



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 AM GMT

PDB ID : 2YQJ
Title : Crystal Structure of uridine-diphospho-N-acetylglucosamine pyrophosphorylase from *Candida albicans*, in the reaction-completed form
Authors : Miki, K.; Maruyama, D.; Nishitani, Y.; Nonaka, T.; Kita, A.
Deposited on : 2007-03-30
Resolution : 2.31 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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

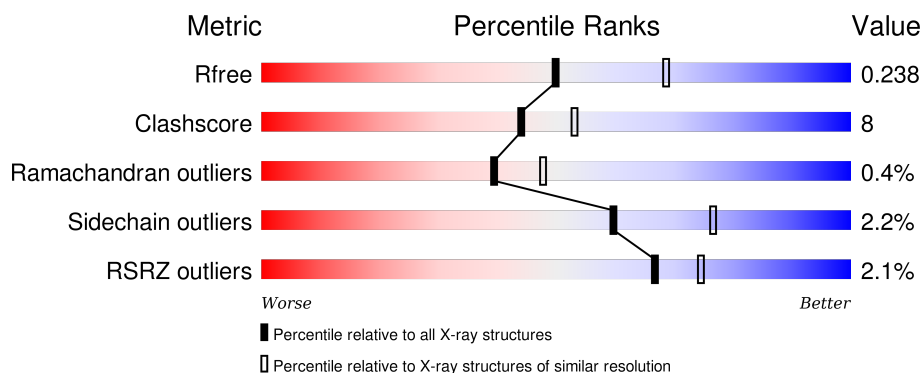
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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. 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	486	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 5%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 5%);"></div> <div style="position: absolute; top: 50%; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 5%);"></div> </div> <div> </div> </div>
1	B	486	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 15%, green 81%, grey 5%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 15%, green 81%, grey 5%);"></div> <div style="position: absolute; top: 50%; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 15%, green 81%, grey 5%);"></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
5	GOL	A	1301	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7615 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.

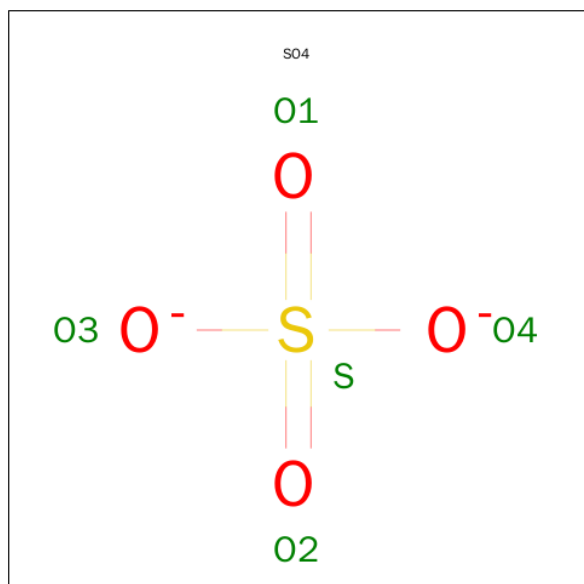
- Molecule 1 is a protein called UDP-N-acetylglucosamine pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3663	2341	613	697	12			
1	B	471	Total	C	N	O	S	0	0	0
			3629	2328	601	688	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	LEU	SER	ENGINEERED	UNP O74933
B	216	LEU	SER	ENGINEERED	UNP O74933

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5	4 1		

Continued on next page...

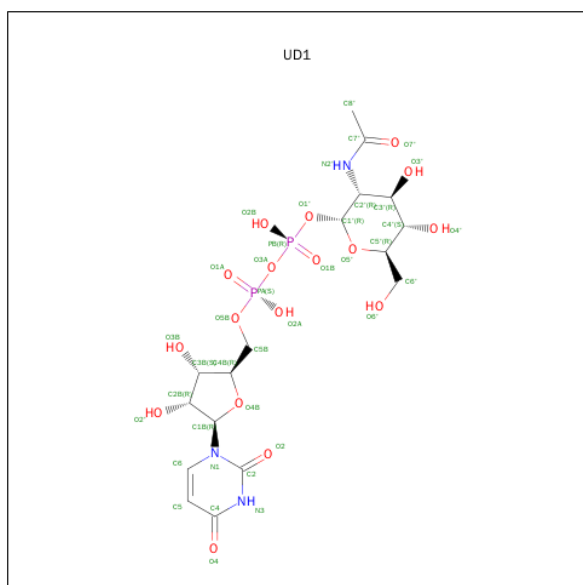
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

