



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2016 – 08:43 PM EDT

PDB ID : 5KWK  
Title : The structure of Arabidopsis thaliana FUT1 in complex with GDP  
Authors : Alahuhta, P.M.; Lunin, V.V.  
Deposited on : 2016-07-18  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (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

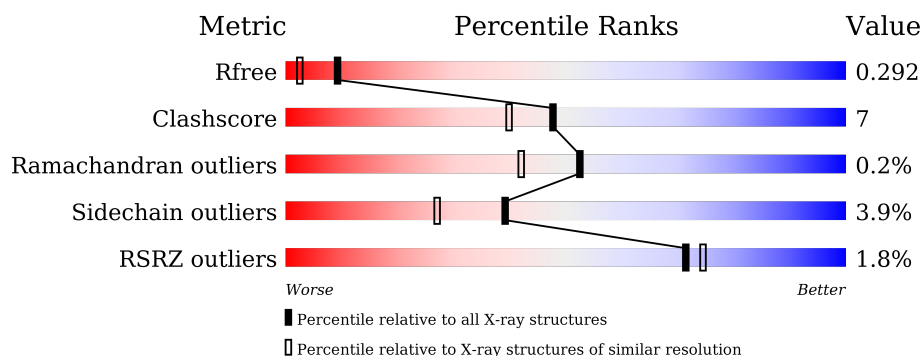
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	B	476	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	603	-	-	X	X
4	EDO	A	605	-	-	-	X
4	EDO	A	606[A]	-	-	-	X
4	EDO	A	606[B]	-	-	-	X
4	EDO	A	607	-	-	-	X
4	EDO	A	608	-	-	-	X
4	EDO	B	606	-	-	-	X
4	EDO	B	607	-	-	-	X
4	EDO	B	608	-	-	-	X
4	EDO	B	610	-	-	-	X
5	GOL	A	611	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8696 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.

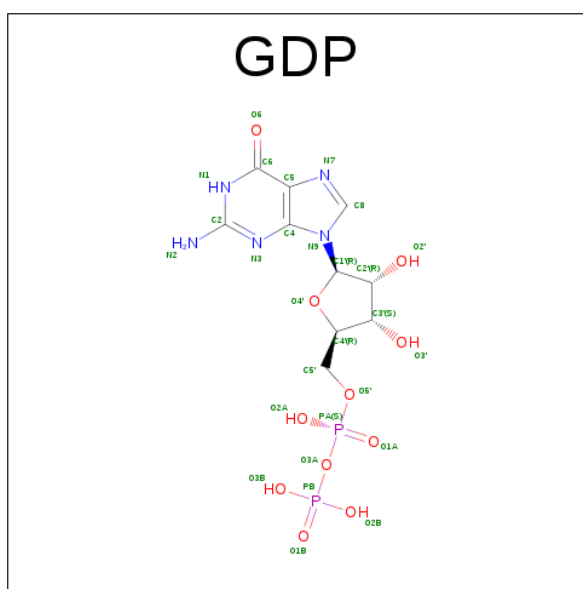
- Molecule 1 is a protein called Galactoside 2- $\alpha$ -L-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	17	0
			3673	2358	616	676	23			
1	B	457	Total	C	N	O	S	0	15	0
			3789	2433	630	703	23			

There are 2 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

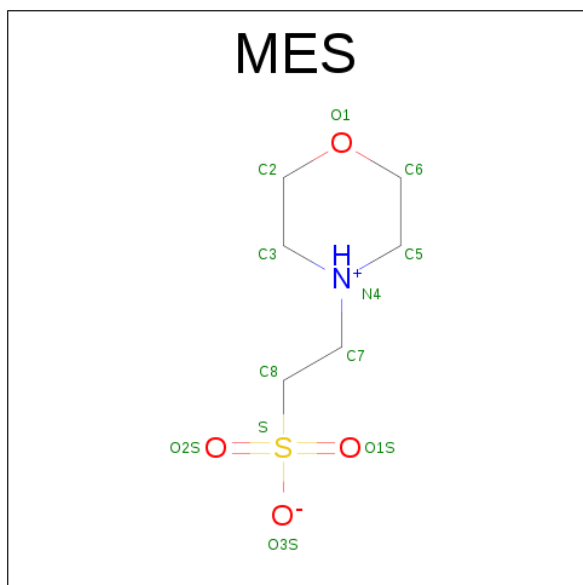
- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



