



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:33 AM GMT

PDB ID : 1JV3  
Title : CRYSTAL STRUCTURE OF HUMAN AGX1 COMPLEXED WITH UDP-GALNAC  
Authors : Peneff, C.; Bourne, Y.  
Deposited on : 2001-08-28  
Resolution : 2.20 Å(reported)

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

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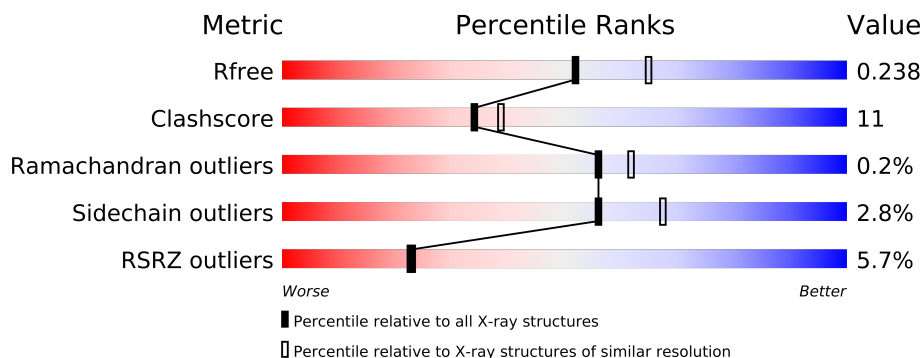
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : 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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 8477 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.

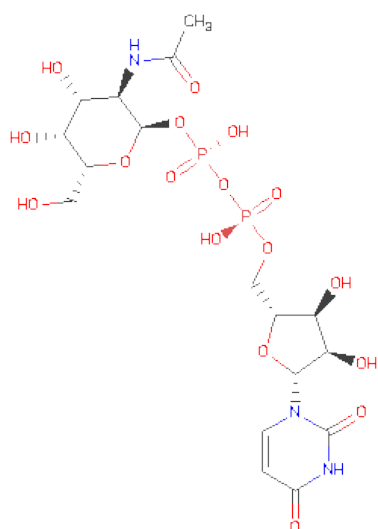
- Molecule 1 is a protein called GlcNAc1P uridyltransferase isoform 1: AGX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	5	0
			3916	2506	668	724	18			
1	B	484	Total	C	N	O	S	0	6	0
			3868	2478	655	717	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	SER	SEE REMARK 999	UNP Q16222
B	445	GLY	SER	SEE REMARK 999	UNP Q16222

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYL GALACTOSAMINE (three-letter code: UD2) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>17</sub>P<sub>2</sub>).



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

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

- Molecule 3 is water.

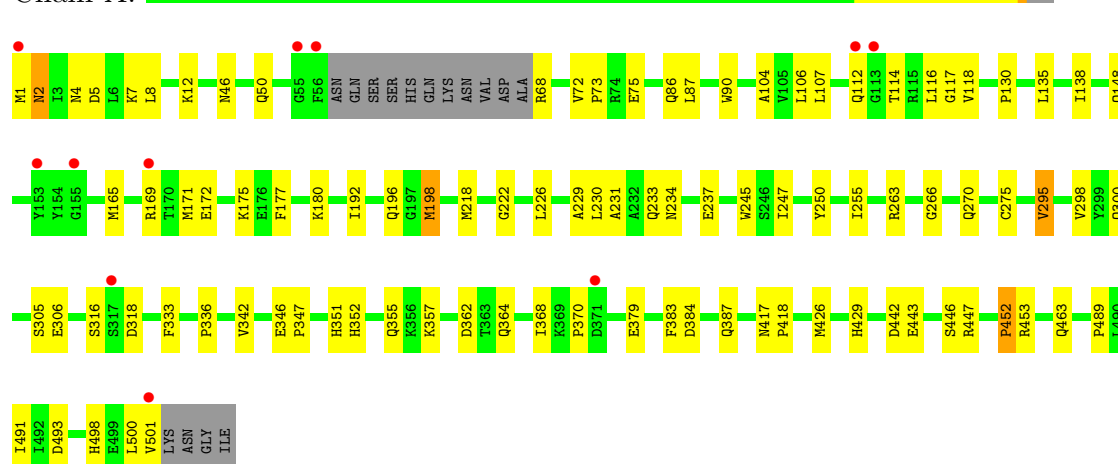
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	361	Total	O	0	0
			361	361		
3	B	254	Total	O	0	0
			254	254		