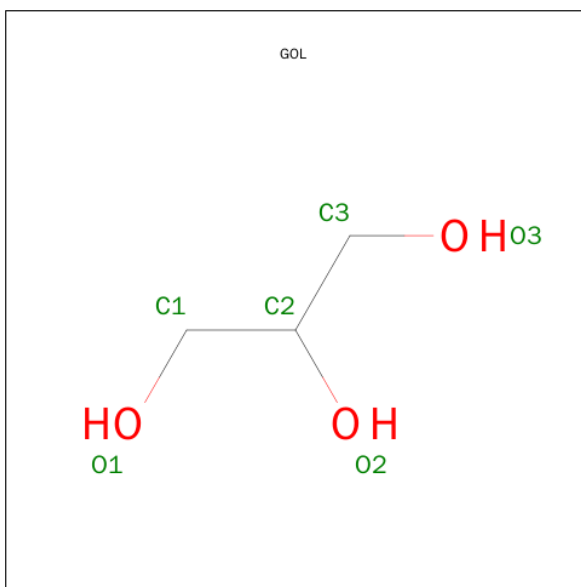
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

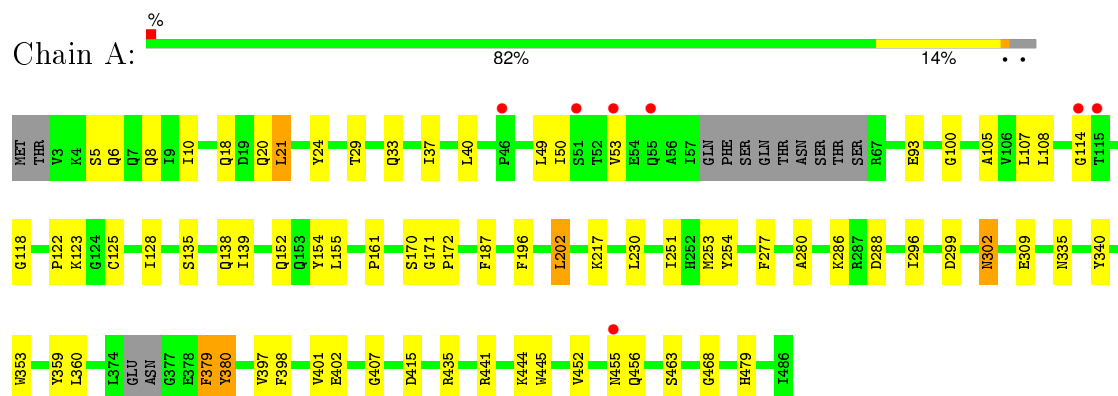
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total	O	0	0
			144	144		
6	B	79	Total	O	0	0
			79	79		

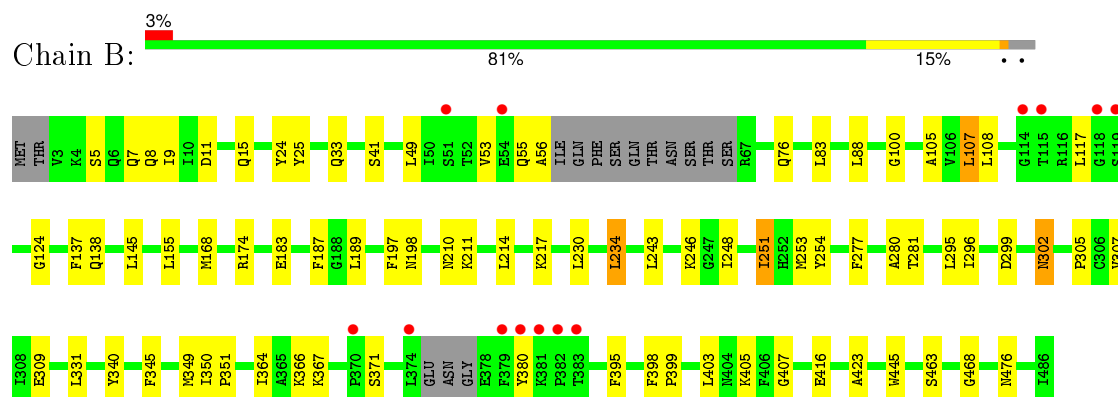
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: UDP-N-acetylglucosamine pyrophosphorylase



