



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2016 – 09:00 PM EDT

PDB ID : 5KOE  
Title : The structure of Arabidopsis thaliana FUT1 in complex with XXLG  
Authors : Alahuhta, P.M.; Lunin, V.V.  
Deposited on : 2016-06-30  
Resolution : 1.79 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

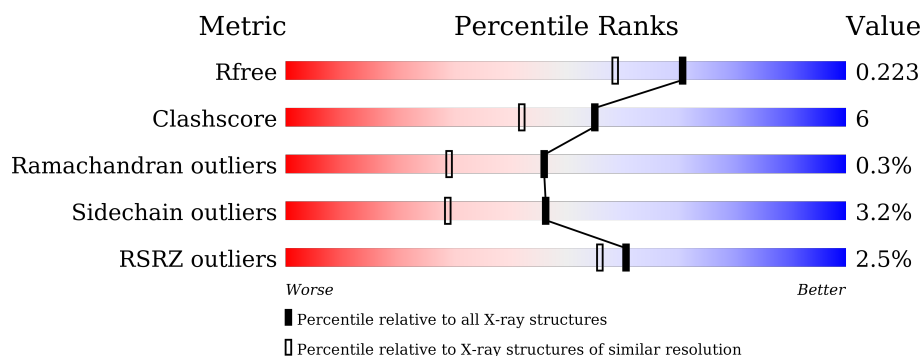
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

i

## X-RAY DIFFRACTION

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div></div> <div>2%</div> <div>82%</div> <div>9%</div> <div>6%</div> </div>
1	B	476	<div> <div></div> <div>3%</div> <div>79%</div> <div>14%</div> <div>5%</div> </div>
1	C	476	<div> <div></div> <div>3%</div> <div>86%</div> <div>10%</div> <div></div> </div>
1	D	476	<div> <div></div> <div>2%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	A	601	-	-	-	X
2	MES	A	602	-	-	-	X
2	MES	C	602	-	-	-	X
5	EDO	C	610	-	-	-	X
6	GAL	A	614	-	-	-	X
7	XYS	A	621	-	-	-	X
9	GOL	D	607	-	-	X	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17403 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.

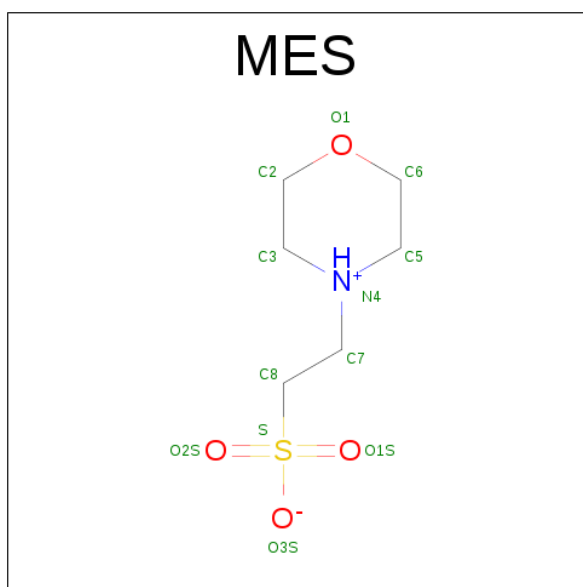
- Molecule 1 is a protein called Galactoside 2-alpha-L-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	17	0
			3700	2379	616	683	22			
1	B	452	Total	C	N	O	S	0	19	0
			3772	2420	625	705	22			
1	C	458	Total	C	N	O	S	0	17	0
			3819	2443	647	707	22			
1	D	454	Total	C	N	O	S	0	19	0
			3768	2416	632	696	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLY	-	expression tag	UNP Q9SWH5
B	83	GLY	-	expression tag	UNP Q9SWH5
C	83	GLY	-	expression tag	UNP Q9SWH5
D	83	GLY	-	expression tag	UNP Q9SWH5

