



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:58 AM GMT

PDB ID : 2D0J  
Title : Crystal Structure of Human GlcAT-S Apo Form  
Authors : Shiba, T.; Kakuda, S.; Ishiguro, M.; Oka, S.; Kawasaki, T.; Wakatsuki, S.; Kato, R.  
Deposited on : 2005-08-03  
Resolution : 2.00 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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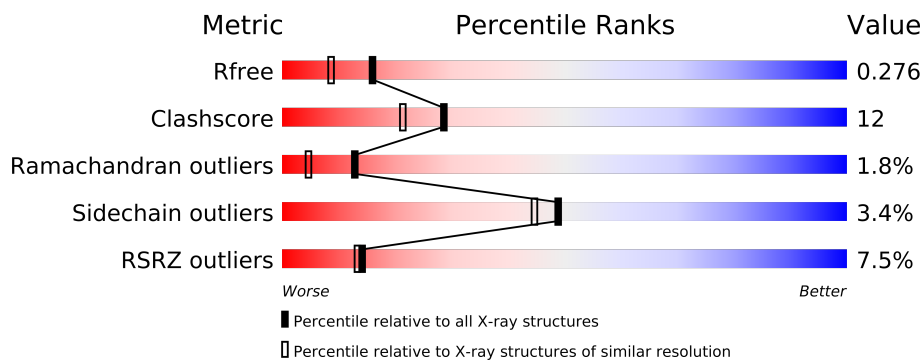
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	246	
1	B	246	
1	C	246	
1	D	246	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8273 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 Galactosylgalactosylxylosylprotein3-beta-glucuronosyltransferase2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1955	1240	365	346	4			
1	B	242	Total	C	N	O	S	0	0	0
			1955	1240	365	346	4			
1	C	242	Total	C	N	O	S	0	0	0
			1955	1240	365	346	4			
1	D	241	Total	C	N	O	S	0	0	0
			1946	1235	363	344	4			

- Molecule 2 is water.

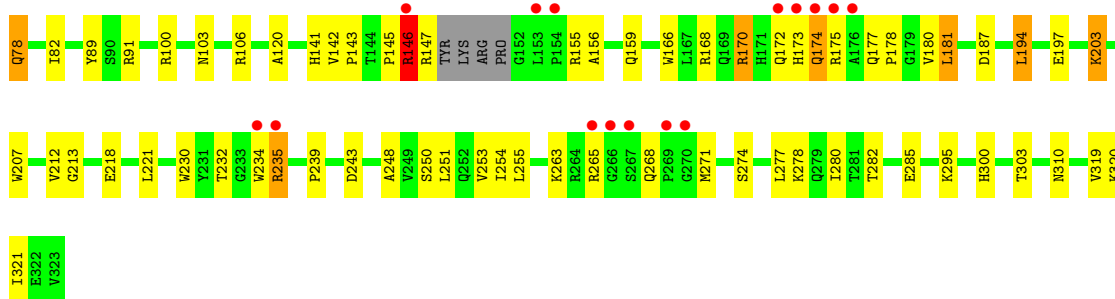
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	127	Total	O	0	0
			127	127		
2	B	113	Total	O	0	0
			113	113		
2	C	119	Total	O	0	0
			119	119		
2	D	103	Total	O	0	0
			103	103		

### 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.

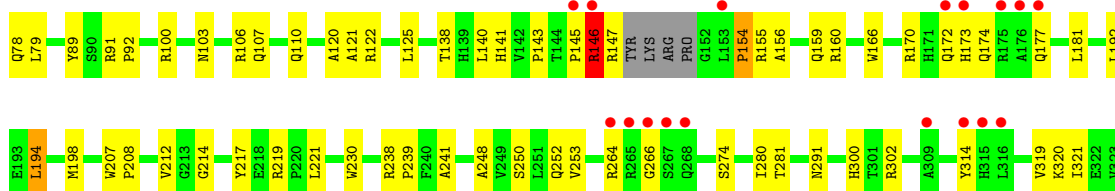
- Molecule 1: Galactosylgalactosylxylosylprotein3-beta-glucuronosyltransferase2

Chain A: 



