



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:56 PM GMT

PDB ID : 2Q4J
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g03250, a putative UDP-glucose pyrophosphorylase
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.86 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

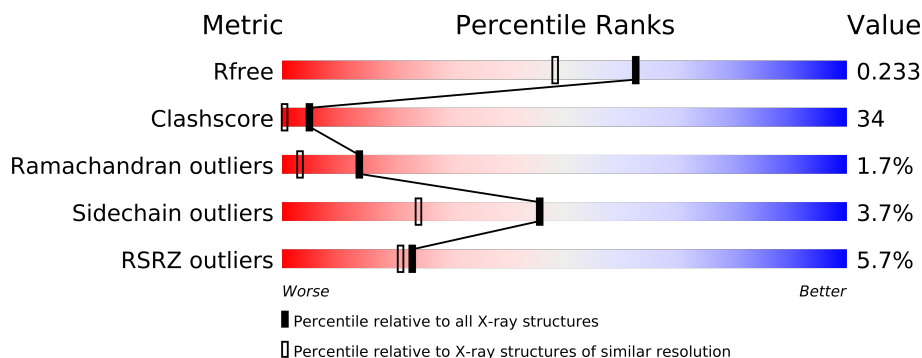
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 1.86 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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	1-A	469	
1	1-B	469	
1	2-A	469	
1	2-B	469	
1	3-A	469	
1	3-B	469	
1	4-A	469	
1	4-B	469	
1	5-A	469	
1	5-B	469	
1	6-A	469	
1	6-B	469	
1	7-A	469	
1	7-B	469	

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Mol	Chain	Length	Quality of chain
1	8-A	469	
1	8-B	469	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 60344 atoms, of which 0 are hydrogen and 0 are deuterium.

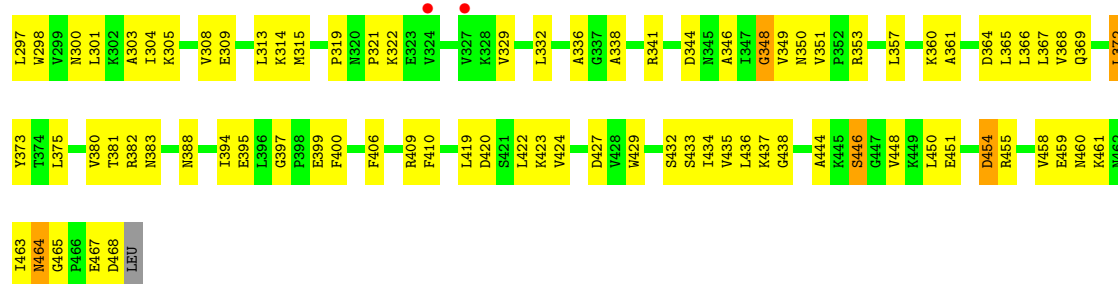
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable UTP-glucose-1-phosphateuridylyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	1-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	2-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	2-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	3-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	3-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	4-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	4-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	5-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	5-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	6-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	6-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	7-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	7-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	8-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	8-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			

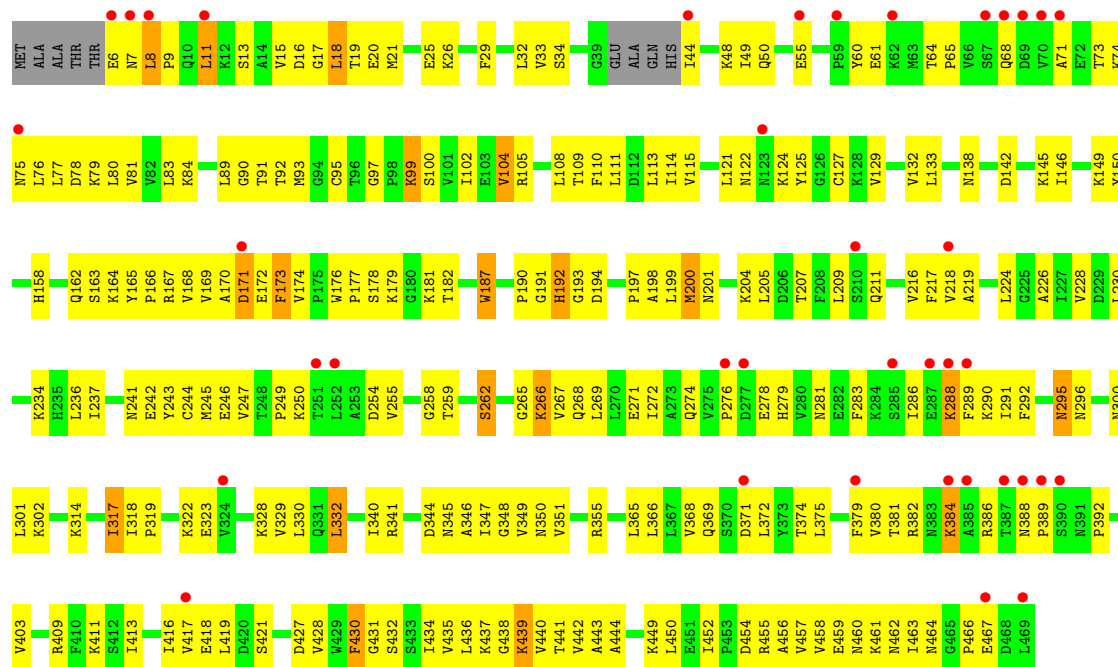
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	180	Total 180	O 180	0	0
2	1-B	241	Total 241	O 241	0	0
2	2-A	182	Total 182	O 182	0	0
2	2-B	239	Total 239	O 239	0	0
2	3-A	182	Total 182	O 182	0	0
2	3-B	239	Total 239	O 239	0	0
2	4-A	183	Total 183	O 183	0	0
2	4-B	238	Total 238	O 238	0	0
2	5-A	182	Total 182	O 182	0	0
2	5-B	239	Total 239	O 239	0	0
2	6-A	182	Total 182	O 182	0	0
2	6-B	239	Total 239	O 239	0	0
2	7-A	183	Total 183	O 183	0	0
2	7-B	238	Total 238	O 238	0	0
2	8-A	183	Total 183	O 183	0	0
2	8-B	238	Total 238	O 238	0	0