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

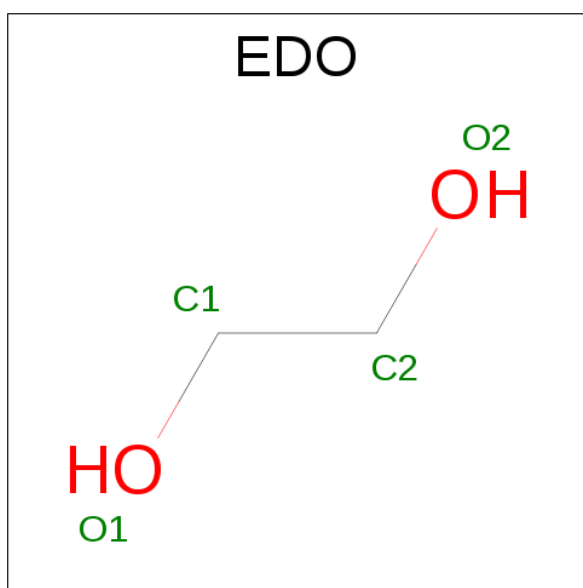
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cl	0	0
			4	4		
3	A	8	Total	Cl	0	0
			8	8		
3	D	3	Total	Cl	0	0
			3	3		
3	C	4	Total	Cl	0	0
			4	4		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

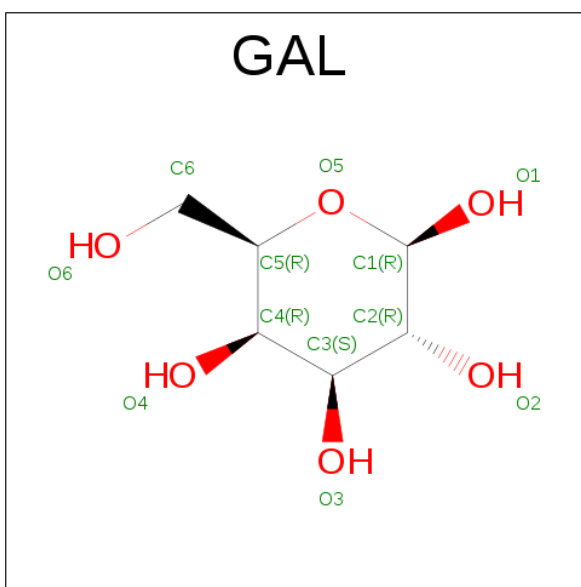
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total K 2 2	0	0
4	A	2	Total K 2 2	0	0
4	D	1	Total K 1 1	0	0
4	C	3	Total K 3 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



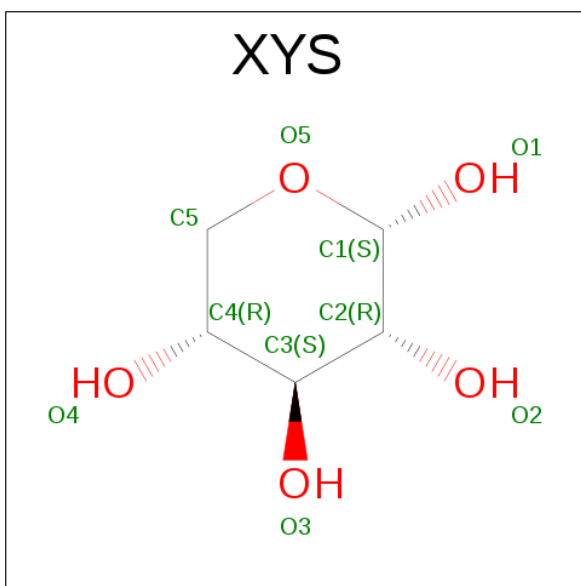
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 8 4 4	0	1

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



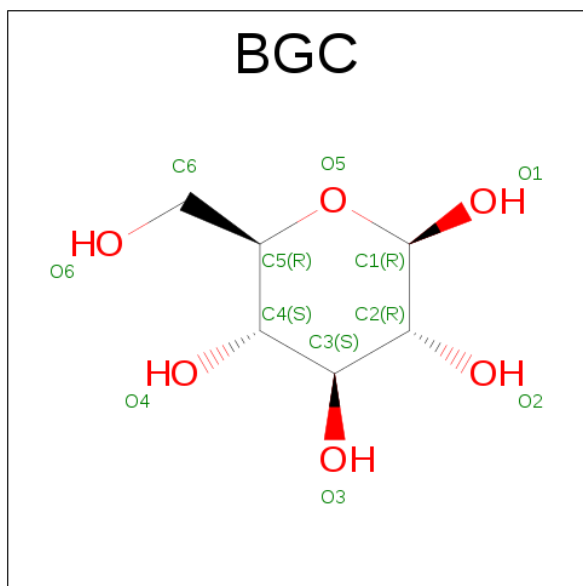
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is XYLOPYRANOSE (three-letter code: XYS) (formula:  $C_5H_{10}O_5$ ).