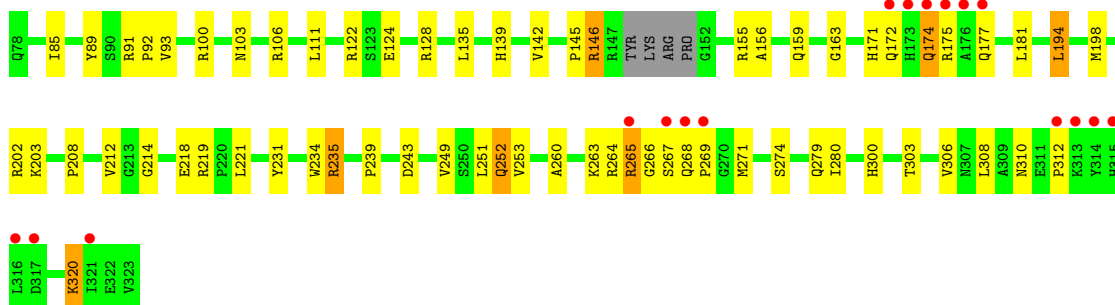
- Molecule 1: Galactosylgalactosylxylosylprotein3-beta-glucuronosyltransferase2

Chain B: 



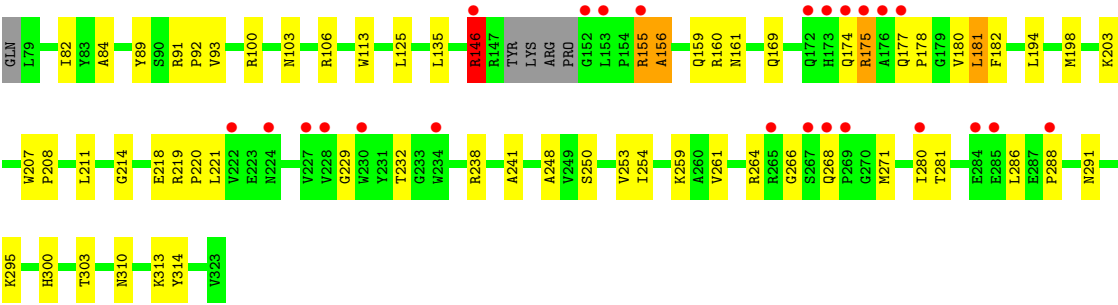
- Molecule 1: Galactosylgalactosylxylosylprotein3-beta-glucuronosyltransferase2

Chain C: 



- Molecule 1: Galactosylgalactosylxylosylprotein3-beta-glucuronosyltransferase2

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.40Å 122.59Å 92.98Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-2.00) 96.0 (40.60-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.69 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.237 , 0.278 0.236 , 0.276	Depositor DCC
$R_{free}$ test set	3836 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 76049 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8273	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 5.95% 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

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	0.33	0/2002	0.58	0/2718
1	B	0.34	0/2002	0.57	0/2718
1	C	0.34	0/2002	0.58	0/2718
1	D	0.30	0/1993	0.53	0/2706
All	All	0.33	0/7999	0.57	0/10860