### 3 Residue-property plots

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

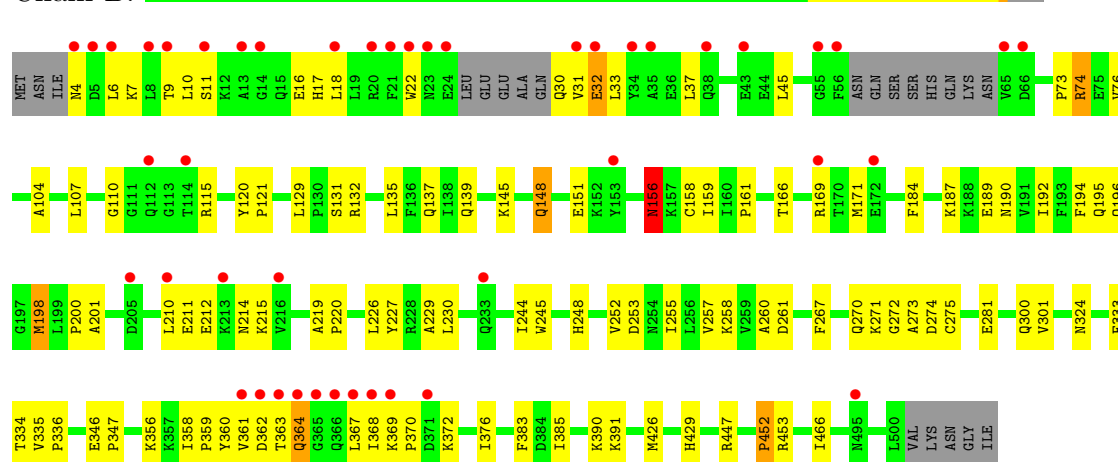
- Molecule 1: GlcNAc1P uridyltransferase isoform 1: AGX1

Chain A:



- Molecule 1: GlcNAc1P uridyltransferase isoform 1: AGX1

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.73Å 70.77Å 95.38Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	19.99 – 2.20 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.99-2.20) 97.5 (19.99-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.190 , 0.234 0.194 , 0.238	Depositor DCC
$R_{free}$ test set	1684 reflections (2.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 64843 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UD2

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	0.60	0/4026	0.69	0/5441
1	B	0.51	0/3980	0.63	0/5379
All	All	0.56	0/8006	0.66	0/10820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	3916	0	3883	88	0
1	B	3868	0	3822	86	0
2	A	39	0	24	1	0
2	B	39	0	24	3	0
3	A	361	0	0	13	0
3	B	254	0	0	10	0
All	All	8477	0	7753	171	0