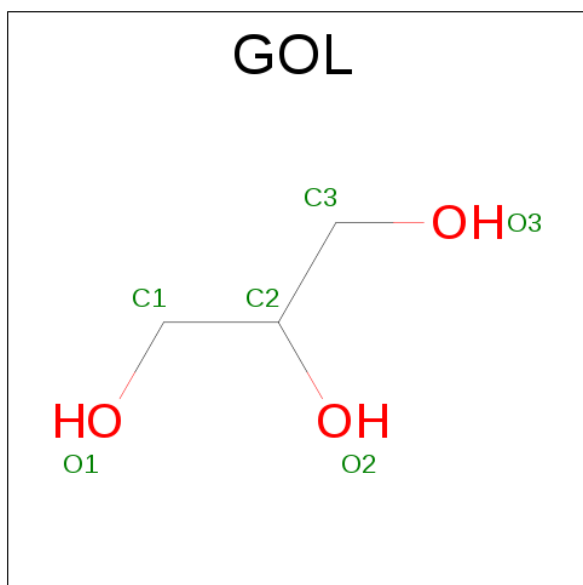
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

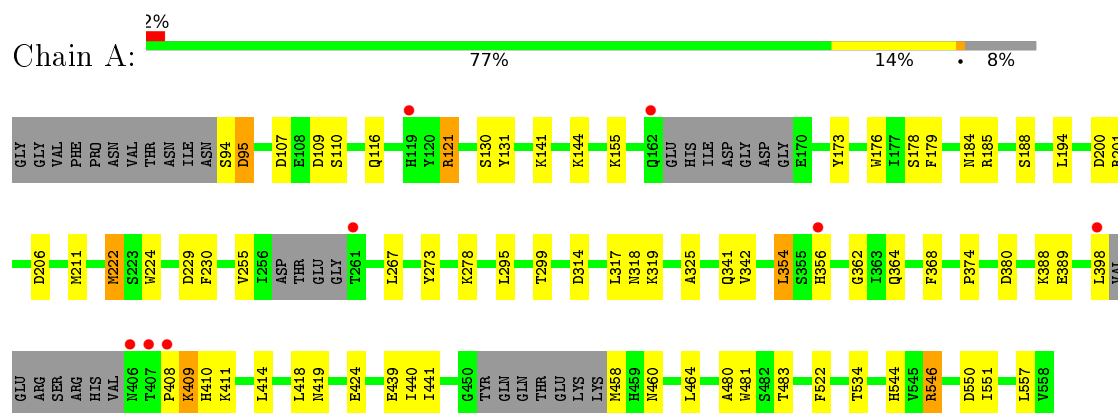
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	541	Total	O	0	29
			570	570		
6	B	491	Total	O	0	15
			506	506		

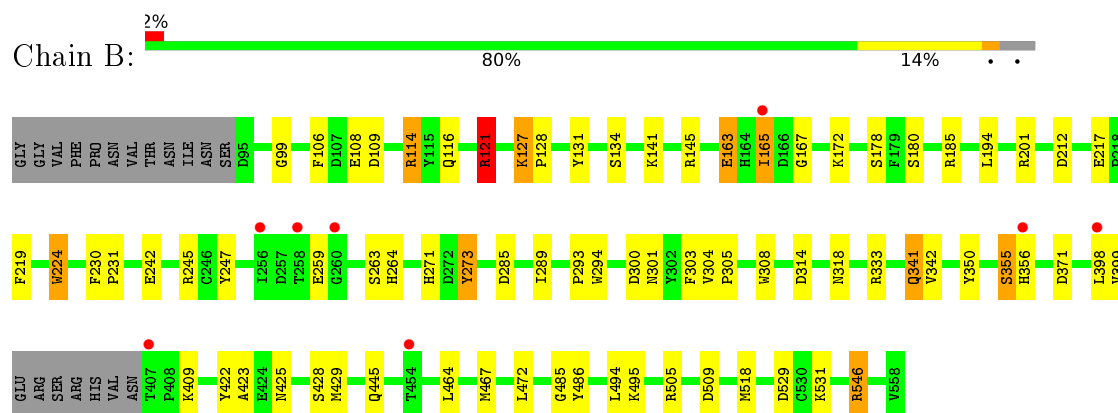
### 3 Residue-property plots [i](#)