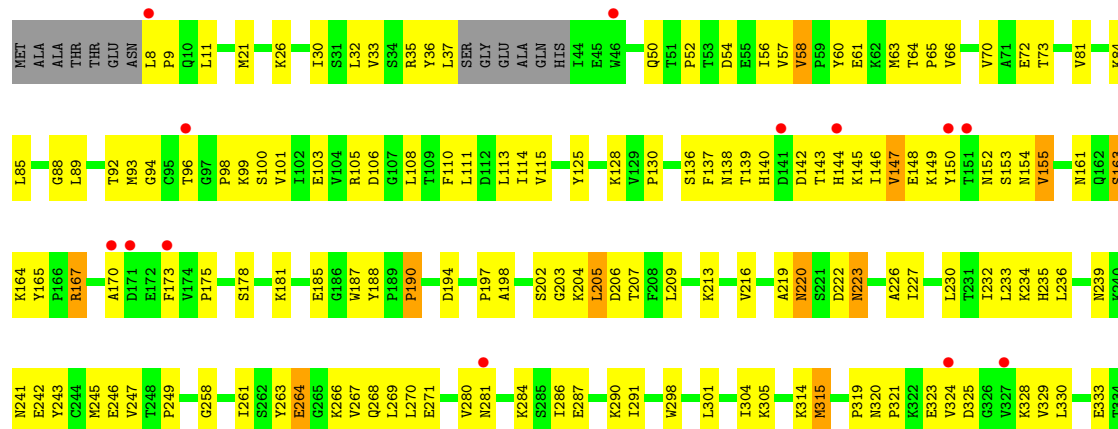
• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

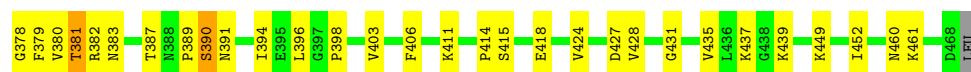
Chain 2-A:



• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

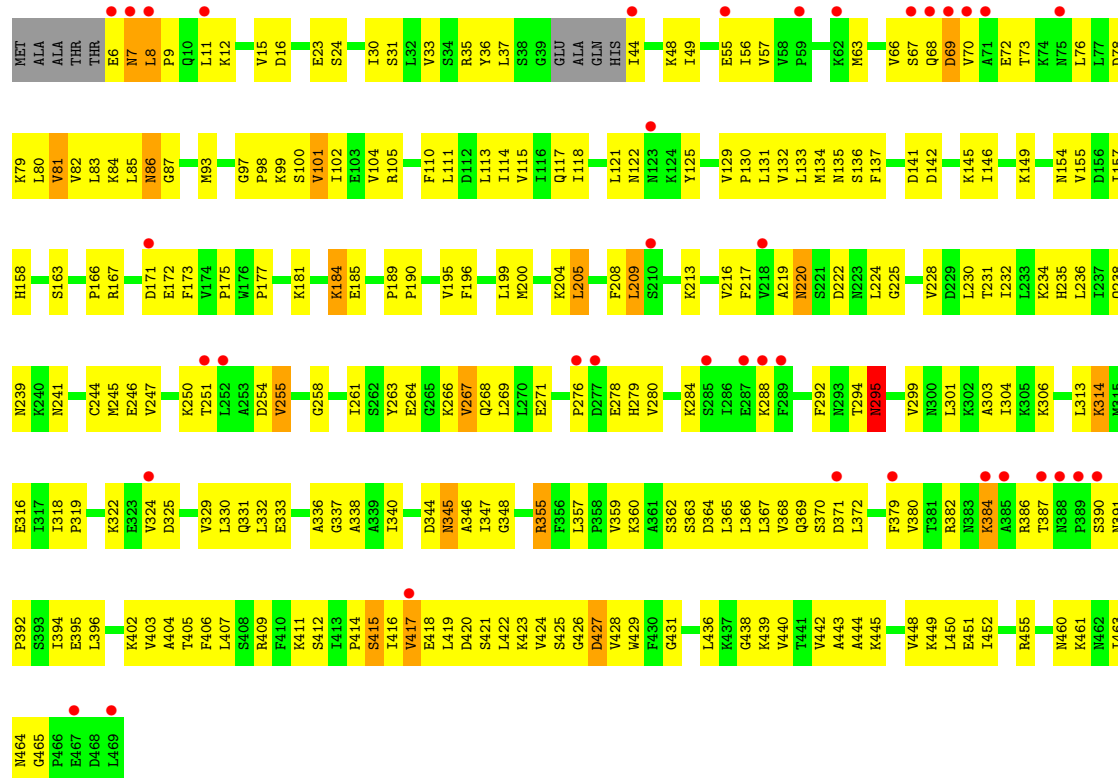
Chain 2-B:





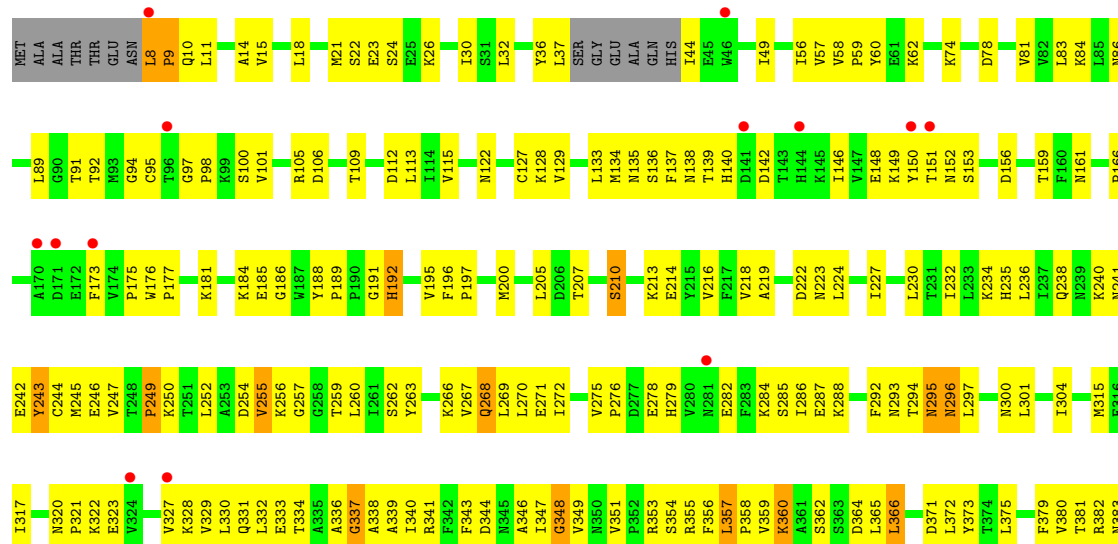
• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

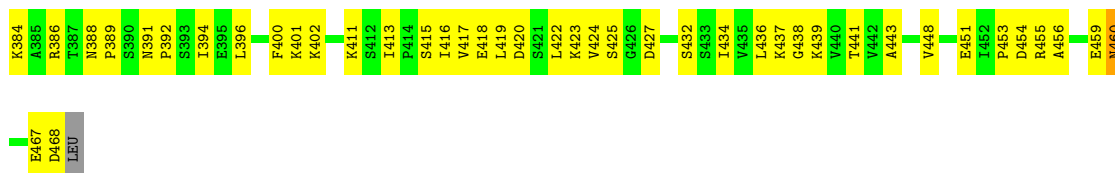
Chain 4-A:



• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

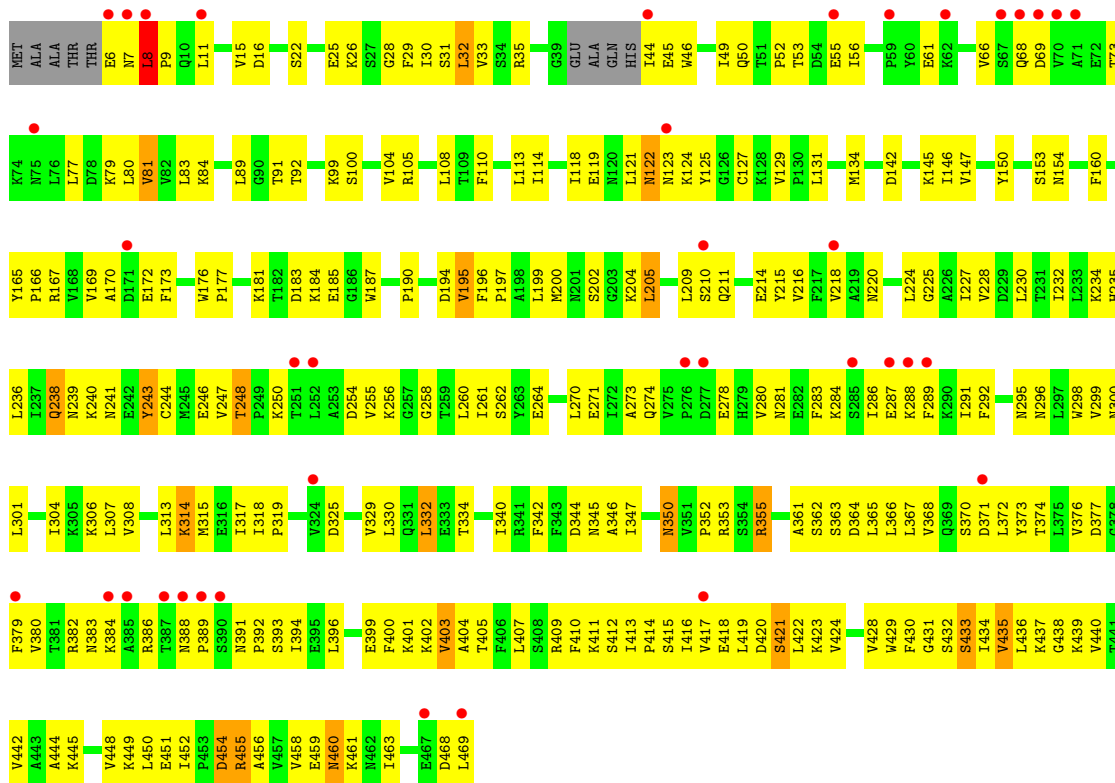
Chain 4-B:





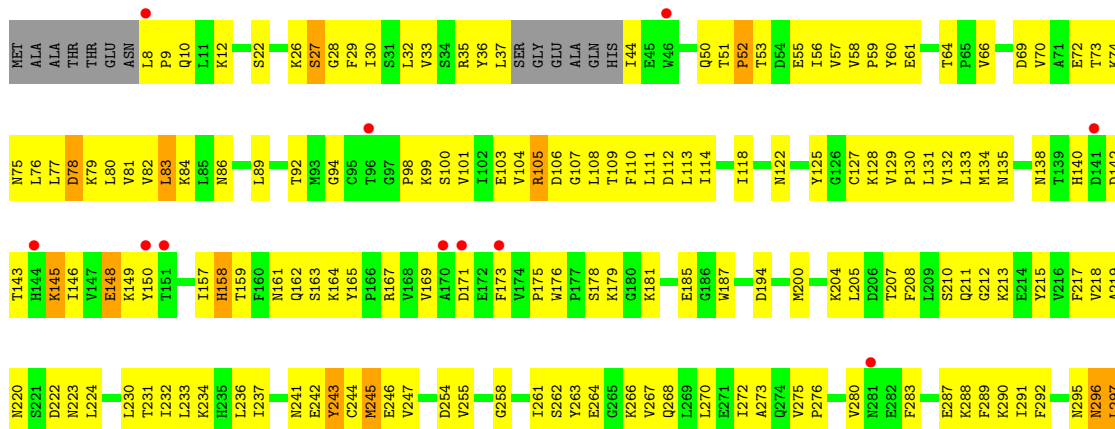
- Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

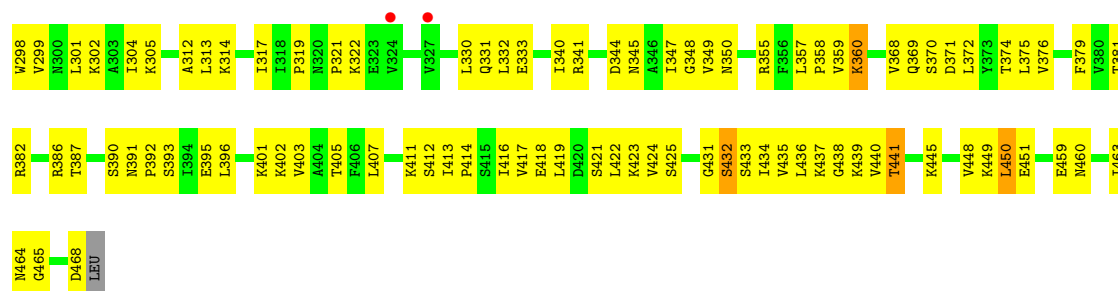
Chain 5-A:



- Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

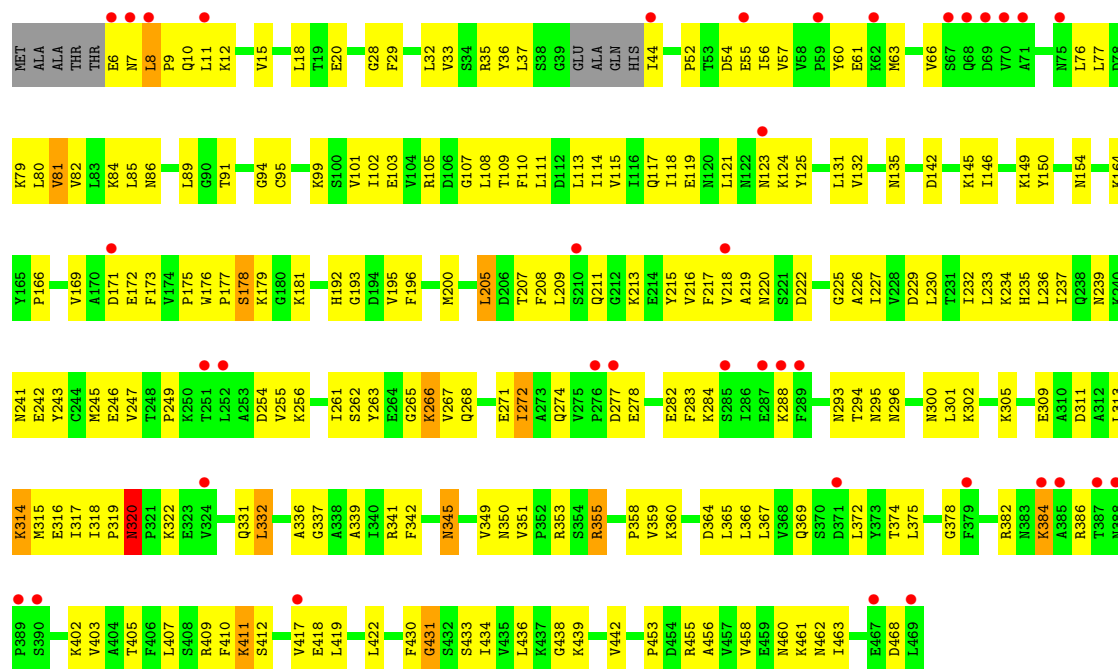
Chain 5-B:





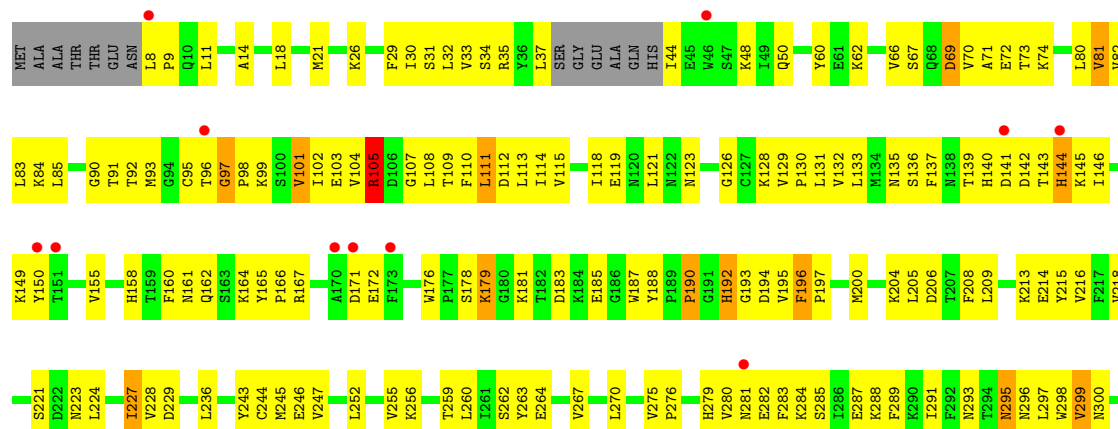
• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

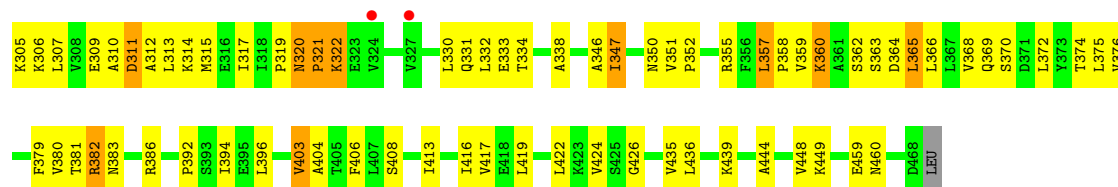
Chain 6-A:



• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

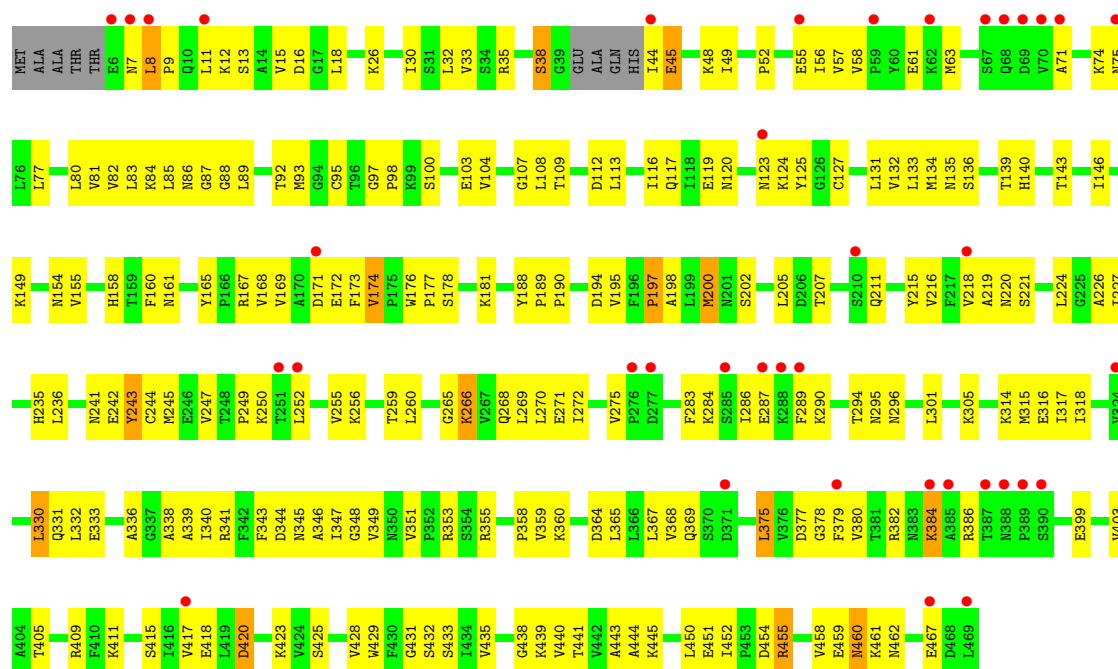
Chain 6-B:





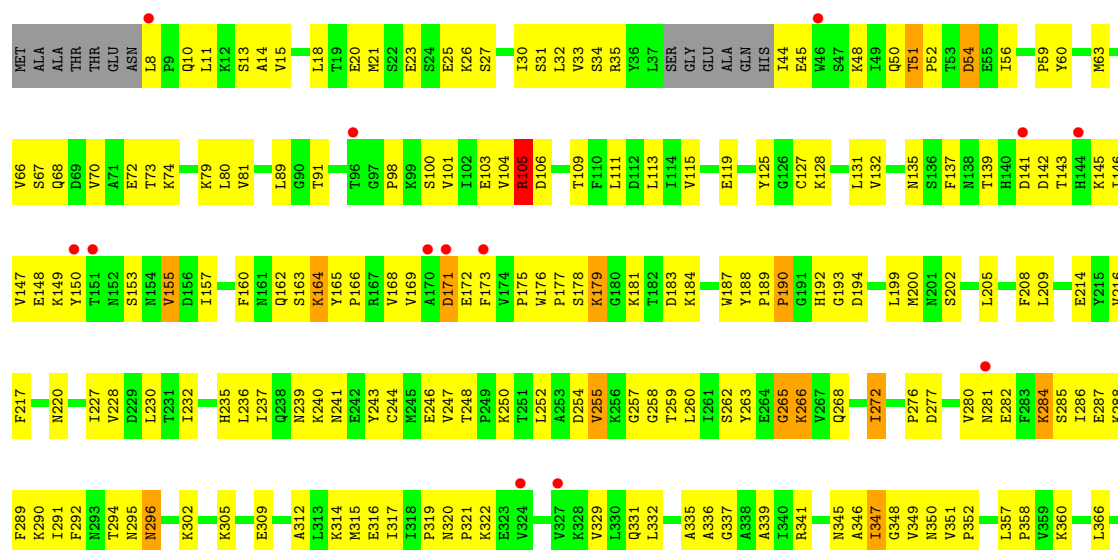
• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

Chain 7-A:



• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

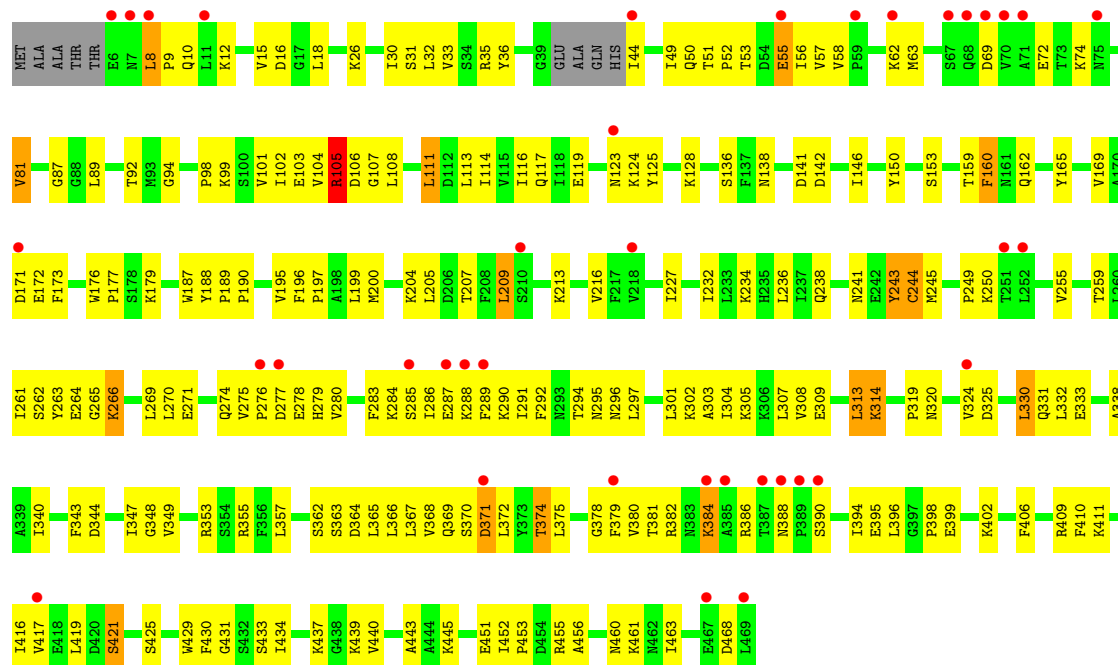
Chain 7-B:





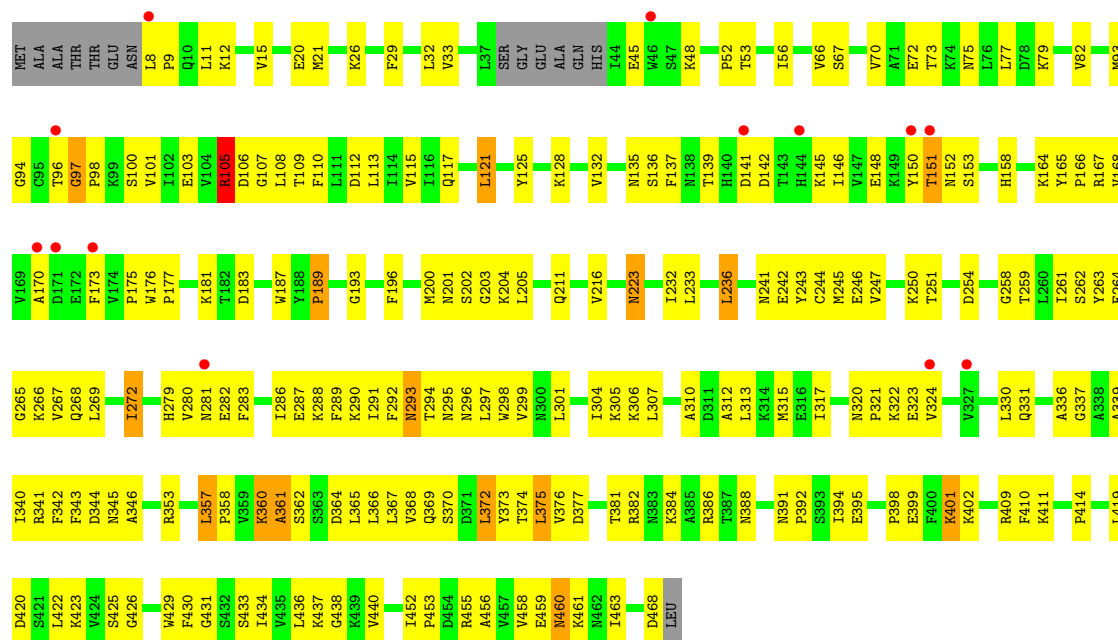
• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

Chain 8-A:



• Molecule 1: Probable UTP-glucose-1-phosphateuridylyltransferase 2

Chain 8-B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.68Å 58.86Å 89.86Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	37.37 – 1.86 37.37 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.6 (37.37-1.86) 97.7 (37.37-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.231 0.175 , 0.233	Depositor DCC
R_{free} test set	3986 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 79504 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60344	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.48	0/3646	0.67	1/4942 (0.0%)
1	1-B	0.56	0/3610	0.73	2/4895 (0.0%)
1	2-A	0.49	0/3646	0.66	0/4942
1	2-B	0.55	1/3610 (0.0%)	0.71	1/4895 (0.0%)
1	3-A	0.47	0/3646	0.66	0/4942
1	3-B	0.55	0/3610	0.71	2/4895 (0.0%)
1	4-A	0.49	0/3646	0.66	0/4942
1	4-B	0.56	0/3610	0.73	2/4895 (0.0%)
1	5-A	0.50	0/3646	0.72	0/4942
1	5-B	0.60	0/3610	0.75	1/4895 (0.0%)
1	6-A	0.50	0/3646	0.68	0/4942
1	6-B	0.60	0/3610	0.76	2/4895 (0.0%)
1	7-A	0.51	0/3646	0.70	0/4942
1	7-B	0.57	0/3610	0.75	3/4895 (0.1%)
1	8-A	0.51	0/3646	0.69	0/4942
1	8-B	0.59	0/3610	0.77	4/4895 (0.1%)
All	All	0.53	1/58048 (0.0%)	0.71	18/78696 (0.0%)

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	3-B	0	1
1	4-B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-B	242	GLU	CG-CD	5.45	1.60	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	348	GLY	N-CA-C	-6.06	97.95	113.10
1	4-B	348	GLY	N-CA-C	-5.87	98.43	113.10
1	4-B	296	ASN	N-CA-C	-5.74	95.52	111.00
1	6-B	105	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	7-B	290	LYS	N-CA-C	5.70	126.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3-B	125	TYR	Sidechain
1	4-B	243	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	3579	0	3652	229	0
1	1-B	3543	0	3621	255	0
1	2-A	3579	0	3652	254	0
1	2-B	3543	0	3621	210	0
1	3-A	3579	0	3652	185	0
1	3-B	3543	0	3621	255	1
1	4-A	3579	0	3652	293	0
1	4-B	3543	0	3621	256	0
1	5-A	3579	0	3652	320	0
1	5-B	3543	0	3621	273	0
1	6-A	3579	0	3652	229	0
1	6-B	3543	0	3621	253	1
1	7-A	3579	0	3652	233	0
1	7-B	3543	0	3621	239	0
1	8-A	3579	0	3652	222	0
1	8-B	3543	0	3621	230	0
2	1-A	180	0	0	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-B	241	0	0	32	0
2	2-A	182	0	0	23	0
2	2-B	239	0	0	38	0
2	3-A	182	0	0	24	0
2	3-B	239	0	0	41	1
2	4-A	183	0	0	32	0
2	4-B	238	0	0	37	0
2	5-A	182	0	0	43	0
2	5-B	239	0	0	37	0
2	6-A	182	0	0	32	0
2	6-B	239	0	0	33	1
2	7-A	183	0	0	27	0
2	7-B	238	0	0	34	0
2	8-A	183	0	0	24	0
2	8-B	238	0	0	41	0
All	All	60344	0	58184	3934	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 3934 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:415:SER:HB3	2:A:486:HOH:O	1.18	1.29
1:A:363:SER:HB3	2:A:605:HOH:O	1.42	1.19
1:B:341:ARG:HA	2:B:568:HOH:O	1.47	1.15
1:A:355:ARG:HH11	1:A:355:ARG:HG3	1.12	1.13
1:A:344:ASP:HB3	2:A:570:HOH:O	1.44	1.13

