



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:36 pm GMT

PDB ID : 1JVG  
Title : CRYSTAL STRUCTURE OF HUMAN AGX2 COMPLEXED WITH UDP-GALNAC  
Authors : Peneff, C.; Bourne, Y.  
Deposited on : 2001-08-30  
Resolution : 2.30 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

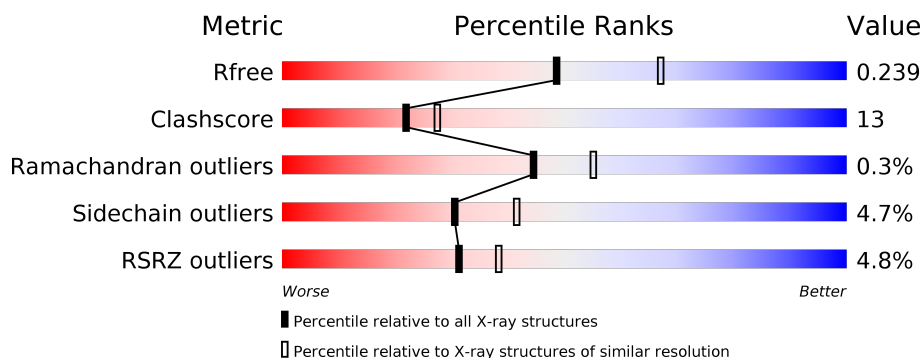
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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	522	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	522	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8040 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.

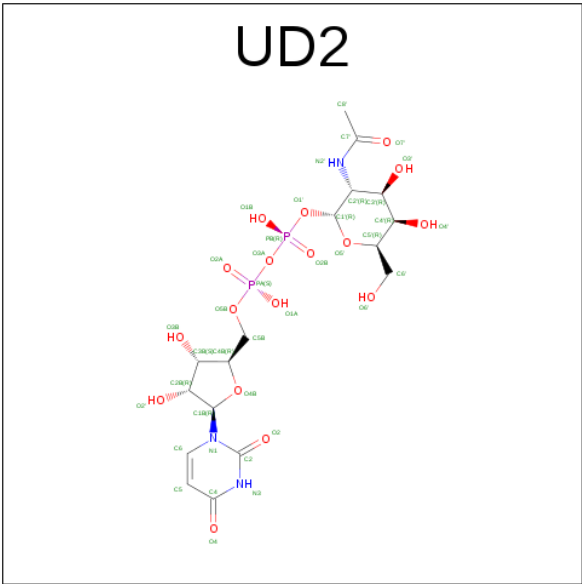
- Molecule 1 is a protein called GLCNAC1P URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	1	0
			3851	2467	654	712	18			
1	B	480	Total	C	N	O	S	0	0	0
			3803	2439	643	703	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	SER	SEE REMARK 999	UNP Q16222
A	454	SER	GLN	SEE REMARK 999	UNP Q16222
B	445	GLY	SER	SEE REMARK 999	UNP Q16222
B	454	SER	GLN	SEE REMARK 999	UNP Q16222

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (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		
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	183	Total	O	0	0
			183	183		
3	B	125	Total	O	0	0
			125	125		



3514	
1517	
VAL	
LYS	
ASN	
GLY	
ILE	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.58Å 71.78Å 93.56Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.94-2.30) 97.6 (19.94-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.201 , 0.240 0.201 , 0.239	Depositor DCC
$R_{free}$ test set	1985 reflections (4.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: 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	0/3940	0.70	3/5324 (0.1%)
1	B	0.54	0/3887	0.63	0/5254
All	All	0.57	0/7827	0.67	3/10578 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	453[A]	ARG	CB-CA-C	5.42	121.25	110.40
1	A	453[B]	ARG	CB-CA-C	5.42	121.25	110.40

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3851	0	3800	93	0
1	B	3803	0	3743	117	0
2	A	39	0	24	0	0
2	B	39	0	25	1	0
3	A	183	0	0	4	0
3	B	125	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8040	0	7592	203	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 13.