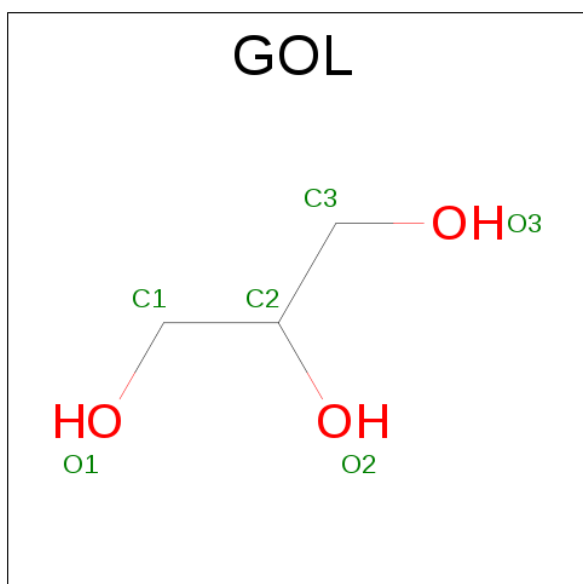
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	5	4		
7	A	1	Total	C	O	0	0
			9	5	4		
7	A	1	Total	C	O	0	0
			9	5	4		

- Molecule 8 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			12	6	6		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

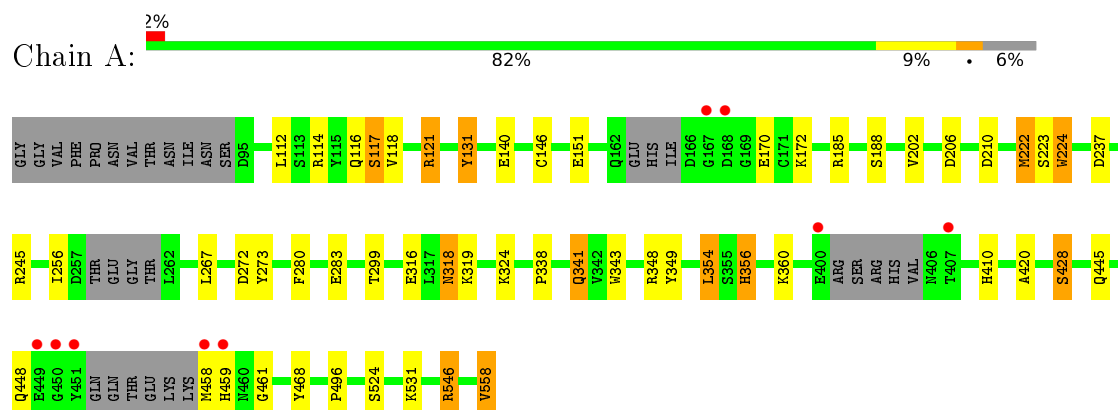
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	544	Total	O	0	24
			568	568		
10	B	492	Total	O	0	14
			506	506		
10	C	546	Total	O	0	18
			564	564		
10	D	495	Total	O	0	13
			508	508		