- Molecule 1: UDP-N-acetylglucosamine pyrophosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.56Å 61.98Å 90.25Å 90.07° 98.11° 92.93°	Depositor
Resolution (Å)	47.02 – 2.31 47.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.02-2.31) 97.1 (47.02-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.237 0.193 , 0.238	Depositor DCC
R_{free} test set	2162 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
Estimated twinning fraction	0.086 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43546 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7615	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, UD1, SO4

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	0.46	0/3734	0.66	0/5056
1	B	0.43	0/3700	0.64	0/5013
All	All	0.45	0/7434	0.65	0/10069

There are no bond length outliers.

There are no bond angle outliers.

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	3663	0	3564	56	0
1	B	3629	0	3506	58	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
4	A	39	0	25	0	0
4	B	39	0	25	0	0
5	A	6	0	8	1	0
6	A	144	0	0	1	0
6	B	79	0	0	2	0
All	All	7615	0	7128	114	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 8.

All (114) 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:B:299:ASP:HB3	1:B:302:ASN:HD21	1.36	0.88
1:A:455:ASN:OD1	1:A:456:GLN:HG2	1.78	0.82
1:A:299:ASP:HB3	1:A:302:ASN:HD21	1.46	0.78
1:A:49:LEU:O	1:A:53:VAL:HG23	1.89	0.73
1:A:5:SER:OG	1:A:8:GLN:HG3	1.91	0.71
1:B:251:ILE:CD1	1:B:253:MET:HG3	2.21	0.70
1:B:299:ASP:HB3	1:B:302:ASN:ND2	2.07	0.69
1:A:6:GLN:HG3	1:A:37:ILE:HG13	1.76	0.67
1:B:251:ILE:HD12	1:B:251:ILE:C	2.16	0.66
1:B:11:ASP:O	1:B:15:GLN:HG3	1.96	0.65
1:A:18:GLN:HB3	1:A:21:LEU:HD22	1.78	0.63
1:A:18:GLN:NE2	1:A:50:ILE:HD13	2.14	0.63
1:A:445:TRP:CH2	1:A:468:GLY:HA2	2.34	0.63
1:A:33:GLN:O	1:A:37:ILE:HG12	1.98	0.62
1:A:302:ASN:HD22	1:A:302:ASN:H	1.48	0.61
1:A:398:PHE:O	1:A:401:VAL:HG12	2.00	0.61
1:B:214:LEU:O	1:B:371:SER:HB2	2.00	0.60
1:B:117:LEU:O	1:B:423:ALA:HB2	2.01	0.60
1:A:379:PHE:O	1:A:380:TYR:HB3	2.01	0.59
1:A:299:ASP:HB3	1:A:302:ASN:ND2	2.18	0.58
1:B:100:GLY:HA3	1:B:155:LEU:HD12	1.85	0.57
1:B:302:ASN:HD22	1:B:302:ASN:H	1.53	0.57
1:B:49:LEU:O	1:B:53:VAL:HG23	2.04	0.57
1:B:210:ASN:ND2	1:B:211:LYS:HD3	2.20	0.57
1:A:24:TYR:CG	1:A:217:LYS:HG3	2.40	0.56
1:B:145:LEU:HD13	1:B:189:LEU:HD23	1.87	0.56
1:B:230:LEU:CD2	1:B:234:LEU:HD22	2.36	0.56
1:B:5:SER:OG	1:B:8:GLN:HG3	2.06	0.55
1:B:107:LEU:HB3	1:B:253:MET:HG2	1.89	0.55
1:A:107:LEU:HB2	1:A:253:MET:HG2	1.88	0.55
1:B:251:ILE:HD11	1:B:253:MET:HG3	1.89	0.54
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.08	0.54
1:A:302:ASN:ND2	1:A:302:ASN:H	2.05	0.54
1:A:108:LEU:HD13	1:A:254:TYR:CE1	2.43	0.54
1:A:230:LEU:C	1:A:230:LEU:HD23	2.28	0.53
1:A:24:TYR:CD1	1:A:217:LYS:HG3	2.44	0.53
1:B:230:LEU:C	1:B:230:LEU:HD23	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD13	1:A:254:TYR:CZ	2.44	0.53
1:B:281:THR:HG21	1:B:296:ILE:HD13	1.90	0.52
1:A:135:SER:O	1:A:139:ILE:HG13	2.08	0.52
1:B:309:GLU:HA	1:B:309:GLU:OE1	2.10	0.52
1:A:20:GLN:NE2	1:A:21:LEU:HD13	2.24	0.52
1:B:416:GLU:HB3	6:B:2148:HOH:O	2.09	0.51
1:B:168:MET:HB2	1:B:197:PHE:CZ	2.44	0.51
1:A:138:GLN:HB2	1:A:187:PHE:CE2	2.46	0.50