All (203) 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:A:15:GLN:NE2	1:A:208:ILE:H	1.66	0.93
1:B:20:ARG:HH21	1:B:363:THR:HA	1.36	0.91
1:A:239:MET:HE3	1:A:335:VAL:HG22	1.54	0.89
1:A:26:GLU:H	1:A:29:GLN:HE21	1.16	0.88
1:A:239:MET:CE	1:A:335:VAL:HG22	2.06	0.85
1:B:15:GLN:HE22	1:B:207:LYS:HA	1.45	0.82
1:A:443:GLU:HB3	1:B:372:LYS:HD2	1.63	0.79
1:A:453[B]:ARG:HB2	1:A:453[B]:ARG:HH11	1.47	0.79
1:B:212:GLU:HB2	1:B:215:LYS:HB3	1.65	0.79
1:B:64:ASN:ND2	1:B:66:ASP:HB2	1.98	0.79
1:B:15:GLN:NE2	1:B:208:ILE:H	1.81	0.78
1:A:175:LYS:O	1:A:179:THR:HG22	1.85	0.76
1:A:47:PHE:CE1	1:A:51:LYS:HE2	2.22	0.75
1:A:284:ASN:HD22	1:A:285:PRO:HD2	1.54	0.72
1:A:72:VAL:HG22	3:A:1930:HOH:O	1.88	0.72
1:B:20:ARG:NH2	1:B:363:THR:HA	2.04	0.72
1:B:417:ASN:ND2	1:B:420:THR:H	1.87	0.72
1:A:28:ALA:O	1:A:31:VAL:HG12	1.89	0.71
1:A:429:HIS:CD2	1:A:483:ILE:H	2.08	0.71
1:B:15:GLN:HG2	1:B:208:ILE:HD12	1.71	0.71
1:A:112:GLN:HB2	1:A:169:ARG:NH1	2.06	0.71
1:A:116:LEU:HD11	1:A:406:LEU:HD22	1.71	0.70
1:A:15:GLN:HE22	1:A:208:ILE:H	1.40	0.69
1:A:248:HIS:HD1	1:A:260:ALA:H	1.39	0.68
1:A:87:LEU:HD22	1:A:263:ARG:HD3	1.75	0.68
1:A:284:ASN:HD22	1:A:285:PRO:CD	2.06	0.68
1:A:8:LEU:HG	1:A:12:LYS:HE3	1.75	0.67
1:A:423:HIS:CD2	1:B:413:ASN:HB3	2.30	0.67
1:B:417:ASN:ND2	1:B:419:THR:HG23	2.09	0.67
1:A:124:MET:HE1	1:A:173:SER:HB3	1.77	0.66
1:B:64:ASN:HD22	1:B:66:ASP:HB2	1.61	0.65
1:B:417:ASN:C	1:B:417:ASN:HD22	2.00	0.64
1:B:248:HIS:HD1	1:B:260:ALA:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HB2	1:B:508:ILE:HD11	1.80	0.64
1:A:408:ASN:HB3	1:A:413:ASN:HD22	1.63	0.64
1:B:442:ASP:OD2	1:B:446:SER:HB2	1.98	0.63
1:B:15:GLN:HE21	1:B:17:HIS:HE1	1.46	0.63
1:A:429:HIS:HD2	1:A:483:ILE:H	1.45	0.62
1:B:84:GLN:HA	1:B:87:LEU:HG	1.81	0.62
1:A:409:ALA:O	1:A:410:ASP:HB2	2.00	0.62
1:A:26:GLU:O	1:A:30:GLN:HG2	2.00	0.62
1:B:235:ILE:HG22	1:B:239:MET:HE3	1.83	0.60
1:B:26:GLU:O	1:B:30:GLN:HG3	2.00	0.60
1:B:340:ASP:O	1:B:344:VAL:HB	2.01	0.60
1:A:346:GLU:HB3	1:A:347:PRO:HD3	1.84	0.59
1:A:66:ASP:HA	1:A:69:MET:HE2	1.83	0.59
1:A:121:PRO:HD2	1:A:124:MET:HE1	1.84	0.59
1:B:97:GLN:HG3	1:B:269:ILE:CD1	2.32	0.59
1:B:324:ASN:HD22	1:B:324:ASN:H	1.50	0.59
1:B:22:TRP:CH2	1:B:30:GLN:HB3	2.37	0.59
1:B:166:THR:HG21	1:B:171:MET:SD	2.43	0.59
1:A:15:GLN:HE22	1:A:207:LYS:HA	1.67	0.59