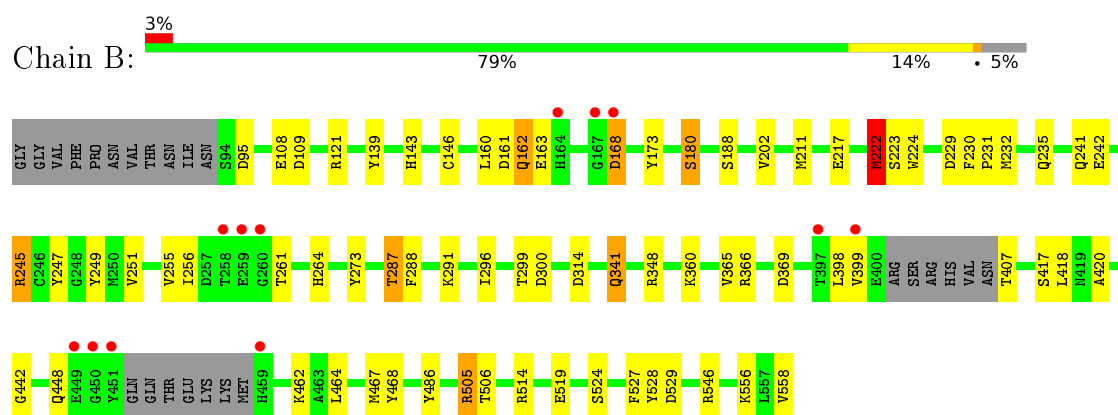
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

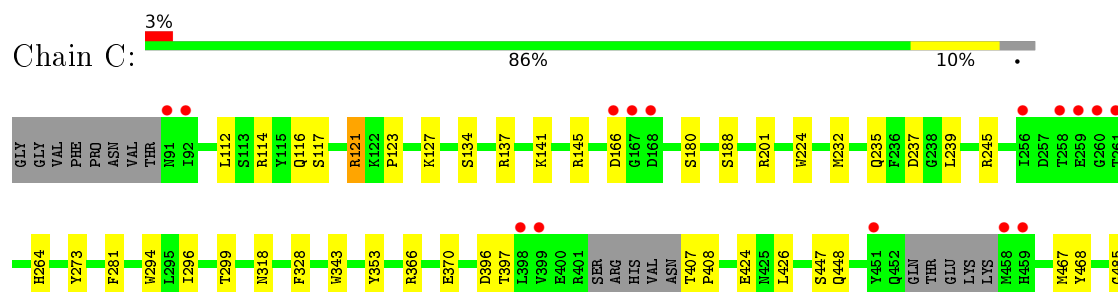
- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

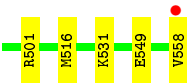


- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase

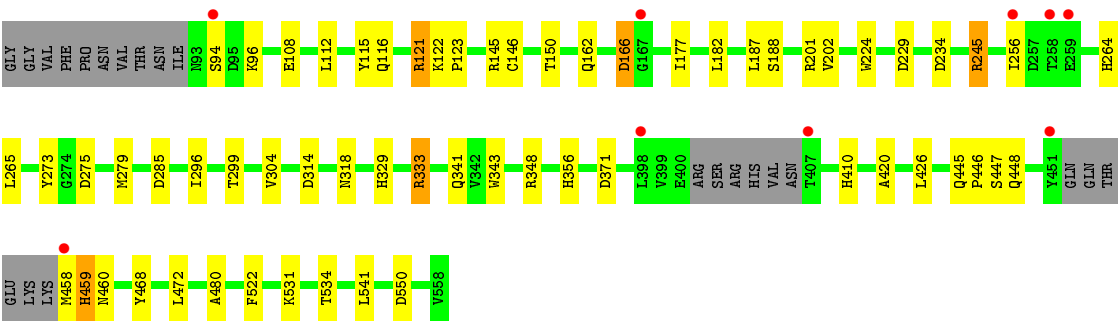
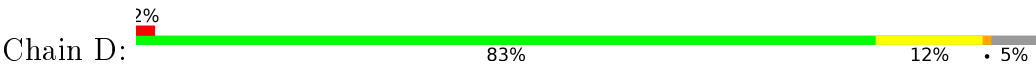