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 11.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453[B]:ARG:HH12	1:B:356:LYS:NZ	1.70	0.90
1:B:429:HIS:CD2	1:B:466:ILE:H	1.92	0.87
1:B:196:GLN:HE22	2:B:902:UD2:HN3	1.18	0.87
1:B:33:LEU:HD22	1:B:214:ASN:HA	1.56	0.86
1:A:90:TRP:HE1	1:A:270[B]:GLN:NE2	1.80	0.80
1:B:248:HIS:HD2	1:B:260:ALA:H	1.31	0.78
1:B:429:HIS:HD2	1:B:466:ILE:H	1.30	0.77
1:B:135:LEU:O	1:B:139:GLN:HG3	1.88	0.74
1:A:72:VAL:HG22	3:A:1055:HOH:O	1.89	0.72
1:A:352:HIS:HE1	1:A:384:ASP:OD1	1.72	0.71
1:A:114:THR:HG21	1:A:118:VAL:HG22	1.71	0.71
1:A:453[B]:ARG:HH12	1:B:356:LYS:HZ1	1.38	0.70
1:B:198:MET:HG3	1:B:219:ALA:O	1.94	0.68
1:A:306:GLU:OE2	1:A:352:HIS:HD2	1.75	0.68
1:B:31:VAL:HG13	1:B:32:GLU:H	1.60	0.67
1:B:73:PRO:HG2	1:B:76:VAL:HG22	1.76	0.66
1:B:107:LEU:HD11	1:B:252:VAL:HB	1.76	0.65
1:B:248:HIS:CD2	1:B:260:ALA:H	2.15	0.64
1:B:166:THR:OG1	3:B:1153:HOH:O	2.14	0.64
1:B:272:GLY:HA2	3:B:1029:HOH:O	1.97	0.64
1:A:171:MET:SD	1:A:175:LYS:HE2	2.38	0.63
2:A:901:UD2:PA	3:A:1241:HOH:O	2.60	0.60
1:B:368:ILE:HG13	1:B:369:LYS:N	2.17	0.59
1:B:110:GLY:HA3	1:B:196:GLN:HE21	1.68	0.59
1:A:86:GLN:HE22	1:A:270[B]:GLN:HE22	1.50	0.59
1:A:114:THR:HB	1:A:118:VAL:O	2.02	0.58
1:A:2:ASN:C	1:A:2:ASN:HD22	2.05	0.58
1:A:107:LEU:HD13	1:A:250:TYR:CE1	2.38	0.58
1:B:426:MET:HE3	3:B:1011:HOH:O	2.03	0.58
1:B:201:ALA:HB1	1:B:358:ILE:HD13	1.85	0.58
1:A:46:ASN:O	1:A:50:GLN:HG3	2.04	0.57
1:A:453[B]:ARG:HH12	1:B:356:LYS:HZ3	1.51	0.57
1:B:189:GLU:H	1:B:189:GLU:CD	2.08	0.57
1:B:367:LEU:HD23	1:B:368:ILE:N	2.20	0.56
1:B:360:TYR:HE1	1:B:362:ASP:HB3	1.69	0.56
1:A:86:GLN:NE2	1:A:270[B]:GLN:HE22	2.04	0.56
1:A:192:ILE:HD12	1:A:192:ILE:N	2.20	0.56
1:A:72:VAL:HG13	3:A:1055:HOH:O	2.05	0.56
1:B:4:ASN:ND2	1:B:7:LYS:HD3	2.20	0.56
1:A:443:GLU:HB3	1:B:372:LYS:HG2	1.87	0.55
1:B:156:ASN:HD22	1:B:156:ASN:N	2.04	0.55
1:A:222:GLY:HA3	1:A:379:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:274:ASP:HA	1:B:334:THR:HG23	1.87	0.55
2:B:902:UD2:PA	3:B:1141:HOH:O	2.64	0.55
1:B:346:GLU:HB3	1:B:347:PRO:HD3	1.88	0.55
1:B:359:PRO:HG2	3:B:1133:HOH:O	2.06	0.54
1:A:177:PHE:HA	1:A:180:LYS:NZ	2.22	0.54
1:B:74:ARG:HB3	1:B:74:ARG:HH11	1.72	0.54
1:B:169:ARG:HD3	1:B:220:PRO:HD3	1.90	0.54
1:B:198:MET:HG3	1:B:219:ALA:C	2.27	0.54
1:A:231:ALA:HB2	1:A:342:VAL:HG13	1.89	0.54
1:A:357:LYS:HB3	1:A:370:PRO:HG2	1.90	0.54
1:A:114:THR:HG21	1:A:118:VAL:H	1.73	0.53
1:A:2:ASN:HD21	1:A:4:ASN:HB2	1.73	0.53
1:A:355:GLN:NE2	3:A:958:HOH:O	2.43	0.52
1:A:417:ASN:HB2	1:A:418:PRO:CD	2.40	0.52