1:B:408:ASN:O	1:B:412:GLN:HG3	2.03	0.58
1:A:453[A]:ARG:HG3	1:B:305:SER:HB3	1.85	0.58
1:A:408:ASN:HB3	1:A:413:ASN:HB2	1.84	0.58
1:A:22:TRP:CH2	1:A:30:GLN:HB2	2.39	0.57
1:B:159:ILE:HD11	3:B:1993:HOH:O	2.03	0.57
1:A:278:LYS:HG2	1:A:328:ILE:HD11	1.86	0.57
1:B:284:ASN:HD22	1:B:285:PRO:HD2	1.69	0.57
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.86	0.57
1:A:121:PRO:HD2	1:A:124:MET:CE	2.35	0.56
1:A:107:LEU:HD13	1:A:250:TYR:CE1	2.41	0.56
1:B:415:LYS:HD3	1:B:415:LYS:H	1.70	0.56
1:B:318:ASP:CG	1:B:320:ARG:HD2	2.25	0.56
1:A:26:GLU:HG3	1:A:29:GLN:NE2	2.21	0.56
1:B:506:PRO:HG2	1:B:517:LEU:HB2	1.88	0.56
1:B:235:ILE:HG22	1:B:239:MET:CE	2.36	0.55
1:A:373:PRO:HD2	1:B:444:ASN:ND2	2.22	0.55
1:B:284:ASN:HD22	1:B:285:PRO:CD	2.19	0.55
1:B:33:LEU:O	1:B:37:LEU:HG	2.06	0.55
1:A:362:ASP:OD1	1:A:368:ILE:HD11	2.07	0.55
1:A:408:ASN:HB3	1:A:413:ASN:ND2	2.21	0.55
1:B:142:ARG:HG2	1:B:485:PRO:HB3	1.88	0.55
1:B:362:ASP:OD2	1:B:366:GLN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:O	1:B:148:GLN:HG3	2.08	0.54
1:B:73:PRO:HB2	1:B:75:GLU:HG2	1.90	0.54
1:B:50:GLN:O	1:B:54:GLU:HG3	2.08	0.53
1:B:417:ASN:HD21	1:B:420:THR:HG23	1.73	0.53
1:B:151:GLU:HG3	1:B:157:LYS:HA	1.90	0.53
1:A:233:GLN:HB2	1:A:235:ILE:HG12	1.91	0.52
1:B:21:PHE:O	1:B:25:LEU:HG	2.08	0.52
1:B:318:ASP:OD2	1:B:320:ARG:HD2	2.10	0.52
1:B:66:ASP:HA	1:B:69:MET:CE	2.39	0.52
1:B:127:VAL:HG13	1:B:418:PRO:O	2.08	0.52
1:A:417:ASN:HB2	1:A:418:PRO:CD	2.40	0.52
1:B:441:ILE:HG13	1:B:504:HIS:CD2	2.45	0.52
1:B:417:ASN:HD21	1:B:419:THR:HG23	1.72	0.52
1:A:318:ASP:OD1	1:A:320:ARG:HG2	2.09	0.51
1:A:112:GLN:HB2	1:A:169:ARG:CZ	2.40	0.51
1:A:254:ASN:ND2	1:A:404:SER:H	2.07	0.51
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.76	0.51
1:B:127:VAL:HG12	1:B:422:ARG:HB2	1.91	0.51
1:A:453[A]:ARG:HG2	1:B:304:TYR:CE1	2.45	0.51
1:A:10:LEU:HD21	1:A:42:PHE:CZ	2.45	0.51
1:A:15:GLN:NE2	1:A:17:HIS:HE1	2.09	0.51
1:B:231:ALA:HB2	1:B:342:VAL:HG13	1.93	0.51
1:A:410:ASP:HA	1:A:417:ASN:HB2	1.93	0.51
1:A:477:VAL:N	1:A:478:PRO:HA	2.26	0.51
1:B:28:ALA:O	1:B:31:VAL:HG12	2.11	0.50
1:B:196:GLN:HE22	2:B:1902:UD2:HN3	1.60	0.50
1:B:257:VAL:HG23	1:B:330:ASN:HD21	1.77	0.50
1:B:362:ASP:OD1	1:B:364:GLN:N	2.44	0.49
1:B:417:ASN:HD22	1:B:420:THR:H	1.60	0.49
1:B:495:GLU:H	1:B:495:GLU:CD	2.14	0.49
1:A:324:ASN:HD22	1:A:324:ASN:C	2.16	0.49