- Molecule 1: Galactoside 2-alpha-L-fucosyltransferase





● Molecule 1: Galactoside 2-alpha-L-fucosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.75Å 80.15Å 157.62Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	157.53 – 1.79 73.54 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (157.53-1.79) 99.6 (73.54-1.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.166 , 0.217 0.174 , 0.223	Depositor DCC
$R_{free}$ test set	9299 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l 0.010 for -k,-h,-l 0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1476e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical 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: GOL, BGC, CL, K, EDO, XYS, MES, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.23	12/3801 (0.3%)	1.10	12/5147 (0.2%)
1	B	1.19	9/3876 (0.2%)	1.14	23/5253 (0.4%)
1	C	1.20	8/3925 (0.2%)	1.11	16/5321 (0.3%)
1	D	1.14	0/3876	1.10	18/5258 (0.3%)
All	All	1.19	29/15478 (0.2%)	1.11	69/20979 (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	B	0	1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	TYR	CE2-CZ	-6.46	1.30	1.38
1	A	428	SER	CB-OG	-6.41	1.33	1.42
1	A	117	SER	CB-OG	5.86	1.49	1.42
1	B	249	TYR	CB-CG	-5.79	1.43	1.51
1	A	343	TRP	CB-CG	-5.78	1.39	1.50

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222[A]	MET	CG-SD-CE	9.57	115.51	100.20
1	B	222[B]	MET	CG-SD-CE	9.57	115.51	100.20
1	C	145	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	245	ARG	NE-CZ-NH1	-8.93	115.83	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASP	CB-CG-OD1	8.02	125.52	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	ASP	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3700	0	3573	44	0
1	B	3772	0	3622	51	0
1	C	3819	0	3663	36	0
1	D	3768	0	3608	46	0
2	A	24	0	26	1	0
2	C	24	0	26	1	0
2	D	12	0	13	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	3	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	6	0	0
5	C	4	0	6	2	0
5	D	8	0	12	0	0
6	A	11	0	10	0	0
7	A	27	0	23	0	0
8	A	45	0	36	0	0
9	C	6	0	8	2	0
9	D	6	0	8	5	0
10	A	568	0	0	27	0
10	B	506	0	0	17	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	564	0	0	18	1
10	D	508	0	0	24	0
All	All	17403	0	14640	186	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516[A]:MET:CE	1:C:558[A]:VAL:HG11	1.49	1.41
9:D:607:GOL:O3	10:D:702:HOH:O	1.54	1.24
1:B:527[A]:PHE:CE1	10:B:730:HOH:O	1.76	1.22
1:C:121[B]:ARG:CG	10:C:1095:HOH:O	1.84	1.22
1:B:527[A]:PHE:CD1	10:B:730:HOH:O	1.74	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:918:HOH:O	10:C:1143:HOH:O[1_655]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/476 (95%)	441 (98%)	11 (2%)	0	100	100
1	B	464/476 (98%)	444 (96%)	17 (4%)	3 (1%)	30	14
1	C	469/476 (98%)	457 (97%)	11 (2%)	1 (0%)	52	35
1	D	466/476 (98%)	449 (96%)	14 (3%)	3 (1%)	30	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1851/1904 (97%)	1791 (97%)	53 (3%)	7 (0%)	46 23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	459[A]	HIS
1	D	459[B]	HIS
1	C	180	SER
1	D	94	SER
1	B	168[A]	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	407/423 (96%)	390 (96%)	17 (4%)	36 18
1	B	416/423 (98%)	396 (95%)	20 (5%)	31 14
1	C	419/423 (99%)	409 (98%)	10 (2%)	57 41
1	D	411/423 (97%)	400 (97%)	11 (3%)	52 36
All	All	1653/1692 (98%)	1595 (96%)	58 (4%)	46 25

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	255	VAL
1	B	399	VAL
1	D	245	ARG
1	B	273	TYR
1	B	341[A]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:



Mol	Chain	Res	Type
1	B	425	ASN
1	D	301	ASN
1	C	276	HIS
1	A	445	GLN
1	C	93	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 27 are monoatomic - leaving 19 for Mogul analysis.

