Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:20 PM 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 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 (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	Percentile Ranks	Value
Rfree		0.235
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		2.8%
RSRZ outliers		6.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
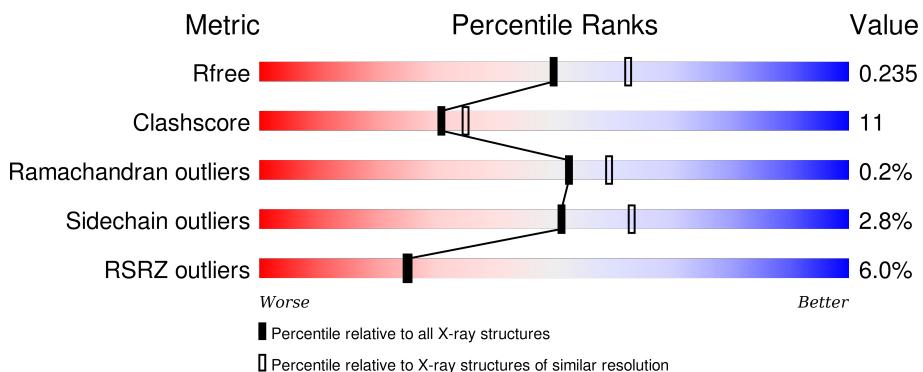
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=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 <=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	505	2% 78% 18% • •
1	B	505	9% 73% 21% • •
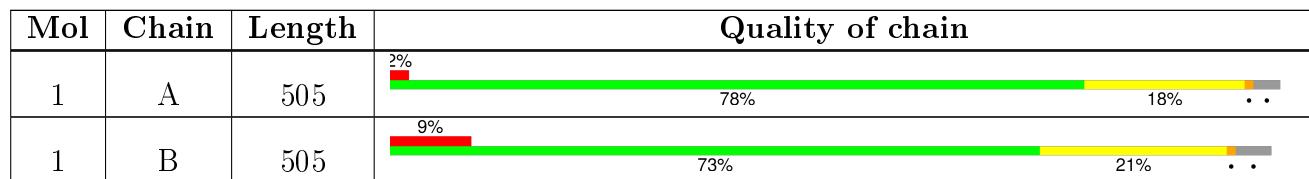
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8477 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 isoform 1: AGX1.

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

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-ACETYLGALACTOSAMINE (three-letter code: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$).

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

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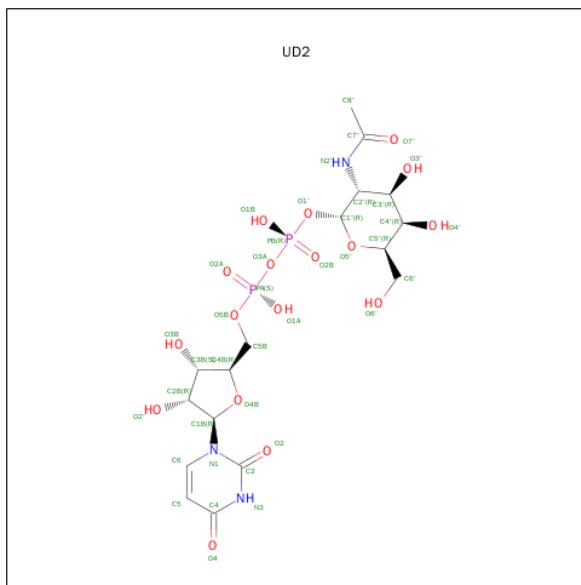
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	39	17	3	17	2	0	0

- Molecule 3 is water.