1:A:231:ALA:HB2	1:A:342:VAL:HG13	1.94	0.49
1:B:15:GLN:NE2	1:B:207:LYS:HA	2.22	0.49
1:A:417:ASN:C	1:A:417:ASN:HD22	2.16	0.48
1:A:71:PRO:HG3	1:A:322:LEU:HD22	1.95	0.48
1:B:367:LEU:C	1:B:368:ILE:HD12	2.32	0.48
1:A:212:GLU:HB2	1:A:215:LYS:HB3	1.95	0.48
1:A:284:ASN:ND2	1:A:285:PRO:HD2	2.26	0.48
1:A:417:ASN:ND2	1:A:420:THR:H	2.12	0.48
1:B:405:PRO:HB2	1:B:407:LYS:HE2	1.94	0.48
1:A:453[B]:ARG:CB	1:A:453[B]:ARG:HH11	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:HD22	1:B:285:PRO:N	2.12	0.48
1:B:127:VAL:HG12	1:B:127:VAL:O	2.14	0.47
1:A:102:LYS:HE3	1:A:243:GLY:O	2.14	0.47
1:A:480:GLN:O	1:A:506:PRO:HA	2.14	0.47
1:B:270:GLN:HG2	3:B:2004:HOH:O	2.15	0.47
1:B:107:LEU:HD13	1:B:250:TYR:CE1	2.50	0.47
1:B:415:LYS:N	1:B:415:LYS:HD3	2.30	0.46
1:B:194:PHE:HB2	1:B:233:GLN:HG3	1.97	0.46
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.79	0.46
1:A:239:MET:HE1	1:A:338:LEU:HD12	1.97	0.46
1:A:408:ASN:CB	1:A:413:ASN:HB2	2.45	0.46
1:B:127:VAL:CG1	1:B:422:ARG:HB2	2.46	0.46
1:B:346:GLU:HB3	1:B:347:PRO:HD3	1.96	0.46
1:A:336:PRO:O	1:A:339:ARG:HB3	2.16	0.46
1:A:441:ILE:HG22	1:A:447:ARG:HA	1.97	0.46
1:B:333:PHE:CE2	1:B:385:ILE:HD11	2.50	0.46
1:A:274:ASP:HA	1:A:334:THR:HG23	1.97	0.46
1:A:26:GLU:HG3	1:A:29:GLN:HE21	1.79	0.46
1:A:66:ASP:C	1:A:68:ARG:H	2.20	0.46
1:B:226:LEU:O	1:B:230:LEU:HG	2.16	0.46
1:A:372:LYS:HG2	1:B:443:GLU:CG	2.46	0.45
1:B:507:LEU:HD11	1:B:514:VAL:HG13	1.99	0.45
1:B:199:LEU:HG	1:B:221:ASP:HB3	1.98	0.45
1:B:192:ILE:HD12	1:B:192:ILE:N	2.31	0.45
1:A:25:LEU:HD22	1:A:214:ASN:HB3	1.99	0.45
1:A:300:GLN:HB2	3:A:1989:HOH:O	2.16	0.45
1:A:372:LYS:HG2	1:B:443:GLU:HG3	1.99	0.45
1:A:176:GLU:HA	1:A:179:THR:CG2	2.46	0.45
1:A:511:GLU:CD	1:A:511:GLU:H	2.20	0.45
1:A:322:LEU:HD13	1:A:323:PHE:CE1	2.52	0.45
1:B:298:VAL:HG22	1:B:387:GLN:HA	1.98	0.45
1:B:477:VAL:N	1:B:478:PRO:CA	2.80	0.45
1:B:201:ALA:HB1	1:B:358:ILE:HD13	1.98	0.45
1:B:15:GLN:NE2	1:B:17:HIS:HE1	2.14	0.44
1:B:105:VAL:CG1	1:B:250:TYR:HE2	2.30	0.44
1:B:142:ARG:HD3	3:B:1912:HOH:O	2.17	0.44
1:A:116:LEU:HD22	1:A:122:LYS:HG2	1.99	0.44
1:A:239:MET:HE1	1:A:247:ILE:HG13	2.00	0.44
1:A:142:ARG:HG2	1:A:485:PRO:HB3	1.98	0.44
1:B:284:ASN:HD22	1:B:284:ASN:C	2.20	0.44
1:B:499:ALA:O	1:B:501:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:NH1	1:B:132:ARG:HG2	2.33	0.44