All (2) 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:B:390:SER:OG	2:B:655:HOH:O[4_545]	2.10	0.10
1:B:305:LYS:NZ	2:B:688:HOH:O[4_555]	2.15	0.05

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	456/469 (97%)	399 (88%)	48 (10%)	9 (2%)	11	2
1	1-B	451/469 (96%)	408 (90%)	38 (8%)	5 (1%)	21	6
1	2-A	456/469 (97%)	407 (89%)	44 (10%)	5 (1%)	21	6
1	2-B	451/469 (96%)	405 (90%)	38 (8%)	8 (2%)	13	2
1	3-A	456/469 (97%)	415 (91%)	33 (7%)	8 (2%)	13	2
1	3-B	451/469 (96%)	410 (91%)	34 (8%)	7 (2%)	14	4
1	4-A	456/469 (97%)	403 (88%)	42 (9%)	11 (2%)	9	1
1	4-B	451/469 (96%)	411 (91%)	33 (7%)	7 (2%)	14	4
1	5-A	456/469 (97%)	406 (89%)	37 (8%)	13 (3%)	7	1
1	5-B	451/469 (96%)	406 (90%)	41 (9%)	4 (1%)	25	8
1	6-A	456/469 (97%)	402 (88%)	48 (10%)	6 (1%)	18	4
1	6-B	451/469 (96%)	399 (88%)	40 (9%)	12 (3%)	8	1
1	7-A	456/469 (97%)	415 (91%)	34 (8%)	7 (2%)	15	4
1	7-B	451/469 (96%)	407 (90%)	38 (8%)	6 (1%)	18	4
1	8-A	456/469 (97%)	403 (88%)	46 (10%)	7 (2%)	15	4
1	8-B	451/469 (96%)	409 (91%)	34 (8%)	8 (2%)	13	2
All	All	7256/7504 (97%)	6505 (90%)	628 (9%)	123 (2%)	14	3

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	8	LEU
1	1-B	170	ALA
1	3-A	38	SER
1	3-A	319	PRO
1	3-B	96	THR

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	408/414 (99%)	394 (97%)	14 (3%)	49	28
1	1-B	404/414 (98%)	390 (96%)	14 (4%)	48	26
1	2-A	408/414 (99%)	389 (95%)	19 (5%)	36	16
1	2-B	404/414 (98%)	392 (97%)	12 (3%)	53	34
1	3-A	408/414 (99%)	396 (97%)	12 (3%)	55	36
1	3-B	404/414 (98%)	389 (96%)	15 (4%)	45	24
1	4-A	408/414 (99%)	388 (95%)	20 (5%)	35	14
1	4-B	404/414 (98%)	392 (97%)	12 (3%)	53	34
1	5-A	408/414 (99%)	392 (96%)	16 (4%)	43	22
1	5-B	404/414 (98%)	385 (95%)	19 (5%)	36	16
1	6-A	408/414 (99%)	395 (97%)	13 (3%)	51	31
1	6-B	404/414 (98%)	389 (96%)	15 (4%)	45	24
1	7-A	408/414 (99%)	395 (97%)	13 (3%)	51	31
1	7-B	404/414 (98%)	385 (95%)	19 (5%)	36	16
1	8-A	408/414 (99%)	392 (96%)	16 (4%)	43	22
1	8-B	404/414 (98%)	391 (97%)	13 (3%)	51	31
All	All	6496/6624 (98%)	6254 (96%)	242 (4%)	45	24

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4-B	192	HIS
1	5-B	52	PRO
1	8-A	314	LYS
1	4-B	268	GLN
1	5-A	81	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-A	75	ASN
1	4-B	138	ASN
1	8-A	238	GLN
1	4-A	120	ASN
1	4-A	279	HIS

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 ⓘ

There are no ligands in this entry.

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	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	1-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	2-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	2-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	3-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	3-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	4-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	4-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	5-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	5-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	6-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	6-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	7-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	7-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
1	8-A	460/469 (98%)	0.33	38 (8%)	11	11	9, 24, 48, 69	460 (100%)
1	8-B	455/469 (97%)	-0.18	13 (2%)	49	45	3, 17, 39, 55	455 (100%)
All	All	7320/7504 (97%)	0.08	408 (5%)	23	21	3, 21, 47, 69	7320 (100%)

The worst 5 of 408 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	385	ALA	6.9
1	2-A	385	ALA	6.9
1	3-A	385	ALA	6.9
1	4-A	385	ALA	6.9
1	5-A	385	ALA	6.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.