1:B:33:LEU:HD13	1:B:214:ASN:C	2.30	0.52
1:A:90:TRP:HE1	1:A:270[B]:GLN:HE22	1.56	0.52
1:B:107:LEU:HD11	1:B:252:VAL:CB	2.40	0.52
1:A:177:PHE:HA	1:A:180:LYS:HZ1	1.74	0.51
1:A:2:ASN:ND2	1:A:5:ASP:H	2.08	0.51
1:B:363:THR:O	1:B:364:GLN:HB2	2.09	0.51
1:A:7:LYS:NZ	3:A:1250:HOH:O	2.43	0.51
1:A:351:HIS:HD2	3:A:1051:HOH:O	1.93	0.51
1:A:346:GLU:HB3	1:A:347:PRO:HD3	1.91	0.51
1:A:138:ILE:CD1	1:A:255:ILE:HD11	2.41	0.50
1:B:6:LEU:HA	1:B:9:THR:OG1	2.11	0.50
1:B:18:LEU:HD13	1:B:37:LEU:HD11	1.92	0.50
1:A:362:ASP:HB3	1:A:368:ILE:HD12	1.94	0.50
1:B:212:GLU:HB2	1:B:215:LYS:HB3	1.93	0.50
1:B:145:LYS:NZ	1:B:148[B]:GLN:HE22	2.10	0.49
1:A:351:HIS:HE1	3:A:1146:HOH:O	1.95	0.49
1:A:130:PRO:HB2	1:A:491:ILE:HD11	1.95	0.49
1:B:120:TYR:HB2	1:B:121:PRO:HD2	1.94	0.49
1:A:73:PRO:HB2	1:A:75:GLU:OE1	2.13	0.49
1:B:196:GLN:HA	1:B:229:ALA:HB2	1.94	0.49
1:A:2:ASN:ND2	1:A:4:ASN:HB2	2.27	0.48
1:B:104:ALA:CB	1:B:161:PRO:HG2	2.43	0.48
1:B:361:VAL:HG23	1:B:361:VAL:O	2.13	0.48
1:B:33:LEU:HD13	1:B:214:ASN:O	2.12	0.48
1:B:11:SER:HA	1:B:16:GLU:HG3	1.95	0.48
1:A:275:CYS:HG	1:A:333:PHE:HE2	1.61	0.48
1:B:359:PRO:HA	1:B:370:PRO:HD3	1.96	0.48
1:B:452:PRO:HD3	3:B:1101:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:TRP:CZ3	1:B:336:PRO:HG2	2.48	0.48
1:A:8:LEU:HG	1:A:12:LYS:HE3	1.96	0.47
1:B:156:ASN:N	1:B:156:ASN:ND2	2.63	0.47
1:A:114:THR:CG2	1:A:116:LEU:HB2	2.44	0.47
1:A:305:SER:HB3	1:B:453:ARG:HG3	1.96	0.47
1:A:387:GLN:NE2	3:A:1252:HOH:O	2.48	0.47
1:B:187:LYS:HB2	1:B:190:ASN:HD22	1.80	0.47
1:B:171:MET:HG2	1:B:195:GLN:HE21	1.79	0.47
1:A:266:GLY:O	1:A:270[A]:GLN:HG2	2.14	0.47
1:B:211:GLU:O	1:B:361:VAL:HG13	2.15	0.47
1:A:295:VAL:CG1	1:A:300[A]:GLN:NE2	2.78	0.47
1:A:104:ALA:HB3	1:A:247:ILE:HD13	1.97	0.47
1:A:295:VAL:HG13	3:A:1054:HOH:O	2.14	0.47
1:A:87:LEU:HD22	1:A:263:ARG:HD3	1.97	0.47
1:A:443:GLU:CB	1:B:372:LYS:HG2	2.44	0.46
1:B:301:VAL:HB	1:B:383:PHE:CD1	2.50	0.46
1:B:359:PRO:HB3	1:B:369:LYS:HD2	1.97	0.46
1:A:114:THR:CG2	1:A:118:VAL:H	2.28	0.46
1:B:104:ALA:HB2	1:B:161:PRO:HG2	1.98	0.46
1:B:31:VAL:HG13	1:B:32:GLU:N	2.29	0.46
1:A:135:LEU:CD2	1:A:255:ILE:HD13	2.45	0.46
1:A:364:GLN:HE21	1:A:364:GLN:N	2.14	0.46
2:B:902:UD2:H6'2	3:B:917:HOH:O	2.14	0.46
1:A:493:ASP:OD1	1:A:498:HIS:HE1	1.99	0.46
1:B:18:LEU:HA	1:B:210:LEU:HD11	1.97	0.46
1:A:295:VAL:HG11	1:A:300[A]:GLN:NE2	2.31	0.46
1:A:245:TRP:CZ3	1:A:336:PRO:HG2	2.50	0.46
1:A:114:THR:HG22	1:A:116:LEU:N	2.31	0.46
1:B:244:ILE:O	1:B:335:VAL:HG21	2.15	0.46
1:A:2:ASN:C	1:A:2:ASN:ND2	2.69	0.45
1:B:275:CYS:HG	1:B:333:PHE:HE1	1.63	0.45
1:A:1:MET:HA	1:A:5:ASP:OD2	2.17	0.45