1:B:137:GLN:O	1:B:141:GLU:HG3	2.17	0.44
1:B:303:GLU:OE1	1:B:303:GLU:HA	2.18	0.44
1:A:142:ARG:HD3	3:A:1944:HOH:O	2.18	0.43
1:A:265:ILE:O	1:A:269:ILE:HG12	2.18	0.43
1:B:412:GLN:O	1:B:415:LYS:HD3	2.19	0.43
1:B:417:ASN:HB2	1:B:418:PRO:HD2	2.00	0.43
1:A:66:ASP:O	1:A:67:ALA:HB3	2.18	0.43
1:B:10:LEU:HB3	1:B:16:GLU:HA	2.00	0.43
1:B:480:GLN:HB2	1:B:506:PRO:HB3	2.00	0.43
1:B:97:GLN:HG3	1:B:269:ILE:HD13	2.01	0.43
1:A:79:SER:HB3	1:A:82:ARG:HB2	2.00	0.43
1:B:417:ASN:ND2	1:B:420:THR:HG23	2.33	0.43
1:B:131:SER:HB3	1:B:482:GLU:OE1	2.18	0.43
1:B:212:GLU:C	1:B:361:VAL:HG21	2.40	0.43
1:B:221:ASP:OD1	1:B:225:GLY:HA3	2.19	0.43
1:A:360:TYR:HB2	3:A:2012:HOH:O	2.19	0.42
1:B:20:ARG:CB	1:B:20:ARG:HH11	2.31	0.42
1:B:443:GLU:H	1:B:443:GLU:CD	2.17	0.42
1:B:426:MET:HE1	1:B:480:GLN:HB3	2.00	0.42
1:B:338:LEU:O	1:B:342:VAL:HG23	2.18	0.42
1:B:350:GLN:HB2	1:B:350:GLN:HE21	1.56	0.42
1:A:181:HIS:O	1:A:182:LYS:HB2	2.20	0.42
1:A:106:LEU:HB3	1:A:249:VAL:HG22	2.00	0.42
1:A:284:ASN:HD22	1:A:285:PRO:N	2.17	0.42
1:A:284:ASN:C	1:A:284:ASN:HD22	2.23	0.42
1:B:299:TYR:C	1:B:300:GLN:HG2	2.39	0.42
1:A:196:GLN:HA	1:A:229:ALA:HB2	2.00	0.42
1:B:324:ASN:N	1:B:324:ASN:HD22	2.13	0.41
1:A:257:VAL:HG23	1:A:330:ASN:HD21	1.85	0.41
1:B:90:TRP:O	1:B:266:GLY:HA3	2.20	0.41
1:B:417:ASN:HB2	1:B:418:PRO:CD	2.50	0.41
1:A:25:LEU:HB3	1:A:29:GLN:HB2	2.03	0.41
1:A:409:ALA:O	1:A:410:ASP:CB	2.67	0.41
1:A:417:ASN:HB2	1:A:418:PRO:HD2	2.02	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.87	0.41
1:A:408:ASN:HB3	1:A:413:ASN:CB	2.50	0.41
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.90	0.41
1:B:510:ASP:C	1:B:512:ASN:H	2.24	0.41
1:B:417:ASN:C	1:B:417:ASN:ND2	2.72	0.41
1:B:415:LYS:HA	1:B:420:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ASP:HB2	1:B:511:GLU:OE1	2.20	0.41
1:A:90:TRP:O	1:A:266:GLY:HA3	2.20	0.40
1:B:254:ASN:ND2	1:B:256:LEU:H	2.19	0.40
1:B:15:GLN:NE2	1:B:208:ILE:N	2.60	0.40
1:B:104:ALA:HB3	1:B:247:ILE:CD1	2.52	0.40
1:B:254:ASN:ND2	1:B:254:ASN:C	2.75	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	480/522 (92%)	462 (96%)	17 (4%)	1 (0%)	51	63
1	B	472/522 (90%)	451 (96%)	19 (4%)	2 (0%)	38	47
All	All	952/1044 (91%)	913 (96%)	36 (4%)	3 (0%)	44	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ASP
1	B	344	VAL
1	B	412	GLN