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

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
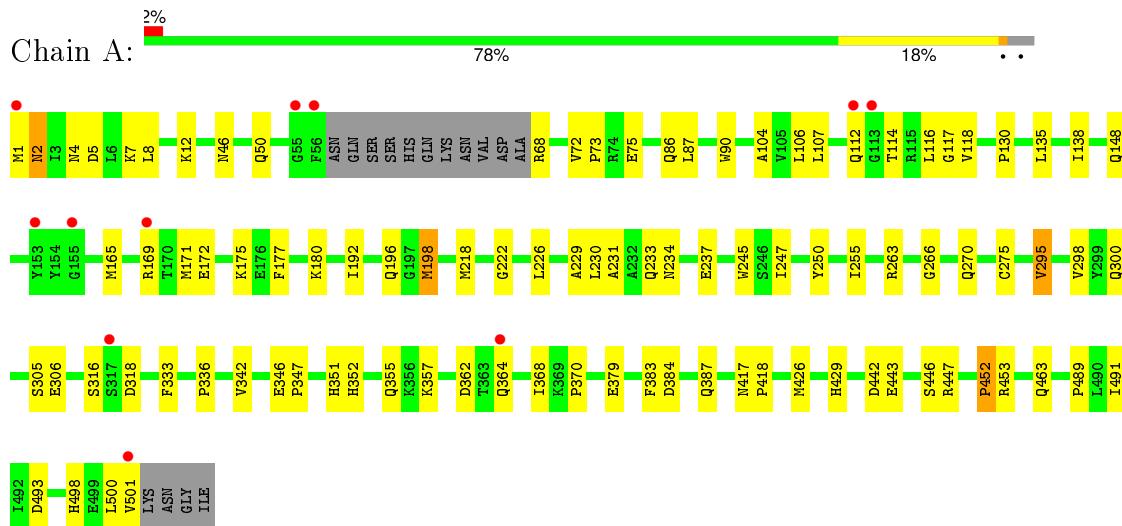
• Molecule 1: GlcNAc1P uridyltransferase isoform 1: AGX1
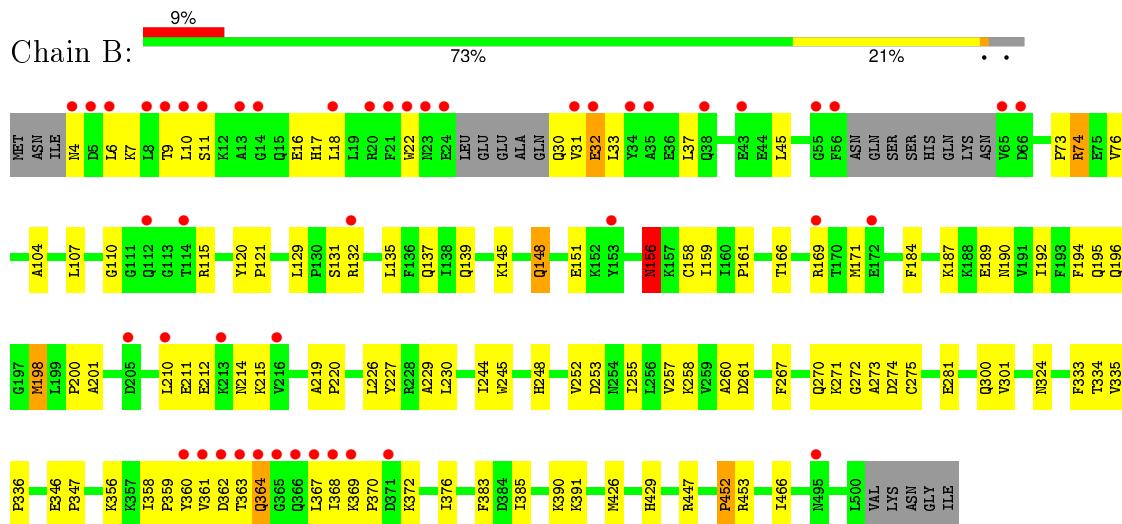
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$<I/\sigma(I)>$ [1]	2.11 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.190 , 0.234 0.192 , 0.235	Depositor DCC
R_{free} test set	1684 reflections (2.99%)	DCC
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	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^2)	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0/4026	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 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	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

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 11.

All (171) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:HA3	1:A:379:GLU:HB2	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	491/505 (97%)	474 (96%)	17 (4%)	0	100	100
1	B	484/505 (96%)	455 (94%)	27 (6%)	2 (0%)	39	42
All	All	975/1010 (96%)	929 (95%)	44 (4%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

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

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/433 (98%)	413 (98%)	10 (2%)	57	69
1	B	418/433 (96%)	404 (97%)	14 (3%)	45	56
All	All	841/866 (97%)	817 (97%)	24 (3%)	51	62

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
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

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Mol	Chain	Res	Type
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
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	-	32,41,41	2.14	5 (15%)	46,62,62	2.78	12 (26%)
2	UD2	B	902	-	32,41,41	2.13	5 (15%)	46,62,62	2.65	10 (21%)