1:B:158:CYS:O	1:B:159:ILE:HD13	2.15	0.45
1:A:452:PRO:HA	3:A:1204:HOH:O	2.16	0.45
1:B:6:LEU:O	1:B:10:LEU:HD13	2.17	0.45
1:A:90:TRP:HD1	1:A:270[A]:GLN:HG3	1.81	0.45
1:B:273:ALA:HA	1:B:391:LYS:HB3	1.99	0.45
1:B:4:ASN:HA	1:B:7:LYS:HB3	1.98	0.45
1:A:426:MET:SD	1:A:463:GLN:HG2	2.57	0.44
1:A:226:LEU:O	1:A:230:LEU:HG	2.17	0.44
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.98	0.44
1:B:151:GLU:HG3	1:B:156:ASN:C	2.37	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:TYR:CZ	1:B:385:ILE:HD13	2.53	0.44
1:A:234:ASN:HA	1:A:237:GLU:OE1	2.17	0.44
1:B:45:LEU:HD13	1:B:200:PRO:HG3	1.99	0.43
1:B:258:LYS:HB3	1:B:261:ASP:HB2	2.00	0.43
1:B:452:PRO:CD	3:B:1101:HOH:O	2.66	0.43
1:A:298:VAL:CG1	1:A:387:GLN:HB2	2.49	0.43
1:A:300[B]:GLN:HB2	3:A:1117:HOH:O	2.18	0.43
1:B:187:LYS:HB2	1:B:190:ASN:ND2	2.34	0.43
1:B:129:LEU:HD11	1:B:255:ILE:HD11	1.99	0.43
1:A:86:GLN:HE22	1:A:270[B]:GLN:NE2	2.15	0.43
1:B:447:ARG:HD2	3:B:1123:HOH:O	2.19	0.43
1:B:137:GLN:HG3	1:B:184:PHE:CD2	2.53	0.43
1:A:306:GLU:OE2	1:A:352:HIS:CD2	2.64	0.43
1:A:165:MET:SD	1:A:226:LEU:HA	2.59	0.43
1:A:198:MET:HE2	1:A:218:MET:HB3	2.01	0.43
1:A:198:MET:HB3	1:A:198:MET:HE3	1.80	0.43
1:A:452:PRO:N	3:A:1133:HOH:O	2.51	0.42
1:A:351:HIS:CE1	3:A:1146:HOH:O	2.72	0.42
1:A:316:SER:OG	1:A:318:ASP:OD1	2.31	0.42
1:A:68:ARG:HA	1:A:68:ARG:HD2	1.82	0.42
1:A:112:GLN:OE1	1:A:169:ARG:HB2	2.20	0.42
1:A:2:ASN:ND2	1:A:4:ASN:H	2.18	0.42
1:A:192:ILE:H	1:A:192:ILE:HD12	1.84	0.42
1:B:267:PHE:O	1:B:271:LYS:HB2	2.20	0.42
1:B:360:TYR:CE1	1:B:362:ASP:HB3	2.53	0.41
1:A:90:TRP:O	1:A:266:GLY:HA3	2.20	0.41
1:A:489:PRO:HB2	1:A:500:LEU:HD12	2.01	0.41
1:B:131:SER:O	1:B:132:ARG:HB2	2.21	0.41
1:A:106:LEU:C	1:A:106:LEU:HD23	2.41	0.41
1:B:429:HIS:HD2	1:B:466:ILE:N	2.09	0.41
1:A:114:THR:HG22	1:A:117:GLY:N	2.35	0.41
1:A:138:ILE:HD12	1:A:255:ILE:HD11	2.03	0.41
1:B:226:LEU:O	1:B:230:LEU:HG	2.21	0.41
1:B:22:TRP:O	1:B:30:GLN:OE1	2.39	0.41
1:B:110:GLY:HA3	1:B:196:GLN:NE2	2.34	0.40
1:B:192:ILE:N	1:B:192:ILE:HD12	2.36	0.40
1:B:281[B]:GLU:CD	1:B:324:ASN:HD22	2.24	0.40
1:A:442:ASP:OD2	1:A:446:SER:HB2	2.21	0.40
1:A:196:GLN:HA	1:A:229:ALA:HB2	2.02	0.40
1:B:257:VAL:HG13	1:B:257:VAL:O	2.21	0.40
1:B:194:PHE:O	3:B:1153:HOH:O	2.22	0.40
1:A:295:VAL:HG12	1:A:300[A]:GLN:CD	2.42	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	491/505 (97%)	474 (96%)	17 (4%)	0	100	100
1	B	484/505 (96%)	455 (94%)	27 (6%)	2 (0%)	43	45
All	All	975/1010 (96%)	929 (95%)	44 (4%)	2 (0%)	56	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	HIS
1	B	156	ASN