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

- Molecule 1: 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, $\alpha$ , $\beta$ , $\gamma$	53.93Å 113.10Å 87.78Å 90.00° 105.01° 90.00°	Depositor
Resolution (Å)	84.78 – 1.90 56.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (84.78-1.90) 97.8 (56.55-1.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.223 , 0.289 0.227 , 0.292	Depositor DCC
$R_{free}$ test set	3790 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, EDO, MES

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	1.25	5/3776 (0.1%)	1.09	8/5115 (0.2%)
1	B	1.31	15/3897 (0.4%)	1.13	21/5283 (0.4%)
All	All	1.28	20/7673 (0.3%)	1.11	29/10398 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	LEU	C-O	-7.75	1.08	1.23
1	B	350	TYR	CE1-CZ	6.84	1.47	1.38
1	A	364	GLN	C-O	6.52	1.35	1.23
1	B	308	TRP	CZ3-CH2	6.42	1.50	1.40
1	B	303	PHE	C-O	6.24	1.35	1.23
1	A	414	LEU	C-O	6.12	1.34	1.23
1	A	173	TYR	CB-CG	-5.97	1.42	1.51
1	B	131	TYR	CE1-CZ	-5.89	1.30	1.38
1	B	185	ARG	C-O	5.88	1.34	1.23
1	B	308	TRP	CG-CD1	5.83	1.45	1.36
1	B	486	TYR	CZ-OH	-5.68	1.28	1.37
1	B	224	TRP	CG-CD1	5.64	1.44	1.36
1	B	219	PHE	CG-CD1	5.61	1.47	1.38
1	A	368	PHE	CG-CD2	-5.44	1.30	1.38
1	B	485	GLY	CA-C	5.44	1.60	1.51
1	B	217	GLU	CD-OE1	5.40	1.31	1.25
1	B	247	TYR	CZ-OH	5.38	1.47	1.37
1	B	422	TYR	CG-CD1	-5.21	1.32	1.39
1	A	362	GLY	C-O	5.13	1.31	1.23
1	B	134	SER	CA-CB	5.02	1.60	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ASP	CB-CG-OD1	13.30	130.27	118.30
1	B	314	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	B	333	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	354	LEU	CB-CG-CD1	7.38	123.55	111.00
1	B	472	LEU	CB-CG-CD1	7.21	123.26	111.00
1	B	467	MET	CG-SD-CE	7.02	111.43	100.20
1	A	314	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	145	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	380	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	114	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	380	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	371	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	486	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	505	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	486	TYR	CB-CG-CD1	5.91	124.54	121.00
1	B	546	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	212	ASP	N-CA-CB	-5.80	100.16	110.60
1	B	333	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	121[A]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	B	121[B]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	121[A]	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	121[B]	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	109	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	509	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	529	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	273	TYR	CB-CG-CD1	5.25	124.15	121.00