### 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	412/447 (92%)	396 (96%)	16 (4%)	37	51
1	B	406/447 (91%)	384 (95%)	22 (5%)	26	35
All	All	818/894 (92%)	780 (95%)	38 (5%)	30	42

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	81	THR
1	A	116	LEU
1	A	156	ASN
1	A	169	ARG
1	A	179	THR
1	A	233	GLN
1	A	284	ASN
1	A	320	ARG
1	A	322	LEU
1	A	324	ASN
1	A	339	ARG
1	A	361	VAL
1	A	406	LEU
1	A	417	ASN
1	A	507	LEU
1	B	6	LEU
1	B	16	GLU
1	B	50	GLN
1	B	95	LEU
1	B	151	GLU
1	B	153	TYR
1	B	157	LYS
1	B	172	GLU
1	B	233	GLN
1	B	254	ASN
1	B	270	GLN
1	B	284	ASN
1	B	298	VAL
1	B	324	ASN
1	B	339	ARG
1	B	350	GLN
1	B	355	GLN
1	B	371	ASP
1	B	405	PRO

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Mol	Chain	Res	Type
1	B	415	LYS
1	B	417	ASN
1	B	419	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	GLN
1	A	38	GLN
1	A	50	GLN
1	A	137	GLN
1	A	139	GLN
1	A	148	GLN
1	A	156	ASN
1	A	233	GLN
1	A	254	ASN
1	A	284	ASN
1	A	300	GLN
1	A	324	ASN
1	A	330	ASN
1	A	343	ASN
1	A	355	GLN
1	A	413	ASN
1	A	417	ASN
1	A	429	HIS
1	A	504	HIS
1	B	15	GLN
1	B	23	ASN
1	B	46	ASN
1	B	50	GLN
1	B	64	ASN
1	B	84	GLN
1	B	137	GLN
1	B	139	GLN
1	B	181	HIS
1	B	195	GLN
1	B	196	GLN
1	B	233	GLN
1	B	254	ASN
1	B	270	GLN
1	B	284	ASN