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	1955	0	1968	55	0
1	B	1955	0	1968	52	0
1	C	1955	0	1968	51	0
1	D	1946	0	1960	50	0
2	A	127	0	0	3	0
2	B	113	0	0	3	0
2	C	119	0	0	1	0
2	D	103	0	0	2	0
All	All	8273	0	7864	196	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 12.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:ASN:HA	1:B:106:ARG:HH12	1.36	0.88
1:C:263:LYS:HE3	1:C:265:ARG:HB2	1.62	0.82
1:A:155:ARG:HB2	2:A:450:HOH:O	1.82	0.80
1:D:238:ARG:NH1	1:D:241:ALA:HA	1.98	0.79
1:D:175:ARG:HD2	1:D:175:ARG:N	1.98	0.77
1:D:280:ILE:HG22	1:D:281:THR:HG23	1.66	0.74
1:C:103:ASN:HA	1:C:106:ARG:HH22	1.53	0.74
1:C:235:ARG:HH21	1:C:269:PRO:HD2	1.51	0.74
1:A:103:ASN:HD22	1:A:106:ARG:HH22	1.34	0.74
1:C:103:ASN:HD22	1:C:106:ARG:HH22	1.37	0.73
1:D:181:LEU:HD21	1:D:254:ILE:HG13	1.70	0.73
1:B:103:ASN:HA	1:B:106:ARG:NH1	2.04	0.72
1:A:203:LYS:HE2	1:A:253:VAL:HG22	1.71	0.72
1:D:291:ASN:HD22	1:D:295:LYS:HD3	1.55	0.71
1:D:103:ASN:ND2	1:D:106:ARG:HH22	1.90	0.70
1:B:103:ASN:HD22	1:B:106:ARG:HH12	1.39	0.69
1:A:181:LEU:HD21	1:A:254:ILE:HG13	1.75	0.69
1:C:103:ASN:HA	1:C:106:ARG:NH2	2.08	0.69
1:D:89:TYR:CZ	1:D:91:ARG:HD3	2.28	0.68
1:B:156:ALA:HA	1:B:159:GLN:OE1	1.96	0.66
1:A:89:TYR:CZ	1:A:91:ARG:HD3	2.30	0.66
1:A:156:ALA:HA	1:A:159:GLN:OE1	1.96	0.66
1:A:277:LEU:HD23	1:A:280:ILE:HD11	1.78	0.66
1:A:250:SER:HB3	1:A:253:VAL:HG23	1.78	0.65
1:B:92:PRO:HG2	2:B:415:HOH:O	1.97	0.64
1:C:235:ARG:NH2	1:C:269:PRO:HD2	2.12	0.63
1:D:103:ASN:ND2	1:D:106:ARG:NH2	2.47	0.63
1:D:135:LEU:O	1:D:135:LEU:HD12	1.99	0.63
1:C:243:ASP:OD1	1:C:300:HIS:HE1	1.82	0.61
1:D:156:ALA:HA	1:D:159:GLN:OE1	2.01	0.61
1:A:106:ARG:HH21	1:B:107:GLN:HE22	1.50	0.60
1:A:239:PRO:HG3	1:A:278:LYS:HD3	1.83	0.60
1:B:146:ARG:HH11	1:B:147:ARG:CZ	2.15	0.60
1:B:174:GLN:HB2	1:B:177:GLN:HG2	1.83	0.60
1:B:146:ARG:NE	1:B:147:ARG:H	1.99	0.59
1:A:146:ARG:H	1:A:146:ARG:HD3	1.68	0.59
1:C:181:LEU:HD23	1:C:249:VAL:O	2.02	0.59
1:D:92:PRO:HG2	2:D:362:HOH:O	2.03	0.59
1:B:146:ARG:CD	1:B:147:ARG:H	2.15	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:93:VAL:HG21	1:D:303:THR:HG21	1.85	0.59
1:A:321:ILE:HD12	1:A:321:ILE:N	2.18	0.59
1:C:156:ALA:HA	1:C:159:GLN:OE1	2.02	0.59
1:B:221:LEU:HD23	1:B:230:TRP:N	2.17	0.58
1:B:250:SER:OG	1:B:253:VAL:HG23	2.03	0.58
1:C:100:ARG:HD2	1:D:100:ARG:HD2	1.86	0.58
1:C:103:ASN:ND2	1:C:106:ARG:HH22	2.01	0.58
1:C:203:LYS:NZ	1:C:252:GLN:HE22	2.01	0.58
1:A:100:ARG:HD2	1:B:100:ARG:HD2	1.84	0.57
