	11-A	108	ASN
1	11-A	128	PHE
1	11-A	209	ILE
1	11-A	219	ASN
1	11-A	239	MET
1	11-A	244	GLU
1	12-A	89	LEU
1	12-A	117	GLU
1	12-A	122	GLU
1	12-A	176	LYS
1	12-A	219	ASN
1	12-A	299	ASP
1	13-A	13	ASP
1	13-A	16	LEU
1	13-A	30	GLU
1	13-A	33	TRP
1	13-A	57	CYS
1	13-A	98	SER
1	13-A	117	GLU
1	13-A	135	ARG
1	13-A	138	ASN
1	13-A	161	CYS
1	13-A	170	SER
1	13-A	173	HIS
1	13-A	174	PHE

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Mol	Chain	Res	Type
1	13-A	200	PHE
1	13-A	248	CYS
1	13-A	251	ILE
1	13-A	318	LYS
1	14-A	19	GLU
1	14-A	35	VAL
1	14-A	36	SER
1	14-A	37	GLU
1	14-A	57	CYS
1	14-A	68	ILE
1	14-A	88	LEU
1	14-A	98	SER
1	14-A	115	PHE
1	14-A	117	GLU
1	14-A	140	HIS
1	14-A	155	CYS
1	14-A	170	SER
1	14-A	200	PHE
1	14-A	241	ARG
1	14-A	251	ILE
1	15-A	29	LYS
1	15-A	42	GLN
1	15-A	90	ASN
1	15-A	95	PRO
1	15-A	112	LEU
1	15-A	148	GLU
1	15-A	153	SER
1	15-A	161	CYS
1	15-A	235	THR
1	15-A	242	ILE
1	15-A	247	GLU
1	15-A	258	GLU
1	15-A	265	PHE
1	15-A	297	TRP
1	15-A	304	SER
1	16-A	80	TRP
1	16-A	93	LYS
1	16-A	108	ASN
1	16-A	114	PRO
1	16-A	117	GLU
1	16-A	138	ASN
1	16-A	139	THR

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Mol	Chain	Res	Type
1	16-A	140	HIS
1	16-A	217	ARG
1	16-A	251	ILE
1	16-A	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	42	GLN
1	1-A	48	GLN
1	1-A	52	GLN
1	1-A	101	ASN
1	1-A	108	ASN
1	1-A	110	HIS
1	1-A	138	ASN
1	1-A	219	ASN
1	2-A	42	GLN
1	2-A	52	GLN
1	2-A	101	ASN
1	2-A	108	ASN
1	2-A	110	HIS
1	2-A	138	ASN
1	2-A	140	HIS
1	2-A	234	GLN
1	3-A	42	GLN
1	3-A	108	ASN
1	3-A	143	HIS
1	3-A	219	ASN
1	3-A	221	ASN
1	4-A	42	GLN
1	4-A	108	ASN
1	4-A	110	HIS
1	4-A	173	HIS
1	4-A	219	ASN
1	5-A	42	GLN
1	5-A	73	ASN
1	5-A	108	ASN
1	5-A	110	HIS
1	5-A	173	HIS
1	5-A	221	ASN
1	5-A	234	GLN
1	6-A	42	GLN

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Mol	Chain	Res	Type
1	6-A	52	GLN
1	6-A	101	ASN
1	6-A	108	ASN
1	6-A	110	HIS
1	6-A	219	ASN
1	6-A	221	ASN
1	7-A	42	GLN
1	7-A	73	ASN
1	7-A	108	ASN
1	7-A	110	HIS
1	7-A	219	ASN
1	8-A	42	GLN
1	8-A	90	ASN
1	8-A	108	ASN
1	8-A	110	HIS
1	8-A	219	ASN
1	8-A	221	ASN
1	9-A	42	GLN
1	9-A	101	ASN
1	9-A	108	ASN
1	9-A	110	HIS
1	9-A	138	ASN
1	9-A	219	ASN
1	9-A	221	ASN
1	10-A	42	GLN
1	10-A	52	GLN
1	10-A	58	GLN
1	10-A	90	ASN
1	10-A	101	ASN
1	10-A	108	ASN
1	10-A	110	HIS
1	10-A	143	HIS
1	10-A	219	ASN
1	10-A	221	ASN
1	11-A	73	ASN
1	11-A	101	ASN
1	11-A	110	HIS
1	11-A	138	ASN
1	11-A	219	ASN
1	11-A	221	ASN
1	12-A	18	GLN
1	12-A	42	GLN