1:B:281:THR:HG21	1:B:296:ILE:CD1	2.42	0.50
1:A:152:GLN:HB2	1:A:161:PRO:HD2	1.95	0.49
1:B:56:ALA:HB1	1:B:364:ILE:HD13	1.95	0.48
1:A:353:TRP:O	1:A:360:LEU:HD12	2.13	0.48
1:A:29:THR:O	1:A:33:GLN:HG3	2.14	0.48
1:B:364:ILE:HD12	1:B:364:ILE:N	2.29	0.48
1:B:302:ASN:H	1:B:302:ASN:ND2	2.11	0.48
1:A:455:ASN:ND2	1:A:456:GLN:HE21	2.12	0.48
1:B:305:PRO:HD3	1:B:403:LEU:HD13	1.94	0.48
1:B:174:ARG:HH11	1:B:198:ASN:ND2	2.12	0.48
1:A:128:ILE:O	1:A:435:ARG:HD3	2.13	0.48
1:A:353:TRP:CE2	1:A:397:VAL:HB	2.49	0.47
1:A:280:ALA:HB3	1:A:340:TYR:HB3	1.95	0.47
1:B:345:PHE:CE1	1:B:349:MET:HG3	2.49	0.47
1:A:277:PHE:CE1	1:A:407:GLY:HA3	2.49	0.47
1:B:246:LYS:HE3	6:B:2178:HOH:O	2.13	0.47
1:B:107:LEU:CB	1:B:253:MET:HG2	2.44	0.47
1:B:25:TYR:CZ	1:B:33:GLN:HB3	2.50	0.47
1:A:122:PRO:HG2	1:A:125:CYS:SG	2.54	0.47
1:B:302:ASN:HD22	1:B:302:ASN:N	2.11	0.46
1:B:210:ASN:O	1:B:211:LYS:HD2	2.16	0.46
1:B:124:GLY:HA3	1:B:137:PHE:CE2	2.50	0.46
1:B:138:GLN:HB2	1:B:187:PHE:CE2	2.52	0.45
1:B:277:PHE:CE1	1:B:407:GLY:HA3	2.52	0.45
1:B:24:TYR:CD2	1:B:217:LYS:HE2	2.52	0.45
1:B:280:ALA:HA	1:B:407:GLY:O	2.18	0.45
1:A:114:GLY:HA2	2:A:1101:SO4:O4	2.17	0.45
1:A:171:GLY:N	1:A:172:PRO:HD2	2.32	0.44
1:B:340:TYR:CD2	1:B:340:TYR:C	2.91	0.44
1:B:230:LEU:HD23	1:B:234:LEU:HD22	1.98	0.44
1:A:302:ASN:N	1:A:302:ASN:HD22	2.07	0.44
1:A:302:ASN:ND2	1:A:302:ASN:N	2.64	0.44
1:B:100:GLY:HA3	1:B:155:LEU:CD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ILE:HD11	1:B:253:MET:HE2	1.99	0.43
1:A:415:ASP:OD2	1:A:441:ARG:HG3	2.18	0.43
1:A:105:ALA:HB3	1:A:251:ILE:CD1	2.48	0.43
1:B:398:PHE:N	1:B:399:PRO:HD2	2.33	0.43
1:A:444:LYS:HE2	1:A:444:LYS:HB3	1.84	0.43
1:A:452:VAL:HG11	1:A:479:HIS:CE1	2.54	0.43
1:B:9:ILE:HD13	1:B:41:SER:HB3	2.01	0.43
1:A:196:PHE:O	5:A:1301:GOL:H2	2.19	0.42
1:A:296:ILE:CD1	1:A:335:ASN:HB2	2.49	0.42
1:A:100:GLY:HA3	1:A:155:LEU:HD12	2.00	0.42
1:A:18:GLN:O	1:A:21:LEU:HB2	2.20	0.42
1:B:307:VAL:HB	1:B:395:PHE:CD1	2.54	0.42
1:B:366:LYS:O	1:B:367:LYS:HD2	2.19	0.42
1:A:445:TRP:CZ2	1:A:468:GLY:HA2	2.54	0.42
1:A:123:LYS:HE3	6:A:1389:HOH:O	2.20	0.42
1:B:105:ALA:HB2	1:B:248:ILE:HD13	2.00	0.42
1:B:230:LEU:HD23	1:B:230:LEU:O	2.20	0.42
1:B:7:GLN:NE2	1:B:11:ASP:OD1	2.51	0.41
1:A:170:SER:OG	1:A:172:PRO:HG2	2.20	0.41
1:A:93:GLU:HG2	1:A:154:TYR:CE1	2.54	0.41
1:A:455:ASN:CG	1:A:456:GLN:HE21	2.24	0.41
1:B:105:ALA:O	1:B:251:ILE:HA	2.21	0.41
1:B:251:ILE:HD11	1:B:253:MET:CE	2.51	0.41
1:A:286:LYS:HE2	1:A:288:ASP:O	2.21	0.41
1:A:202:LEU:HA	1:A:202:LEU:HD12	1.88	0.41
1:A:18:GLN:NE2	1:A:50:ILE:CD1	2.83	0.41
1:B:83:LEU:HB2	1:B:88:LEU:HD21	2.03	0.41
1:B:108:LEU:HD13	1:B:254:TYR:CZ	2.55	0.41
1:A:296:ILE:HD12	1:A:296:ILE:N	2.36	0.41
1:B:445:TRP:CH2	1:B:468:GLY:HA2	2.56	0.41
1:B:76:GLN:HA	1:B:76:GLN:NE2	2.36	0.41
1:B:350:ILE:N	1:B:351:PRO:CD	2.84	0.40
1:A:455:ASN:HD21	1:A:456:GLN:HE21	1.68	0.40
1:A:6:GLN:O	1:A:10:ILE:HG13	2.22	0.40
1:B:230:LEU:HD21	1:B:234:LEU:HD22	2.03	0.40
1:B:295:LEU:HD13	1:B:331:LEU:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/486 (96%)	453 (97%)	11 (2%)	3 (1%)	30	35
1	B	465/486 (96%)	443 (95%)	21 (4%)	1 (0%)	52	64
All	All	932/972 (96%)	896 (96%)	32 (3%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	A	380	TYR
1	A	379	PHE
1	A	118	GLY