1:A:203:LYS:HE2	1:A:253:VAL:CG2	2.35	0.57
1:D:313:LYS:HD2	1:D:314:TYR:CE2	2.40	0.56
1:C:85:ILE:HD12	1:C:163:GLY:HA3	1.86	0.56
1:D:250:SER:OG	1:D:253:VAL:HG23	2.05	0.56
1:D:146:ARG:H	1:D:146:ARG:NE	2.03	0.56
1:C:253:VAL:CG1	1:C:280:ILE:HG23	2.35	0.56
1:D:286:LEU:O	1:D:288:PRO:HD3	2.06	0.56
1:A:282:THR:OG1	1:A:285:GLU:HG3	2.06	0.55
1:B:125:LEU:C	1:B:125:LEU:HD23	2.26	0.55
1:B:120:ALA:HA	1:B:143:PRO:HG3	1.89	0.55
1:C:268:GLN:HB2	1:C:271:MET:HG2	1.89	0.54
1:B:145:PRO:O	1:B:147:ARG:HG2	2.07	0.54
1:A:103:ASN:HA	1:A:106:ARG:HH22	1.72	0.54
1:C:155:ARG:O	1:C:156:ALA:HB3	2.08	0.54
1:A:170:ARG:HD3	1:A:170:ARG:O	2.08	0.54
1:C:264:ARG:O	1:C:266:GLY:N	2.41	0.53
1:C:194:LEU:HD13	1:C:198:MET:CE	2.38	0.53
1:A:235:ARG:HH21	1:A:235:ARG:HG2	1.73	0.53
1:B:155:ARG:O	1:B:156:ALA:HB3	2.09	0.53
1:C:93:VAL:HG12	1:D:211:LEU:HD13	1.91	0.53
1:C:221:LEU:HD11	1:C:231:TYR:HB2	1.90	0.53
1:B:194:LEU:HD13	1:B:198:MET:CE	2.40	0.52
1:A:251:LEU:O	1:A:255:LEU:HG	2.09	0.52
1:D:156:ALA:O	1:D:160:ARG:HG3	2.10	0.52
1:A:155:ARG:O	1:A:156:ALA:HB3	2.10	0.52
1:A:120:ALA:HA	1:A:143:PRO:HG3	1.92	0.52
1:A:177:GLN:N	1:A:178:PRO:CD	2.73	0.51
1:C:263:LYS:HE3	1:C:265:ARG:CB	2.38	0.51
1:C:124:GLU:O	1:C:128:ARG:HG3	2.11	0.51
1:A:155:ARG:HD2	2:A:332:HOH:O	2.10	0.51
1:A:194:LEU:O	1:A:197:GLU:HB2	2.11	0.50
1:D:103:ASN:HD22	1:D:106:ARG:NH2	2.08	0.50
1:C:260:ALA:CB	1:C:280:ILE:HD11	2.40	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ARG:N	1:A:146:ARG:HD3	2.24	0.50
1:A:218:GLU:HG3	1:A:232:THR:HB	1.94	0.50
1:A:320:LYS:C	1:A:321:ILE:HD12	2.31	0.50
1:C:310:ASN:O	1:C:312:PRO:HD3	2.12	0.49
1:D:218:GLU:HG2	1:D:232:THR:HA	1.95	0.49
1:B:89:TYR:CZ	1:B:91:ARG:HD3	2.47	0.49
1:A:268:GLN:HG2	1:A:271:MET:HE2	1.93	0.49
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.78	0.49
1:C:122:ARG:HG2	1:C:139:HIS:CD2	2.48	0.49
1:D:219:ARG:O	1:D:219:ARG:HD2	2.13	0.48
1:B:221:LEU:CD2	1:B:230:TRP:C	2.81	0.48
1:D:194:LEU:HD13	1:D:198:MET:CE	2.44	0.48
1:B:170:ARG:HH21	1:B:170:ARG:HG2	1.78	0.48
1:D:259:LYS:HB2	2:D:389:HOH:O	2.12	0.48
1:B:121:ALA:HA	1:B:141:HIS:CE1	2.48	0.48
1:B:221:LEU:HD23	1:B:230:TRP:CA	2.43	0.48
1:C:320:LYS:HD3	1:C:320:LYS:C	2.34	0.48
1:B:207:TRP:HH2	1:B:248:ALA:HB2	1.78	0.48
1:D:207:TRP:HH2	1:D:248:ALA:HB2	1.79	0.48
1:B:320:LYS:NZ	1:B:320:LYS:HB3	2.28	0.47
1:A:103:ASN:HA	1:A:106:ARG:NH2	2.28	0.47
1:B:194:LEU:HD13	1:B:198:MET:HE2	1.96	0.47
1:C:92:PRO:HB2	1:C:306:VAL:HG21	1.96	0.47