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	MES	A	601	-	12,12,12	1.53	1 (8%)	15,16,16	1.62	4 (26%)
2	MES	A	602	-	12,12,12	1.75	1 (8%)	15,16,16	1.66	3 (20%)
5	EDO	A	613	-	3,3,3	0.39	0	2,2,2	0.76	0
6	GAL	A	614	7	11,11,12	1.98	2 (18%)	15,15,17	1.12	1 (6%)
7	XYS	A	615	8,6	9,9,10	1.68	2 (22%)	12,12,14	1.23	2 (16%)
8	BGC	A	616	8,7	11,11,12	0.90	0	15,15,17	1.21	1 (6%)
8	BGC	A	617	8	12,12,12	0.81	0	17,17,17	1.26	1 (5%)
8	BGC	A	618	8,7	11,11,12	1.13	1 (9%)	15,15,17	1.34	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	XYS	A	619	8	9,9,10	1.60	2 (22%)	12,12,14	1.87	4 (33%)
8	BGC	A	620	8,7	11,11,12	1.11	1 (9%)	15,15,17	0.96	1 (6%)
7	XYS	A	621	8	9,9,10	1.03	0	12,12,14	1.18	1 (8%)
2	MES	C	601	-	12,12,12	1.71	1 (8%)	15,16,16	2.26	4 (26%)
2	MES	C	602	-	12,12,12	2.02	1 (8%)	15,16,16	2.36	6 (40%)
5	EDO	C	610	-	3,3,3	0.48	0	2,2,2	0.76	0
9	GOL	C	611	-	5,5,5	0.31	0	5,5,5	0.56	0
2	MES	D	601	-	12,12,12	2.08	1 (8%)	15,16,16	1.69	2 (13%)
5	EDO	D	606[A]	-	3,3,3	0.59	0	2,2,2	0.14	0
5	EDO	D	606[B]	-	3,3,3	0.48	0	2,2,2	0.29	0
9	GOL	D	607	-	5,5,5	0.23	0	5,5,5	0.54	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	MES	A	601	-	-	0/6/14/14	0/1/1/1
2	MES	A	602	-	-	0/6/14/14	0/1/1/1
5	EDO	A	613	-	-	0/1/1/1	0/0/0/0
6	GAL	A	614	7	-	0/2/19/22	0/1/1/1
7	XYS	A	615	8,6	-	0/0/14/17	0/1/1/1
8	BGC	A	616	8,7	-	0/2/19/22	0/1/1/1
8	BGC	A	617	8	-	0/2/22/22	0/1/1/1
8	BGC	A	618	8,7	-	0/2/19/22	0/1/1/1
7	XYS	A	619	8	-	0/0/14/17	1/1/1/1
8	BGC	A	620	8,7	-	0/2/19/22	0/1/1/1
7	XYS	A	621	8	-	0/0/14/17	0/1/1/1
2	MES	C	601	-	-	0/6/14/14	0/1/1/1
2	MES	C	602	-	-	0/6/14/14	0/1/1/1
5	EDO	C	610	-	-	0/1/1/1	0/0/0/0
9	GOL	C	611	-	-	0/4/4/4	0/0/0/0
2	MES	D	601	-	-	0/6/14/14	0/1/1/1
5	EDO	D	606[A]	-	-	0/1/1/1	0/0/0/0
5	EDO	D	606[B]	-	-	0/1/1/1	0/0/0/0
9	GOL	D	607	-	-	0/4/4/4	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	MES	C8-S	-6.76	1.67	1.77
2	C	602	MES	C8-S	-6.59	1.67	1.77
2	A	602	MES	C8-S	-5.46	1.69	1.77
2	C	601	MES	C8-S	-5.13	1.69	1.77
2	A	601	MES	C8-S	-4.74	1.70	1.77

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MES	O3S-S-O1S	-3.48	103.56	111.26
7	A	619	XYS	C4-C3-C2	-3.40	107.25	111.02
7	A	619	XYS	C1-C2-C3	-3.02	105.89	109.55
7	A	615	XYS	O4-C4-C3	-2.94	104.26	110.19
8	A	618	BGC	C6-C5-C4	-2.82	105.92	112.99