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	391/432 (90%)	384 (98%)	7 (2%)	66	81
1	B	380/432 (88%)	370 (97%)	10 (3%)	54	71
All	All	771/864 (89%)	754 (98%)	17 (2%)	60	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	202	LEU
1	A	302	ASN
1	A	359	TYR
1	A	402	GLU
1	A	463	SER
1	B	107	LEU
1	B	183	GLU
1	B	234	LEU
1	B	243	LEU
1	B	251	ILE
1	B	302	ASN
1	B	380	TYR
1	B	405	LYS
1	B	463	SER
1	B	476	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	23	GLN
1	A	101	ASN
1	A	140	GLN
1	A	164	ASN
1	A	190	ASN
1	A	198	ASN
1	A	222	GLN
1	A	302	ASN
1	A	357	GLN
1	A	436	ASN
1	A	456	GLN
1	A	479	HIS
1	B	17	ASN
1	B	149	GLN
1	B	152	GLN
1	B	153	GLN
1	B	185	ASN
1	B	198	ASN
1	B	302	ASN
1	B	357	GLN
1	B	456	GLN
1	B	476	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
4	UD1	A	1001	-	32,41,41	1.48	3 (9%)	46,62,62	2.31	6 (13%)
2	SO4	A	1101	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	A	1102	-	4,4,4	0.23	0	6,6,6	0.24	0
5	GOL	A	1301	-	5,5,5	0.28	0	5,5,5	0.21	0
4	UD1	B	2001	-	32,41,41	1.55	3 (9%)	46,62,62	2.17	6 (13%)
2	SO4	B	2102	-	4,4,4	0.20	0	6,6,6	0.12	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
4	UD1	A	1001	-	-	0/22/63/63	0/3/3/3
2	SO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1301	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UD1	B	2001	-	-	0/22/63/63	0/3/3/3
2	SO4	B	2102	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	UD1	C6-C5	-2.45	1.32	1.38
4	A	1001	UD1	C6-C5	-2.07	1.33	1.38
4	B	2001	UD1	C6-N1	4.07	1.41	1.35
4	A	1001	UD1	C6-N1	4.25	1.41	1.35
4	A	1001	UD1	C4-N3	4.75	1.41	1.33
4	B	2001	UD1	C4-N3	5.52	1.43	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	UD1	C5-C4-N3	-3.00	115.43	123.12
4	A	1001	UD1	C5-C4-N3	-2.95	115.56	123.12
4	A	1001	UD1	C4'-C3'-C2'	-2.38	107.13	110.43
4	B	2001	UD1	C2'-N2'-C7'	-2.35	117.06	123.10
4	A	1001	UD1	C2'-N2'-C7'	-2.06	117.81	123.10
4	B	2001	UD1	C4'-C3'-C2'	-2.05	107.59	110.43
4	B	2001	UD1	PB-O3A-PA	2.53	139.84	132.73
4	A	1001	UD1	O3A-PB-O1'	2.73	111.48	103.63
4	B	2001	UD1	O3A-PB-O1'	2.96	112.14	103.63
4	A	1001	UD1	PB-O3A-PA	3.95	143.81	132.73
4	B	2001	UD1	C4-N3-C2	12.51	126.53	114.14
4	A	1001	UD1	C4-N3-C2	13.17	127.19	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	SO4	1	0
5	A	1301	GOL	1	0

