



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:41 am BST

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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

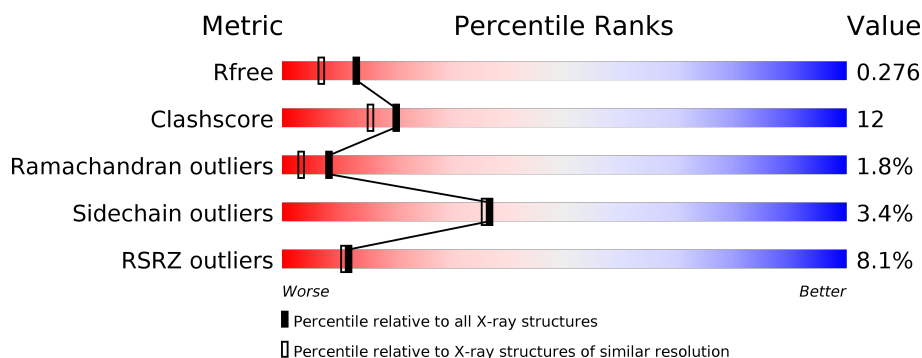
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	246	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	246	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	246	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	246	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8273 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 Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2.

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			

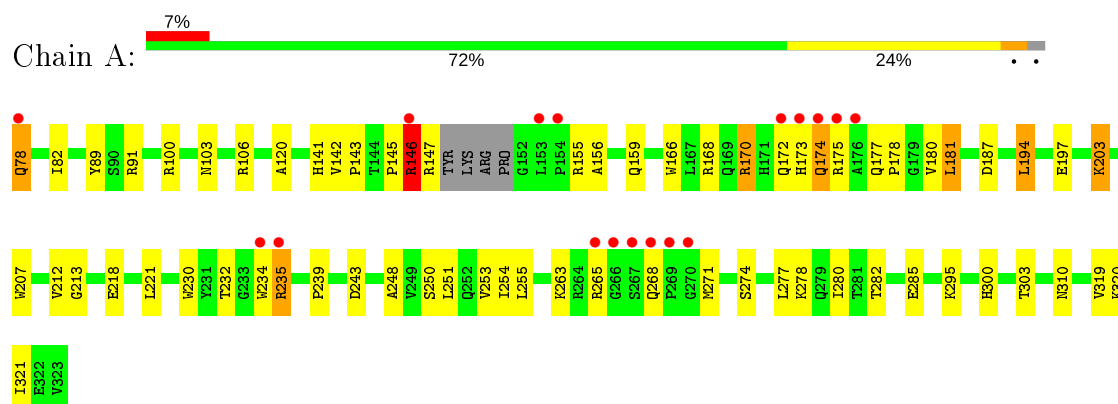
- Molecule 2 is water.

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		

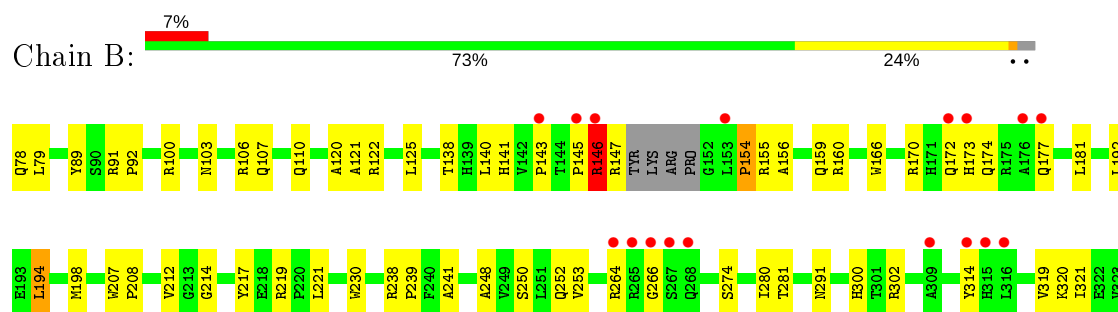
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