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	619	XYS	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	MES	1	0
2	C	602	MES	1	0
5	C	610	EDO	2	0
9	C	611	GOL	2	0
9	D	607	GOL	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	446/476 (93%)	-0.37	9 (2%) 68 64	9, 19, 45, 82	3 (0%)
1	B	452/476 (94%)	-0.32	12 (2%) 58 53	9, 20, 57, 94	0
1	C	458/476 (96%)	-0.20	16 (3%) 48 42	11, 22, 54, 87	1 (0%)
1	D	454/476 (95%)	-0.22	9 (1%) 68 64	11, 22, 52, 90	1 (0%)
All	All	1810/1904 (95%)	-0.28	46 (2%) 61 56	9, 21, 53, 94	5 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	THR	11.4
1	A	451	TYR	7.1
1	D	256	ILE	6.2
1	C	459	HIS	5.4
1	D	258	THR	5.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	GOL	D	607	6/6	0.87	0.24	8.36	24,28,28,29	6
7	XYS	A	621	9/10	0.89	0.13	6.03	22,24,26,29	9
2	MES	A	601	12/12	0.94	0.12	4.26	25,32,35,36	12
2	MES	A	602	12/12	0.92	0.17	3.46	26,33,39,41	12
6	GAL	A	614	11/12	0.91	0.11	2.96	15,17,19,19	11
2	MES	C	602	12/12	0.88	0.16	2.86	38,44,48,50	12
5	EDO	C	610	4/4	0.90	0.18	2.14	7,7,7,7	4
4	K	B	606	1/1	0.98	0.13	1.88	40,40,40,40	0
4	K	A	612	1/1	0.97	0.12	0.84	38,38,38,38	0
2	MES	D	601	12/12	0.95	0.13	0.80	49,50,52,53	0
2	MES	C	601	12/12	0.96	0.12	0.27	39,43,50,50	0
4	K	C	608	1/1	0.94	0.09	0.02	43,43,43,43	0
5	EDO	D	606[B]	4/4	0.94	0.11	-0.38	15,16,16,16	4
5	EDO	D	606[A]	4/4	0.94	0.11	-0.61	37,41,45,46	4
3	CL	A	603	1/1	0.99	0.05	-0.77	18,18,18,18	0
3	CL	B	602	1/1	0.99	0.05	-1.68	29,29,29,29	0
4	K	A	611	1/1	0.98	0.05	-1.88	20,20,20,20	0
3	CL	D	603	1/1	1.00	0.04	-1.99	26,26,26,26	0
3	CL	A	605	1/1	0.99	0.04	-2.03	29,29,29,29	0
4	K	B	605	1/1	0.99	0.06	-2.39	23,23,23,23	0
4	K	D	605	1/1	0.99	0.04	-2.78	25,25,25,25	0
4	K	C	607	1/1	0.99	0.05	-3.55	26,26,26,26	0
3	CL	A	608	1/1	0.99	0.04	-4.24	27,27,27,27	0
3	CL	A	607	1/1	0.99	0.07	-	44,44,44,44	0
3	CL	A	609	1/1	0.97	0.07	-	42,42,42,42	0
9	GOL	C	611	6/6	0.66	0.27	-	35,36,37,39	6
8	BGC	A	620	11/12	0.88	0.14	-	24,27,31,32	11
3	CL	A	610	1/1	0.94	0.11	-	41,41,41,41	1
3	CL	D	602	1/1	0.99	0.06	-	33,33,33,33	0
3	CL	C	604	1/1	0.99	0.12	-	21,21,21,21	1
3	CL	A	604	1/1	0.98	0.04	-	32,32,32,32	0
8	BGC	A	616	11/12	0.89	0.15	-	25,31,37,39	11
3	CL	B	603	1/1	0.96	0.09	-	48,48,48,48	0
5	EDO	A	613	4/4	0.92	0.15	-	33,34,34,36	4
3	CL	C	606	1/1	0.95	0.08	-	39,39,39,39	0
3	CL	C	603	1/1	0.98	0.04	-	32,32,32,32	0
4	K	C	609	1/1	0.92	0.09	-	40,40,40,40	1
7	XYS	A	615	9/10	0.93	0.12	-	19,24,25,25	9
3	CL	D	604	1/1	0.93	0.08	-	40,40,40,40	0
7	XYS	A	619	9/10	0.68	0.30	-	48,51,55,56	9
3	CL	B	601	1/1	0.97	0.05	-	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	B	604	1/1	0.99	0.05	-	28,28,28,28	0
3	CL	C	605	1/1	0.98	0.07	-	36,36,36,36	0
3	CL	A	606	1/1	0.97	0.08	-	37,37,37,37	0
8	BGC	A	618	11/12	0.88	0.09	-	23,27,34,39	11
8	BGC	A	617	12/12	0.61	0.26	-	46,57,61,63	12

## 6.5 Other polymers [i](#)

There are no such residues in this entry.