1	B	529	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	201	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	206	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3673	0	3540	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3789	0	3654	57	0
2	A	28	0	12	1	0
2	B	28	0	12	0	0
3	A	12	0	13	1	0
3	B	12	0	13	0	0
4	A	40	0	60	7	0
4	B	32	0	48	0	0
5	A	6	0	8	3	0
6	A	570	0	0	24	0
6	B	506	0	0	27	0
All	All	8696	0	7360	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:602:MES:H52	6:A:914:HOH:O	1.26	1.28
1:A:410[A]:HIS:NE2	6:A:705:HOH:O	1.61	1.21
1:B:108[A]:GLU:OE1	6:B:705:HOH:O	1.67	1.12
1:B:356[B]:HIS:CD2	6:B:711:HOH:O	2.07	1.06
4:A:603:EDO:H12	6:A:1017:HOH:O	1.56	1.06
1:A:200[A]:ASP:OD2	6:A:706[A]:HOH:O	1.74	1.04
1:A:200[B]:ASP:OD2	6:A:707:HOH:O	1.75	1.02
1:B:341[A]:GLN:NE2	6:B:706:HOH:O	1.75	0.99
1:A:200[B]:ASP:CG	6:A:707:HOH:O	2.04	0.96
1:B:259:GLU:OE1	6:B:707:HOH:O	1.84	0.95
1:B:108[B]:GLU:OE2	6:B:708:HOH:O	1.85	0.93
1:B:108[A]:GLU:CD	6:B:705:HOH:O	2.00	0.91
1:A:318[A]:ASN:OD1	6:A:708:HOH:O	1.88	0.91
4:A:603:EDO:H21	6:A:1017:HOH:O	1.71	0.90
1:B:116[B]:GLN:OE1	6:B:705:HOH:O	1.89	0.90
1:A:222[B]:MET:HE1	6:A:1011[B]:HOH:O	1.73	0.86
1:B:108[A]:GLU:CG	6:B:705:HOH:O	2.28	0.79
1:B:494:LEU:C	1:B:518[B]:MET:HG2	2.03	0.79
4:A:603:EDO:C1	6:A:1017:HOH:O	2.20	0.77
1:B:116[B]:GLN:OE1	6:B:710:HOH:O	2.01	0.77
1:B:356[A]:HIS:CD2	6:B:715:HOH:O	2.38	0.76
1:B:356[B]:HIS:CD2	6:B:717:HOH:O	2.39	0.76
1:B:141[B]:LYS:NZ	6:B:709:HOH:O	1.88	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355[A]:SER:OG	6:B:711:HOH:O	2.04	0.73
4:A:603:EDO:C2	6:A:1017:HOH:O	2.27	0.72
1:A:388[A]:LYS:NZ	1:A:389:GLU:OE2	2.23	0.72
1:A:410[A]:HIS:CD2	6:A:705:HOH:O	2.27	0.70
1:A:318[A]:ASN:CG	6:A:708:HOH:O	2.28	0.68
1:B:108[A]:GLU:HG2	6:B:705:HOH:O	1.92	0.67
1:B:127[B]:LYS:N	1:B:127[B]:LYS:HD3	2.11	0.66
1:A:318[A]:ASN:ND2	6:A:708:HOH:O	2.30	0.64
1:B:121[B]:ARG:O	6:B:712:HOH:O	2.10	0.64
1:B:341[A]:GLN:O	1:B:341[A]:GLN:NE2	2.31	0.63
1:A:185:ARG:NH1	1:A:211:MET:SD	2.71	0.63
5:A:611:GOL:C3	6:A:922:HOH:O	2.46	0.63
1:B:341[A]:GLN:OE1	6:B:706:HOH:O	2.16	0.62
1:B:356[A]:HIS:NE2	6:B:715:HOH:O	2.31	0.60
1:B:108[B]:GLU:CD	6:B:708:HOH:O	2.36	0.60
1:B:355[A]:SER:HB2	6:B:715:HOH:O	2.02	0.60
1:A:534:THR:HG21	6:B:791:HOH:O	2.02	0.59
1:A:222[B]:MET:CE	6:A:1011[B]:HOH:O	2.40	0.58
1:B:356[B]:HIS:H	1:B:356[B]:HIS:CD2	2.21	0.58
1:B:127[B]:LYS:N	1:B:127[B]:LYS:CD	2.67	0.57
1:B:495:LYS:N	1:B:518[B]:MET:HG2	2.19	0.57
1:A:325:ALA:HB3	4:A:605:EDO:H22	1.87	0.57
1:B:495:LYS:HB2	1:B:518[B]:MET:HG3	1.87	0.56
1:A:109[A]:ASP:OD1	1:A:110:SER:N	2.39	0.56
1:B:341[A]:GLN:CD	6:B:706:HOH:O	2.22	0.56
5:A:611:GOL:H31	6:A:922:HOH:O	2.06	0.55
1:B:99:GLY:HA3	1:B:127[A]:LYS:HE2	1.87	0.55
1:A:130[A]:SER:HB2	4:A:606[A]:EDO:H12	1.89	0.55
1:B:264:HIS:HA	1:B:294:TRP:O	2.07	0.54