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Mol	Chain	Res	Type
1	B	313	GLN
1	B	324	ASN
1	B	330	ASN
1	B	350	GLN
1	B	355	GLN
1	B	387	GLN
1	B	412	GLN
1	B	413	ASN
1	B	417	ASN
1	B	439	HIS

### 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 ⓘ

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	1901	-	34,41,41	2.51	6 (17%)	43,62,62	3.13	13 (30%)
2	UD2	B	1902	-	34,41,41	2.23	4 (11%)	43,62,62	3.16	12 (27%)

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	1901	-	-	0/22/63/63	0/3/3/3
2	UD2	B	1902	-	-	0/22/63/63	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	UD2	O4'-C4'	-3.31	1.35	1.43
2	B	1902	UD2	O4'-C4'	-2.62	1.36	1.43
2	B	1902	UD2	C1'-C2'	2.64	1.57	1.53
2	A	1901	UD2	C2'-N2'	2.84	1.50	1.45
2	A	1901	UD2	C3'-C2'	2.86	1.58	1.53
2	A	1901	UD2	O5'-C1'	3.00	1.49	1.41
2	B	1902	UD2	C3'-C2'	3.18	1.59	1.53
2	A	1901	UD2	C1'-C2'	5.20	1.62	1.53
2	B	1902	UD2	C6-N1	10.72	1.50	1.35
2	A	1901	UD2	C6-N1	11.10	1.50	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	UD2	C4'-C3'-C2'	-7.92	98.58	110.33
2	B	1902	UD2	C4'-C3'-C2'	-7.47	99.24	110.33
2	B	1902	UD2	C3'-C4'-C5'	-4.01	103.15	110.22
2	B	1902	UD2	C1'-C2'-N2'	-3.75	104.69	111.03
2	A	1901	UD2	C1'-C2'-N2'	-3.43	105.22	111.03
2	B	1902	UD2	O3'-C3'-C2'	-3.42	102.67	109.61
2	A	1901	UD2	O3'-C3'-C2'	-3.33	102.86	109.61
2	A	1901	UD2	C3'-C4'-C5'	-3.08	104.79	110.22
2	A	1901	UD2	O1'-C1'-C2'	-2.84	103.27	108.40
2	B	1902	UD2	O5'-C5'-C4'	-2.66	104.76	109.66
2	A	1901	UD2	C6'-C5'-C4'	-2.38	107.44	113.00
2	A	1901	UD2	O5'-C5'-C4'	-2.17	105.67	109.66
2	B	1902	UD2	O1'-C1'-C2'	-2.01	104.76	108.40
2	A	1901	UD2	C3'-C2'-N2'	2.10	114.64	110.61
2	B	1902	UD2	O5'-C1'-O1'	2.20	114.24	111.36
2	B	1902	UD2	C3'-C2'-N2'	2.45	115.30	110.61
2	A	1901	UD2	O5'-C1'-O1'	3.00	115.28	111.36
2	A	1901	UD2	O3A-PB-O1'	3.80	108.83	102.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1902	UD2	O3A-PB-O1'	4.58	110.24	102.05
2	A	1901	UD2	O4'-C4'-C3'	5.11	121.47	110.36
2	B	1902	UD2	O4'-C4'-C5'	5.64	123.50	109.28
2	A	1901	UD2	O4'-C4'-C5'	5.77	123.82	109.28
2	B	1902	UD2	O4'-C4'-C3'	5.93	123.26	110.36
2	B	1902	UD2	C4-N3-C2	13.77	125.96	114.13
2	A	1901	UD2	C4-N3-C2	13.89	126.06	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1902	UD2	1	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 ⓘ

### 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	485/522 (92%)	-0.32	10 (2%) 64 70	13, 27, 56, 74	0
1	B	480/522 (91%)	0.13	36 (7%) 15 20	14, 38, 70, 85	0
All	All	965/1044 (92%)	-0.10	46 (4%) 31 38	13, 32, 64, 85	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	10.7
1	B	56	PHE	7.0
1	B	2	ASN	6.9
1	B	412	GLN	6.1
1	B	119	ALA	5.7
1	B	414	GLY	5.7
1	B	411	SER	5.7
1	B	410	ASP	4.8
1	B	477	VAL	4.4
1	B	31	VAL	4.3
1	A	413	ASN	4.2
1	B	65	VAL	4.2
1	B	27	GLU	4.1
1	A	454	SER	4.0
1	B	4	ASN	4.0
1	B	153	TYR	3.9
1	A	169	ARG	3.8
1	B	363	THR	3.8
1	B	120	TYR	3.8
1	B	169	ARG	3.8
1	B	64	ASN	3.7
1	A	411	SER	3.5
1	B	413	ASN	3.5
1	B	55	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	3.4
1	A	453[A]	ARG	3.3
1	B	28	ALA	3.2
1	B	3	ILE	3.1
1	B	26	GLU	3.1
1	B	35	ALA	3.0
1	B	6	LEU	3.0
1	A	414	GLY	2.8
1	A	66	ASP	2.8
1	B	478	PRO	2.7
1	B	408	ASN	2.7
1	B	18	LEU	2.7
1	B	371	ASP	2.6
1	A	412	GLN	2.6
1	B	369	LYS	2.5
1	B	5	ASP	2.4
1	A	363	THR	2.3
1	A	56	PHE	2.2
1	B	20	ARG	2.2
1	B	205	ASP	2.2
1	B	33	LEU	2.0
1	B	12	LYS	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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UD2	A	1901	39/39	0.93	0.10	0.08	17,25,38,41	0
2	UD2	B	1902	39/39	0.92	0.10	-0.30	16,29,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.