### 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	423/433 (98%)	413 (98%)	10 (2%)	61	73
1	B	418/433 (96%)	404 (97%)	14 (3%)	50	60
All	All	841/866 (97%)	817 (97%)	24 (3%)	56	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	148	GLN
1	A	172	GLU
1	A	198	MET

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	295	VAL
1	A	383	PHE
1	A	447	ARG
1	A	452	PRO
1	A	501	VAL
1	B	32	GLU
1	B	74	ARG
1	B	115	ARG
1	B	148[A]	GLN
1	B	148[B]	GLN
1	B	156	ASN
1	B	198	MET
1	B	253	ASP
1	B	270	GLN
1	B	300	GLN
1	B	364	GLN
1	B	376	ILE
1	B	390	LYS
1	B	452	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	38	GLN
1	A	84	GLN
1	A	137	GLN
1	A	156	ASN
1	A	331	HIS
1	A	348	GLN
1	A	352	HIS
1	A	355	GLN
1	A	364	GLN
1	A	429	HIS
1	A	498	HIS
1	B	4	ASN
1	B	23	ASN
1	B	30	GLN
1	B	38	GLN
1	B	84	GLN
1	B	112	GLN

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Mol	Chain	Res	Type
1	B	139	GLN
1	B	156	ASN
1	B	195	GLN
1	B	196	GLN
1	B	248	HIS
1	B	300	GLN
1	B	331	HIS
1	B	348	GLN
1	B	351	HIS
1	B	423	HIS
1	B	429	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 ⓘ

2 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	UD2	A	901	-	41,41,41	2.15	9 (21%)	58,62,62	2.04	12 (20%)
2	UD2	B	902	-	41,41,41	2.19	9 (21%)	58,62,62	1.87	9 (15%)