1:A:131:TYR:CD1	1:A:319[B]:LYS:HE3	2.42	0.54
1:B:423:ALA:HB2	1:B:445:GLN:HE21	1.74	0.52
1:B:425:ASN:O	1:B:428[A]:SER:OG	2.26	0.52
1:A:342:VAL:HG11	1:A:464:LEU:HD23	1.90	0.52
1:A:388[B]:LYS:NZ	6:A:719:HOH:O	2.43	0.52
1:B:242:GLU:OE1	6:B:713:HOH:O	2.19	0.51
1:A:176:TRP:CH2	1:A:178:SER:HA	2.46	0.50
1:B:99:GLY:HA3	1:B:127[A]:LYS:CE	2.41	0.50
1:A:318[B]:ASN:ND2	6:A:722:HOH:O	2.44	0.50
1:B:163:GLU:HG2	1:B:245:ARG:NH2	2.26	0.50
1:A:229:ASP:O	1:A:230:PHE:C	2.51	0.49
1:B:356[B]:HIS:NE2	6:B:717:HOH:O	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PRO:HD3	6:A:1066:HOH:O	2.13	0.48
1:A:440:ILE:C	1:A:441:ILE:HD13	2.33	0.48
1:B:172[A]:LYS:HB3	1:B:201:ARG:HG2	1.96	0.48
1:B:172[B]:LYS:N	1:B:172[B]:LYS:HD3	2.29	0.48
1:A:424:GLU:OE2	4:A:608:EDO:O2	2.31	0.47
1:B:518[B]:MET:SD	6:B:957:HOH:O	2.61	0.47
1:A:144:LYS:HA	1:A:222[A]:MET:HG3	1.97	0.47
1:B:108[B]:GLU:CD	1:B:108[B]:GLU:H	2.18	0.47
1:A:409:LYS:HG2	1:A:439:GLU:HG2	1.97	0.47
1:A:184:ASN:ND2	1:A:483:THR:HG21	2.30	0.47
1:B:356[B]:HIS:N	1:B:356[B]:HIS:CD2	2.83	0.47
1:B:165:ILE:HD11	1:B:293:PRO:CG	2.45	0.47
1:B:165:ILE:CD1	1:B:263:SER:HA	2.45	0.46
1:B:141[B]:LYS:HE2	6:B:1074:HOH:O	2.16	0.46
1:B:428[A]:SER:OG	1:B:429:MET:N	2.48	0.46
1:A:94:SER:N	6:A:733:HOH:O	2.50	0.45
1:A:188:SER:HB2	1:A:299:THR:HG23	1.99	0.45
1:A:480:ALA:HB1	1:A:550:ASP:HB2	1.98	0.45
5:A:611:GOL:H32	6:A:922:HOH:O	2.12	0.44
1:B:304:VAL:HB	1:B:305:PRO:HD3	1.99	0.44
1:B:127[A]:LYS:HD3	1:B:128:PRO:HD2	1.99	0.44
1:B:546:ARG:NH2	6:B:731:HOH:O	2.50	0.44
1:A:95:ASP:OD1	1:A:95:ASP:N	2.49	0.44
1:B:518[B]:MET:CG	6:B:957:HOH:O	2.65	0.44
1:B:165:ILE:HG23	1:B:167:GLY:O	2.18	0.44
1:A:546:ARG:NH1	6:A:738:HOH:O	2.51	0.43
1:A:441:ILE:N	1:A:441:ILE:HD13	2.34	0.43
1:A:481:TRP:CZ3	1:A:551:ILE:HD12	2.53	0.43
1:B:106:PHE:CD2	1:B:114:ARG:HD3	2.53	0.43
1:A:411:LYS:HB2	1:A:441:ILE:HD12	1.99	0.43
1:A:194:LEU:HD21	1:A:317:LEU:HD21	2.01	0.42
1:A:480:ALA:O	1:A:481:TRP:HB2	2.19	0.42
1:A:374:PRO:HG3	1:A:419:ASN:OD1	2.20	0.42
1:A:460:ASN:HA	1:A:460:ASN:HD22	1.68	0.42
1:A:278:LYS:NZ	6:A:729:HOH:O	2.48	0.41
1:B:116[B]:GLN:HE21	1:B:116[B]:GLN:HA	1.85	0.41
1:B:165:ILE:HD12	1:B:263:SER:HA	2.03	0.41
1:A:107:ASP:OD2	1:A:110:SER:HB3	2.20	0.41
1:B:342:VAL:HG11	1:B:464:LEU:HD23	2.01	0.41
1:A:418:LEU:HD21	2:A:601:GDP:C4	2.56	0.41
1:A:179:PHE:O	1:A:185:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:ND1	1:B:300:ASP:OD2	2.48	0.41
1:A:544:HIS:O	1:A:557:LEU:HA	2.21	0.41
1:A:267:LEU:HD11	1:A:295:LEU:HD13	2.03	0.40
1:B:341[A]:GLN:C	1:B:341[A]:GLN:NE2	2.74	0.40
1:B:285:ASP:O	1:B:289:ILE:HG13	2.22	0.40
1:B:230:PHE:HA	1:B:231:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/476 (94%)	431 (96%)	15 (3%)	1 (0%)	52	42
1	B	468/476 (98%)	451 (96%)	16 (3%)	1 (0%)	52	42
All	All	915/952 (96%)	882 (96%)	31 (3%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	SER
1	A	255	VAL