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Mol	Chain	Res	Type
1	12-A	138	ASN
1	12-A	143	HIS
1	12-A	219	ASN
1	12-A	221	ASN
1	13-A	90	ASN
1	13-A	108	ASN
1	13-A	163	ASN
1	13-A	234	GLN
1	14-A	42	GLN
1	14-A	48	GLN
1	14-A	52	GLN
1	14-A	101	ASN
1	14-A	108	ASN
1	14-A	110	HIS
1	14-A	140	HIS
1	14-A	173	HIS
1	14-A	234	GLN
1	15-A	18	GLN
1	15-A	42	GLN
1	15-A	90	ASN
1	15-A	101	ASN
1	15-A	108	ASN
1	15-A	140	HIS
1	15-A	234	GLN
1	16-A	42	GLN
1	16-A	52	GLN
1	16-A	108	ASN
1	16-A	110	HIS
1	16-A	143	HIS
1	16-A	221	ASN
1	16-A	234	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	1-A	901	-	6,6,6	0.88	0	7,7,7	1.06	0
2	MLA	10-A	901	-	6,6,6	1.36	1 (16%)	7,7,7	1.18	1 (14%)
2	MLA	11-A	901	-	6,6,6	1.76	2 (33%)	7,7,7	1.30	1 (14%)
2	MLA	12-A	901	-	6,6,6	1.18	1 (16%)	7,7,7	1.03	0
2	MLA	13-A	901	-	6,6,6	1.66	1 (16%)	7,7,7	1.28	1 (14%)
2	MLA	14-A	901	-	6,6,6	1.43	1 (16%)	7,7,7	1.41	1 (14%)
2	MLA	15-A	901	-	6,6,6	0.92	0	7,7,7	0.93	0
2	MLA	16-A	901	-	6,6,6	1.97	2 (33%)	7,7,7	1.51	1 (14%)
2	MLA	2-A	901	-	6,6,6	1.12	1 (16%)	7,7,7	1.31	1 (14%)
2	MLA	3-A	901	-	6,6,6	1.38	1 (16%)	7,7,7	1.27	1 (14%)
2	MLA	4-A	901	-	6,6,6	1.65	1 (16%)	7,7,7	1.21	0
2	MLA	5-A	901	-	6,6,6	1.11	1 (16%)	7,7,7	1.23	0
2	MLA	6-A	901	-	6,6,6	0.98	0	7,7,7	1.30	1 (14%)
2	MLA	7-A	901	-	6,6,6	0.94	0	7,7,7	1.12	0
2	MLA	8-A	901	-	6,6,6	1.38	1 (16%)	7,7,7	1.27	0
2	MLA	9-A	901	-	6,6,6	0.96	0	7,7,7	1.22	0

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	1-A	901	-	-	0/4/4/4	0/0/0/0

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	16-A	901	MLA	C2-C3	3.87	1.56	1.51
2	13-A	901	MLA	C2-C1	3.84	1.56	1.51
2	11-A	901	MLA	C2-C3	3.18	1.55	1.51
2	8-A	901	MLA	C2-C1	3.00	1.55	1.51
2	4-A	901	MLA	C2-C1	2.95	1.55	1.51
2	11-A	901	MLA	O1A-C1	2.65	1.40	1.30
2	10-A	901	MLA	C2-C1	2.54	1.54	1.51
2	14-A	901	MLA	C2-C1	2.54	1.54	1.51
2	12-A	901	MLA	C2-C3	-2.53	1.47	1.51
2	2-A	901	MLA	C2-C3	2.44	1.54	1.51
2	3-A	901	MLA	C2-C3	2.32	1.54	1.51
2	5-A	901	MLA	C2-C1	2.31	1.54	1.51
2	16-A	901	MLA	C2-C1	2.17	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-A	901	MLA	O1A-C1-O1B	-2.32	117.39	123.30
2	2-A	901	MLA	C3-C2-C1	2.32	119.11	112.77
2	14-A	901	MLA	O1A-C1-O1B	-2.22	117.65	123.30
2	6-A	901	MLA	O1A-C1-O1B	-2.22	117.66	123.30
2	11-A	901	MLA	O3B-C3-O3A	-2.19	117.73	123.30
2	13-A	901	MLA	O1A-C1-O1B	-2.16	117.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-A	901	MLA	O3B-C3-O3A	-2.04	118.11	123.30
2	3-A	901	MLA	O1A-C1-O1B	-2.00	118.20	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.