1:D:221:LEU:HD23	1:D:229:GLY:C	2.35	0.47
1:A:78:GLN:OE1	1:A:78:GLN:N	2.48	0.47
1:C:208:PRO:HG3	1:C:219:ARG:HB2	1.97	0.47
1:B:146:ARG:HH11	1:B:147:ARG:NE	2.12	0.47
1:A:207:TRP:HH2	1:A:248:ALA:HB2	1.80	0.47
1:A:310:ASN:HD22	1:B:214:GLY:HA3	1.80	0.47
1:C:212:VAL:HG13	1:C:218:GLU:HG3	1.97	0.47
1:A:103:ASN:ND2	1:A:106:ARG:HH22	2.08	0.47
1:B:146:ARG:HE	1:B:147:ARG:H	1.63	0.47
1:C:93:VAL:HG11	1:C:303:THR:HG21	1.96	0.46
1:C:203:LYS:HZ2	1:C:252:GLN:HE22	1.63	0.46
1:C:111:LEU:C	1:C:111:LEU:HD23	2.36	0.46
1:D:291:ASN:HD22	1:D:295:LYS:CD	2.25	0.46
1:B:239:PRO:HG2	1:B:274:SER:OG	2.15	0.46
1:D:156:ALA:HB3	1:D:160:ARG:NH1	2.31	0.46
1:C:194:LEU:HD13	1:C:198:MET:HE2	1.98	0.46
1:A:172:GLN:C	1:A:174:GLN:H	2.19	0.46
1:C:93:VAL:HG12	1:D:211:LEU:CD1	2.45	0.46
1:D:82:ILE:HG12	1:D:180:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:219:ARG:HA	1:D:220:PRO:HD3	1.85	0.46
1:B:78:GLN:HG2	1:B:79:LEU:N	2.31	0.46
1:B:319:VAL:O	1:B:321:ILE:HD12	2.16	0.46
1:A:187:ASP:HB2	2:A:424:HOH:O	2.16	0.46
1:D:155:ARG:O	1:D:156:ALA:HB2	2.16	0.46
1:A:263:LYS:HG3	1:A:265:ARG:HG3	1.97	0.46
1:B:122:ARG:HG3	1:B:141:HIS:CD2	2.52	0.45
1:A:268:GLN:HG2	1:A:271:MET:CE	2.45	0.45
1:A:172:GLN:HG3	1:A:173:HIS:N	2.32	0.45
1:C:174:GLN:HB2	1:C:177:GLN:HG2	1.99	0.45
1:D:291:ASN:ND2	1:D:295:LYS:HD3	2.28	0.45
1:B:166:TRP:CH2	1:B:170:ARG:HD2	2.51	0.45
1:B:79:LEU:HD23	1:B:110:GLN:CG	2.47	0.45
1:C:239:PRO:HG2	1:C:274:SER:OG	2.17	0.45
1:C:103:ASN:HD22	1:C:106:ARG:NH2	2.09	0.45
1:B:250:SER:HG	1:B:253:VAL:HG23	1.82	0.45
1:C:214:GLY:HA3	1:D:310:ASN:HD22	1.81	0.45
1:D:313:LYS:HD2	1:D:314:TYR:CZ	2.51	0.45
1:A:146:ARG:CD	1:A:146:ARG:H	2.26	0.45
1:A:141:HIS:O	1:A:142:VAL:HG23	2.17	0.44
1:A:82:ILE:HG12	1:A:180:VAL:CG2	2.47	0.44
1:D:268:GLN:HB3	1:D:271:MET:HB2	1.99	0.44
1:C:146:ARG:HD2	1:C:146:ARG:O	2.16	0.44
1:C:122:ARG:HG2	1:C:139:HIS:NE2	2.33	0.44
1:D:125:LEU:C	1:D:125:LEU:HD23	2.38	0.44
1:B:302:ARG:HD3	2:B:344:HOH:O	2.16	0.44
1:C:135:LEU:HD23	1:C:135:LEU:N	2.32	0.44
1:D:253:VAL:HG11	1:D:280:ILE:HG23	2.00	0.44
1:B:238:ARG:CZ	1:B:241:ALA:HA	2.48	0.44
1:C:308:LEU:HA	1:D:214:GLY:O	2.18	0.43
1:D:113:TRP:HE3	1:D:135:LEU:HD11	1.82	0.43
1:B:208:PRO:HG3	1:B:219:ARG:HB2	2.00	0.43
1:D:208:PRO:CB	1:D:219:ARG:HB3	2.47	0.43
1:D:208:PRO:HB3	1:D:219:ARG:HB3	2.00	0.43
1:A:145:PRO:O	1:A:147:ARG:N	2.52	0.43
1:A:303:THR:HA	1:B:302:ARG:O	2.19	0.43
1:A:221:LEU:HD23	1:A:230:TRP:N	2.33	0.43