### 5.3.2 Protein sidechains [i](#)

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	406/423 (96%)	386 (95%)	20 (5%)	31	18
1	B	418/423 (99%)	399 (96%)	19 (4%)	34	21
All	All	824/846 (97%)	785 (95%)	39 (5%)	39	20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	116	GLN
1	A	121[A]	ARG
1	A	121[B]	ARG
1	A	141	LYS
1	A	155	LYS
1	A	222[A]	MET
1	A	222[B]	MET
1	A	224	TRP
1	A	273	TYR
1	A	341[A]	GLN
1	A	341[B]	GLN
1	A	354	LEU
1	A	356[A]	HIS
1	A	356[B]	HIS
1	A	398	LEU
1	A	409	LYS
1	A	458	MET
1	A	522	PHE
1	A	546	ARG
1	B	121[A]	ARG
1	B	121[B]	ARG
1	B	127[A]	LYS
1	B	127[B]	LYS
1	B	163	GLU
1	B	165	ILE
1	B	178	SER
1	B	224	TRP
1	B	273	TYR
1	B	301	ASN
1	B	318	ASN
1	B	341[A]	GLN
1	B	341[B]	GLN
1	B	355[A]	SER
1	B	355[B]	SER

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Mol	Chain	Res	Type
1	B	398	LEU
1	B	399	VAL
1	B	409	LYS
1	B	531	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	323	GLN
1	A	460	ASN
1	B	323	GLN
1	B	445	GLN
1	B	448	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