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	A	473/486 (97%)	0.00	7 (1%) 76 82	8, 21, 51, 62	3 (0%)
1	B	471/486 (96%)	0.11	13 (2%) 56 66	11, 26, 56, 77	0
All	All	944/972 (97%)	0.06	20 (2%) 67 74	8, 24, 53, 77	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	SER	3.7
1	B	118	GLY	3.5
1	B	374	LEU	3.5
1	B	383	THR	3.5
1	A	114	GLY	3.4
1	B	382	PRO	3.2
1	B	380	TYR	3.1
1	B	381	LYS	3.1
1	B	379	PHE	2.9
1	A	51	SER	2.7
1	B	114	GLY	2.7
1	A	46	PRO	2.7
1	A	53	VAL	2.5
1	B	119	SER	2.5
1	A	115	THR	2.4
1	B	115	THR	2.3
1	A	55	GLN	2.3
1	B	370	PRO	2.2
1	A	455	ASN	2.1
1	B	54	GLU	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	1301	6/6	0.89	0.24	8.54	37,40,41,42	6
2	SO4	A	1101	5/5	0.83	0.29	1.32	45,46,47,48	5
4	UD1	B	2001	39/39	0.95	0.13	-0.09	15,29,39,40	0
4	UD1	A	1001	39/39	0.95	0.12	-0.17	12,22,30,32	0
2	SO4	B	2102	5/5	0.95	0.17	-	33,35,35,38	5
3	MG	A	1201	1/1	0.83	0.17	-	28,28,28,28	1
2	SO4	A	1102	5/5	0.94	0.18	-	31,32,35,36	5

6.5 Other polymers [i](#)

There are no such residues in this entry.