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	UD2	A	901	-	-	0/25/63/63	0/3/3/3
2	UD2	B	902	-	-	0/25/63/63	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	UD2	C6-N1	8.03	1.48	1.35
2	B	902	UD2	C6-N1	7.97	1.48	1.35
2	B	902	UD2	PA-O3A	-5.43	1.50	1.59
2	A	901	UD2	PA-O3A	-4.94	1.50	1.59
2	A	901	UD2	PB-O3A	-4.82	1.51	1.59
2	B	902	UD2	PB-O3A	-4.65	1.51	1.59
2	B	902	UD2	O4'-C4'	-3.76	1.33	1.43
2	A	901	UD2	C1'-C2'	3.63	1.59	1.53
2	B	902	UD2	C5-C4	3.37	1.49	1.40
2	A	901	UD2	O4'-C4'	-3.20	1.35	1.43
2	A	901	UD2	C3'-C2'	3.01	1.59	1.53
2	A	901	UD2	C5-C4	2.74	1.47	1.40
2	B	902	UD2	C2'-N2'	2.65	1.50	1.45
2	B	902	UD2	C4'-C5'	2.52	1.58	1.53
2	B	902	UD2	C1'-C2'	2.47	1.57	1.53
2	B	902	UD2	C2-N1	2.23	1.40	1.38
2	A	901	UD2	O1'-C1'	2.23	1.46	1.42
2	A	901	UD2	O5'-C1'	2.21	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	UD2	C4'-C3'-C2'	-8.52	98.35	110.44
2	B	902	UD2	C4'-C3'-C2'	-6.11	101.77	110.44
2	B	902	UD2	O4'-C4'-C3'	5.67	123.06	110.35
2	A	901	UD2	O4'-C4'-C5'	5.32	123.30	109.28
2	B	902	UD2	O4'-C4'-C5'	5.27	123.17	109.28
2	A	901	UD2	O4'-C4'-C3'	5.10	121.79	110.35
2	B	902	UD2	C3'-C4'-C5'	-4.18	102.74	110.20
2	B	902	UD2	O3'-C3'-C2'	-3.49	102.45	109.61
2	A	901	UD2	C1'-C2'-N2'	-3.40	104.58	111.02
2	A	901	UD2	O1'-C1'-C2'	-3.24	102.76	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	UD2	O5'-C5'-C4'	-3.18	103.88	109.76
2	A	901	UD2	O3'-C3'-C2'	-3.17	103.09	109.61
2	A	901	UD2	C3'-C4'-C5'	-3.06	104.74	110.20
2	A	901	UD2	O5'-C1'-O1'	2.94	115.21	111.36
2	A	901	UD2	O5'-C5'-C4'	-2.86	104.47	109.76
2	B	902	UD2	C1'-C2'-N2'	-2.79	105.75	111.02
2	B	902	UD2	O1'-C1'-C2'	-2.77	103.50	107.91
2	A	901	UD2	C6'-C5'-C4'	-2.38	107.24	113.00
2	B	902	UD2	C5-C6-N1	-2.28	118.63	121.21
2	A	901	UD2	O1A-PA-O3A	2.07	114.98	105.14
2	A	901	UD2	C5-C6-N1	-2.04	118.90	121.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	490/505 (97%)	-0.31	11 (2%) 59 59	14, 29, 49, 70	0
1	B	484/505 (95%)	0.26	45 (9%) 9 8	17, 40, 78, 92	0
All	All	974/1010 (96%)	-0.03	56 (5%) 23 23	14, 34, 68, 92	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	GLY	8.1
1	B	364	GLN	7.5
1	B	6	LEU	6.2
1	B	4	ASN	6.1
1	B	8	LEU	6.1
1	B	363	THR	5.9
1	B	5	ASP	5.3
1	B	22	TRP	4.9
1	B	31	VAL	4.9
1	B	65	VAL	4.7
1	B	56	PHE	4.6
1	B	18	LEU	4.5
1	B	35	ALA	4.2
1	A	169	ARG	4.0
1	A	501	VAL	3.9
1	B	34	TYR	3.8
1	B	366	GLN	3.7
1	A	1	MET	3.6
1	B	20	ARG	3.5
1	B	362	ASP	3.5
1	B	371	ASP	3.4
1	B	9	THR	3.3
1	B	38	GLN	3.2
1	B	112	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	153	TYR	3.1
1	B	367	LEU	3.1
1	B	369	LYS	3.1
1	B	11	SER	3.0
1	B	23	ASN	3.0
1	A	113	GLY	2.9
1	B	153	TYR	2.9
1	B	32	GLU	2.7
1	B	213	LYS	2.7
1	B	205	ASP	2.6
1	A	317	SER	2.6
1	B	43	GLU	2.5
1	B	114	THR	2.4
1	A	112	GLN	2.4
1	B	24	GLU	2.4
1	B	365	GLY	2.4
1	B	14	GLY	2.3
1	B	368	ILE	2.3
1	A	55	GLY	2.3
1	B	169	ARG	2.2
1	A	56	PHE	2.2
1	B	172	GLU	2.2
1	B	21	PHE	2.1
1	B	361	VAL	2.1
1	A	371	ASP	2.1
1	B	233	GLN	2.1
1	B	66	ASP	2.1
1	B	495	ASN	2.1
1	B	13	ALA	2.1
1	A	155	GLY	2.0
1	B	210	LEU	2.0
1	B	216	VAL	2.0

## 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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UD2	A	901	39/39	0.10	0.23	21,26,40,45	0
2	UD2	B	902	39/39	0.10	0.06	25,33,41,45	0

## 6.5 Other polymers

There are no such residues in this entry.