23 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	GDP	A	601	-	24,30,30	0.98	1 (4%)	26,47,47	2.33	9 (34%)
3	MES	A	602	-	12,12,12	2.04	1 (8%)	15,16,16	1.82	2 (13%)
4	EDO	A	603	-	3,3,3	0.27	0	2,2,2	0.62	0
4	EDO	A	604	-	3,3,3	0.38	0	2,2,2	0.73	0
4	EDO	A	605	-	3,3,3	0.37	0	2,2,2	0.90	0
4	EDO	A	606[A]	-	3,3,3	0.44	0	2,2,2	0.44	0
4	EDO	A	606[B]	-	3,3,3	0.53	0	2,2,2	0.25	0
4	EDO	A	607	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	A	608	-	3,3,3	0.53	0	2,2,2	0.26	0
4	EDO	A	609[A]	-	3,3,3	0.55	0	2,2,2	0.43	0
4	EDO	A	609[B]	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	610	-	3,3,3	0.46	0	2,2,2	0.33	0
5	GOL	A	611	-	5,5,5	0.22	0	5,5,5	0.27	0
2	GDP	B	601	-	24,30,30	1.07	2 (8%)	26,47,47	2.34	6 (23%)
3	MES	B	602	-	12,12,12	2.18	1 (8%)	15,16,16	1.37	1 (6%)
4	EDO	B	603	-	3,3,3	0.38	0	2,2,2	0.42	0
4	EDO	B	604	-	3,3,3	0.38	0	2,2,2	0.63	0
4	EDO	B	605	-	3,3,3	0.43	0	2,2,2	0.23	0
4	EDO	B	606	-	3,3,3	0.58	0	2,2,2	0.86	0
4	EDO	B	607	-	3,3,3	0.41	0	2,2,2	0.34	0
4	EDO	B	608	-	3,3,3	0.27	0	2,2,2	0.54	0
4	EDO	B	609	-	3,3,3	0.51	0	2,2,2	0.16	0
4	EDO	B	610	-	3,3,3	0.47	0	2,2,2	0.21	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	GDP	A	601	-	-	0/12/32/32	0/3/3/3
3	MES	A	602	-	-	0/6/14/14	0/1/1/1
4	EDO	A	603	-	-	0/1/1/1	0/0/0/0
4	EDO	A	604	-	-	0/1/1/1	0/0/0/0
4	EDO	A	605	-	-	0/1/1/1	0/0/0/0
4	EDO	A	606[A]	-	-	0/1/1/1	0/0/0/0
4	EDO	A	606[B]	-	-	0/1/1/1	0/0/0/0
4	EDO	A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	A	608	-	-	0/1/1/1	0/0/0/0
4	EDO	A	609[A]	-	-	0/1/1/1	0/0/0/0
4	EDO	A	609[B]	-	-	0/1/1/1	0/0/0/0
4	EDO	A	610	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	611	-	-	0/4/4/4	0/0/0/0
2	GDP	B	601	-	-	0/12/32/32	0/3/3/3
3	MES	B	602	-	-	0/6/14/14	0/1/1/1
4	EDO	B	603	-	-	0/1/1/1	0/0/0/0
4	EDO	B	604	-	-	0/1/1/1	0/0/0/0
4	EDO	B	605	-	-	0/1/1/1	0/0/0/0
4	EDO	B	606	-	-	0/1/1/1	0/0/0/0
4	EDO	B	607	-	-	0/1/1/1	0/0/0/0
4	EDO	B	608	-	-	0/1/1/1	0/0/0/0
4	EDO	B	609	-	-	0/1/1/1	0/0/0/0
4	EDO	B	610	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	MES	C8-S	-7.33	1.66	1.77
3	A	602	MES	C8-S	-6.84	1.67	1.77
2	B	601	GDP	C5-C4	2.06	1.45	1.40
2	A	601	GDP	C6-C5	2.77	1.46	1.41
2	B	601	GDP	C6-C5	3.01	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GDP	N3-C2-N1	-5.11	120.60	127.56
2	A	601	GDP	C6-C5-C4	-4.70	115.49	120.86
2	A	601	GDP	C1'-N9-C4	-4.53	121.75	126.81
2	B	601	GDP	C6-C5-C4	-4.44	115.78	120.86
2	B	601	GDP	C5-C6-N1	-4.38	117.80	123.52
2	A	601	GDP	N3-C2-N1	-4.14	121.93	127.56
2	A	601	GDP	C5-C6-N1	-3.96	118.34	123.52
2	B	601	GDP	C1'-N9-C4	-2.39	124.14	126.81
2	A	601	GDP	C2'-C1'-N9	-2.04	108.01	113.47
2	A	601	GDP	O2B-PB-O1B	2.05	117.32	110.63
2	A	601	GDP	O3'-C3'-C4'	2.47	118.38	111.01
2	A	601	GDP	N2-C2-N1	2.49	121.31	117.20
2	B	601	GDP	N2-C2-N1	3.35	122.72	117.20
3	A	602	MES	O2S-S-C8	3.54	109.37	106.87
3	B	602	MES	O3S-S-C8	3.78	112.85	104.99
3	A	602	MES	O1S-S-C8	5.24	110.57	106.87
2	A	601	GDP	C6-N1-C2	5.95	122.85	115.88
2	B	601	GDP	C6-N1-C2	6.59	123.61	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GDP	1	0
3	A	602	MES	1	0
4	A	603	EDO	4	0
4	A	605	EDO	1	0
4	A	606[A]	EDO	1	0
4	A	608	EDO	1	0
5	A	611	GOL	3	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	440/476 (92%)	-0.15	8 (1%) 71 74	16, 22, 46, 75	0
1	B	457/476 (96%)	-0.12	8 (1%) 71 74	17, 22, 47, 71	1 (0%)
All	All	897/952 (94%)	-0.14	16 (1%) 71 74	16, 22, 47, 75	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	THR	3.4
1	A	406	ASN	3.4
1	B	454	THR	2.9
1	A	119[A]	HIS	2.8
1	B	398	LEU	2.8
1	B	356[A]	HIS	2.8
1	A	398	LEU	2.7
1	B	165	ILE	2.6
1	A	261	THR	2.5
1	A	162	GLN	2.4
1	B	256	ILE	2.4
1	B	407	THR	2.2
1	B	260	GLY	2.2
1	B	258	THR	2.1
1	A	356[A]	HIS	2.0
1	A	408	PRO	2.0