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	-	-	0/22/63/63	0/3/3/3
2	UD2	B	902	-	-	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	B	902	UD2	O4'-C4'	-3.79	1.33	1.43
2	A	901	UD2	O4'-C4'	-3.23	1.35	1.43
2	A	901	UD2	O5'-C1'	2.21	1.47	1.41
2	B	902	UD2	C1'-C2'	2.53	1.57	1.53
2	B	902	UD2	C4'-C5'	2.58	1.58	1.53
2	B	902	UD2	C2'-N2'	2.77	1.50	1.45
2	A	901	UD2	C3'-C2'	3.16	1.59	1.53
2	A	901	UD2	C1'-C2'	3.73	1.59	1.53
2	B	902	UD2	C6-N1	9.21	1.48	1.35
2	A	901	UD2	C6-N1	9.28	1.48	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	A	901	UD2	C4'-C3'-C2'	-8.71	98.35	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	902	UD2	C4'-C3'-C2'	-6.25	101.77	110.43
2	B	902	UD2	C3'-C4'-C5'	-4.28	102.74	110.20
2	B	902	UD2	O3'-C3'-C2'	-3.54	102.45	109.66
2	A	901	UD2	C1'-C2'-N2'	-3.42	104.58	111.01
2	A	901	UD2	O3'-C3'-C2'	-3.22	103.09	109.66
2	A	901	UD2	C3'-C4'-C5'	-3.13	104.74	110.20
2	B	902	UD2	O5'-C5'-C4'	-3.09	103.88	109.68
2	A	901	UD2	O1'-C1'-C2'	-3.07	102.76	108.42
2	B	902	UD2	C1'-C2'-N2'	-2.80	105.75	111.01
2	A	901	UD2	O5'-C5'-C4'	-2.78	104.47	109.68
2	B	902	UD2	O1'-C1'-C2'	-2.67	103.50	108.42
2	A	901	UD2	C6'-C5'-C4'	-2.34	107.24	113.02
2	B	902	UD2	O1A-PA-O3A	2.09	114.59	105.09
2	A	901	UD2	O1A-PA-O3A	2.18	114.98	105.09
2	A	901	UD2	O5'-C1'-O1'	2.92	115.21	111.36
2	A	901	UD2	O4'-C4'-C3'	5.09	121.79	110.34
2	B	902	UD2	O4'-C4'-C5'	5.26	123.17	109.24
2	A	901	UD2	O4'-C4'-C5'	5.31	123.30	109.24
2	B	902	UD2	O4'-C4'-C3'	5.65	123.06	110.34
2	A	901	UD2	C4-N3-C2	11.22	125.25	114.14
2	B	902	UD2	C4-N3-C2	11.60	125.63	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	UD2	1	0
2	B	902	UD2	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	490/505 (97%)	-0.31	11 (2%)	65	64	14, 29, 49, 70	0
1	B	484/505 (95%)	0.28	47 (9%)	10	9	17, 40, 78, 92	0
All	All	974/1010 (96%)	-0.02	58 (5%)	25	25	14, 34, 68, 92	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	GLY	8.3
1	B	364	GLN	7.5
1	B	8	LEU	6.9
1	B	6	LEU	6.6
1	B	363	THR	6.0
1	B	4	ASN	5.8
1	B	5	ASP	5.7
1	B	31	VAL	5.2
1	B	65	VAL	5.1
1	B	22	TRP	5.1
1	B	18	LEU	4.6
1	B	56	PHE	4.6
1	B	35	ALA	4.4
1	A	169	ARG	4.2
1	B	366	GLN	4.1
1	A	501	VAL	4.1
1	B	34	TYR	4.0
1	B	20	ARG	3.9
1	A	1	MET	3.7
1	B	362	ASP	3.7
1	B	9	THR	3.7
1	B	371	ASP	3.6
1	A	153	TYR	3.5
1	B	369	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	11	SER	3.4
1	A	113	GLY	3.2
1	B	112	GLN	3.1
1	B	38	GLN	3.1
1	B	153	TYR	3.0
1	B	23	ASN	2.9
1	B	367	LEU	2.9
1	B	32	GLU	2.9
1	B	66	ASP	2.9
1	B	213	LYS	2.8
1	B	24	GLU	2.7
1	A	317	SER	2.7
1	B	43	GLU	2.6
1	A	55	GLY	2.6
1	B	172	GLU	2.6
1	B	114	THR	2.6
1	A	112	GLN	2.6
1	B	169	ARG	2.6
1	B	205	ASP	2.5
1	B	368	ILE	2.5
1	B	216	VAL	2.5
1	B	14	GLY	2.4
1	B	361	VAL	2.4
1	B	210	LEU	2.4
1	A	56	PHE	2.4
1	B	13	ALA	2.3
1	B	360	TYR	2.2
1	B	21	PHE	2.2
1	B	365	GLY	2.2
1	A	155	GLY	2.1
1	A	364	GLN	2.1
1	B	132	ARG	2.1
1	B	495	ASN	2.1
1	B	10	LEU	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(Å^2)	Q<0.9
2	UD2	A	901	39/39	0.95	0.10	0.31	21,26,40,45	0
2	UD2	B	902	39/39	0.95	0.11	0.14	25,33,41,45	0

6.5 Other polymers (i)

There are no such residues in this entry.