1:A:321:ILE:HD13	1:B:217:TYR:OH	2.18	0.43
1:C:234:TRP:HE1	1:D:310:ASN:ND2	2.16	0.43
1:D:161:ASN:OD1	1:D:261:VAL:HG22	2.18	0.43
1:B:146:ARG:HD2	1:B:147:ARG:H	1.83	0.43
1:A:295:LYS:HE2	1:A:295:LYS:HB3	1.87	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:235:ARG:CG	1:C:235:ARG:HH11	2.31	0.42
1:B:147:ARG:CZ	1:B:264:ARG:HG2	2.49	0.42
1:B:154:PRO:HG3	2:B:420:HOH:O	2.18	0.42
1:C:128:ARG:HB3	1:C:128:ARG:NH2	2.34	0.42
1:B:138:THR:HG22	1:B:140:LEU:HG	2.02	0.42
1:B:89:TYR:CE1	1:B:91:ARG:HD3	2.54	0.42
1:B:145:PRO:O	1:B:146:ARG:C	2.56	0.42
1:B:253:VAL:CG1	1:B:280:ILE:HG13	2.50	0.42
1:C:202:ARG:NH1	2:C:369:HOH:O	2.52	0.42
1:D:264:ARG:C	1:D:266:GLY:H	2.24	0.42
1:A:212:VAL:HG22	1:A:213:GLY:N	2.35	0.42
1:A:166:TRP:CH2	1:A:170:ARG:HG3	2.55	0.41
1:D:194:LEU:HD13	1:D:194:LEU:O	2.19	0.41
1:A:239:PRO:HG2	1:A:274:SER:OG	2.20	0.41
1:A:168:ARG:HG2	1:A:255:LEU:HD23	2.02	0.41
1:C:171:HIS:CD2	1:C:251:LEU:HD21	2.55	0.41
1:C:260:ALA:HB3	1:C:280:ILE:HD11	2.01	0.41
1:B:156:ALA:O	1:B:160:ARG:HG3	2.21	0.41
1:A:321:ILE:HD13	1:B:217:TYR:CZ	2.55	0.41
1:D:146:ARG:N	1:D:146:ARG:NE	2.68	0.41
1:C:142:VAL:HG13	1:C:142:VAL:O	2.20	0.41
1:A:243:ASP:OD1	1:A:300:HIS:NE2	2.54	0.41
1:C:89:TYR:CZ	1:C:91:ARG:HD3	2.55	0.41
1:D:84:ALA:HB2	1:D:182:PHE:CE1	2.55	0.41
1:A:181:LEU:HD21	1:A:254:ILE:CG1	2.46	0.41
1:B:280:ILE:HG22	1:B:281:THR:HG22	2.03	0.40
1:D:221:LEU:HB2	1:D:229:GLY:HA3	2.02	0.40
1:D:177:GLN:N	1:D:178:PRO:CD	2.84	0.40
1:A:319:VAL:HG12	1:A:320:LYS:N	2.36	0.40
1:B:212:VAL:HB	1:B:300:HIS:HD2	1.85	0.40
1:A:221:LEU:HD22	1:A:221:LEU:N	2.37	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	238/246 (97%)	226 (95%)	9 (4%)	3 (1%)	18	8
1	B	238/246 (97%)	223 (94%)	11 (5%)	4 (2%)	14	5
1	C	238/246 (97%)	217 (91%)	14 (6%)	7 (3%)	7	2
1	D	237/246 (96%)	216 (91%)	18 (8%)	3 (1%)	18	8
All	All	951/984 (97%)	882 (93%)	52 (6%)	17 (2%)	13	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	A	174	GLN
1	C	172	GLN
1	C	175	ARG
1	D	156	ALA
1	B	314	TYR
1	C	267	SER
1	D	174	GLN
1	C	265	ARG
1	D	146	ARG
1	C	146	ARG
1	C	174	GLN
1	A	235	ARG
1	B	146	ARG
1	C	145	PRO
1	B	154	PRO
1	B	266	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	208/212 (98%)	200 (96%)	8 (4%)	44	39
1	B	208/212 (98%)	200 (96%)	8 (4%)	44	39
1	C	208/212 (98%)	203 (98%)	5 (2%)	61	61
1	D	207/212 (98%)	200 (97%)	7 (3%)	49	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	831/848 (98%)	803 (97%)	28 (3%)	49 45