### 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 ⓘ

There are no carbohydrates 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. 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
5	GOL	A	611	6/6	0.82	0.31	16.99	29,30,31,31	6
4	EDO	A	603	4/4	0.87	0.29	16.43	18,22,22,25	4
4	EDO	A	605	4/4	0.78	0.21	8.77	27,29,29,30	4
4	EDO	A	607	4/4	0.85	0.15	5.51	33,33,34,35	4
4	EDO	A	608	4/4	0.62	0.27	4.75	36,37,38,39	4
4	EDO	A	606[A]	4/4	0.78	0.19	4.61	31,31,32,32	4
4	EDO	A	606[B]	4/4	0.78	0.19	4.04	30,30,31,31	4
4	EDO	B	608	4/4	0.79	0.34	3.75	25,27,27,31	4
4	EDO	B	610	4/4	0.77	0.22	3.10	47,47,48,48	4
4	EDO	B	606	4/4	0.87	0.13	3.01	24,26,28,28	0
4	EDO	B	607	4/4	0.86	0.15	2.57	42,44,45,46	0
3	MES	B	602	12/12	0.91	0.18	1.96	34,38,40,40	12
4	EDO	B	604	4/4	0.86	0.12	1.92	38,42,42,44	0
2	GDP	A	601	28/28	0.88	0.11	0.67	18,30,45,50	0
2	GDP	B	601	28/28	0.90	0.12	0.38	20,27,41,47	0
4	EDO	B	605	4/4	0.89	0.12	0.27	35,36,36,39	0
4	EDO	A	610	4/4	0.77	0.17	-	26,26,27,27	4
4	EDO	A	609[A]	4/4	0.78	0.27	-	34,34,34,35	4
4	EDO	A	604	4/4	0.84	0.19	-	27,27,27,29	4
3	MES	A	602	12/12	0.79	0.20	-	38,40,43,43	12
4	EDO	A	609[B]	4/4	0.78	0.27	-	30,31,32,33	4
4	EDO	B	603	4/4	0.74	0.25	-	27,28,30,30	4
4	EDO	B	609	4/4	0.81	0.11	-	56,59,61,63	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.