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	146	ARG
1	A	170	ARG
1	A	175	ARG
1	A	181	LEU
1	A	194	LEU
1	A	203	LYS
1	A	234	TRP
1	B	146	ARG
1	B	172	GLN
1	B	173	HIS
1	B	181	LEU
1	B	192	LEU
1	B	194	LEU
1	B	252	GLN
1	B	291	ASN
1	C	194	LEU
1	C	235	ARG
1	C	252	GLN
1	C	279	GLN
1	C	320	LYS
1	D	146	ARG
1	D	155	ARG
1	D	169	GLN
1	D	175	ARG
1	D	181	LEU
1	D	203	LYS
1	D	300	HIS

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	103	ASN
1	A	141	HIS
1	A	174	GLN
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	310	ASN
1	B	78	GLN
1	B	103	ASN
1	B	107	GLN
1	B	141	HIS
1	B	171	HIS
1	B	188	ASN
1	B	196	GLN
1	B	224	ASN
1	B	252	GLN
1	B	279	GLN
1	B	310	ASN
1	C	103	ASN
1	C	188	ASN
1	C	252	GLN
1	C	257	ASN
1	C	268	GLN
1	C	300	HIS
1	D	103	ASN
1	D	172	GLN
1	D	188	ASN
1	D	196	GLN
1	D	291	ASN
1	D	300	HIS
1	D	310	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	242/246 (98%)	0.27	15 (6%) 20 19	12, 30, 59, 81	0
1	B	242/246 (98%)	0.33	17 (7%) 16 15	12, 30, 62, 75	0
1	C	242/246 (98%)	0.38	17 (7%) 16 15	13, 28, 65, 86	0
1	D	241/246 (97%)	0.61	24 (9%) 8 7	13, 39, 75, 88	0
All	All	967/984 (98%)	0.40	73 (7%) 14 13	12, 31, 67, 88	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	TYR	11.4
1	C	173	HIS	10.5
1	D	176	ALA	10.0
1	A	176	ALA	8.8
1	B	267	SER	7.8
1	C	315	HIS	7.1
1	D	269	PRO	7.0
1	D	268	GLN	6.6
1	D	173	HIS	6.6
1	A	175	ARG	6.3
1	C	265	ARG	6.1
1	B	265	ARG	5.8
1	C	267	SER	5.8
1	C	176	ALA	5.5
1	D	267	SER	5.5
1	D	280	ILE	5.2
1	C	316	LEU	5.2
1	A	269	PRO	4.9
1	B	314	TYR	4.8
1	C	175	ARG	4.5
1	B	316	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	234	TRP	4.4
1	A	173	HIS	4.3
1	D	174	GLN	4.3
1	D	230	TRP	4.0
1	B	268	GLN	3.6
1	A	154	PRO	3.6
1	D	172	GLN	3.5
1	B	315	HIS	3.5
1	B	176	ALA	3.4
1	A	266	GLY	3.4
1	C	269	PRO	3.4
1	C	268	GLN	3.3
1	D	175	ARG	3.3
1	D	228	VAL	3.2
1	C	313	LYS	3.1
1	B	309	ALA	3.1
1	A	146	ARG	3.1
1	A	265	ARG	2.9
1	A	234	TRP	2.9
1	A	267	SER	2.9
1	A	153	LEU	2.9
1	A	174	GLN	2.9
1	D	227	VAL	2.9
1	B	172	GLN	2.9
1	B	146	ARG	2.8
1	A	235	ARG	2.8
1	D	265	ARG	2.8
1	C	317	ASP	2.6
1	D	224	ASN	2.6
1	D	153	LEU	2.6
1	C	174	GLN	2.5
1	D	222	VAL	2.4
1	D	152	GLY	2.4
1	C	321	ILE	2.4
1	B	264	ARG	2.3
1	C	172	GLN	2.3
1	A	270	GLY	2.3
1	C	312	PRO	2.3
1	B	175	ARG	2.2
1	D	146	ARG	2.2
1	D	155	ARG	2.2
1	D	285	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	177	GLN	2.2
1	B	145	PRO	2.2
1	A	172	GLN	2.2
1	D	288	PRO	2.2
1	C	177	GLN	2.1
1	D	284	GLU	2.1
1	B	173	HIS	2.1
1	D	177	GLN	2.1
1	B	153	LEU	2.0
1	B	266	GLY	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.