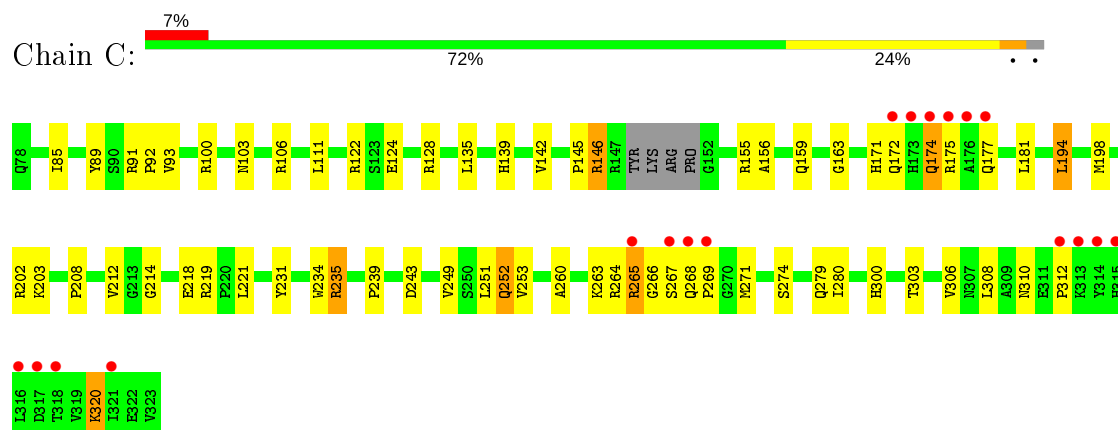
- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2




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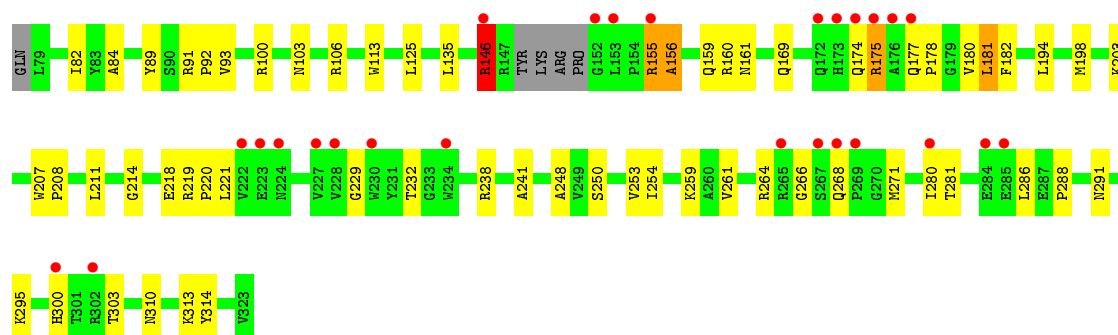


- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2



• Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2

Chain D:  11% 73% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.40 Å 122.59 Å 92.98 Å 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
$\langle I/\sigma(I) \rangle$ ¹	5.69 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.278 0.236 , 0.276	Depositor DCC
R_{free} test set	3837 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8273	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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 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	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

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 12.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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
1:D:93:VAL:HG21	1:D:303:THR:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:85:ILE:HD12	1:C:163:GLY:HA3	1.86	0.56
1:D:313:LYS:HD2	1:D:314:TYR:CE2	2.40	0.56
1:D:146:ARG:H	1:D:146:ARG:NE	2.03	0.56
1:D:250:SER:OG	1:D:253:VAL:HG23	2.05	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:A:170:ARG:HD3	1:A:170:ARG:O	2.08	0.54
1:C:155:ARG:O	1:C:156:ALA:HB3	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:124:GLU:O	1:C:128:ARG:HG3	2.11	0.51
1:C:263:LYS:HE3	1:C:265:ARG:CB	2.38	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:C:260:ALA:CB	1:C:280:ILE:HD11	2.40	0.50
1:D:103:ASN:HD22	1:D:106:ARG:NH2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:122:ARG:HG2	1:C:139:HIS:CD2	2.48	0.49
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.78	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:B:207:TRP:HH2	1:B:248:ALA:HB2	1.78	0.48
1:C:320:LYS:HD3	1:C:320:LYS:C	2.34	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:A:207:TRP:HH2	1:A:248:ALA:HB2	1.80	0.47
1:B:146:ARG:HH11	1:B:147:ARG:NE	2.12	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:HD23	1:C:111:LEU:C	2.36	0.46
1:B:239:PRO:HG2	1:B:274:SER:OG	2.15	0.46
1:D:291:ASN:HD22	1:D:295:LYS:CD	2.25	0.46
1:A:172:GLN:C	1:A:174:GLN:H	2.19	0.46
1:C:194:LEU:HD13	1:C:198:MET:HE2	1.98	0.46
1:D:156:ALA:HB3	1:D:160:ARG:NH1	2.31	0.46
1:C:93:VAL:HG12	1:D:211:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HG12	1:D:180:VAL:CG1	2.46	0.46
1:B:78:GLN:HG2	1:B:79:LEU:N	2.31	0.46
1:D:219:ARG:HA	1:D:220:PRO:HD3	1.85	0.46
1:A:187:ASP:HB2	2:A:424:HOH:O	2.16	0.46
1:B:319:VAL:O	1:B:321:ILE:HD12	2.16	0.46
1:A:263:LYS:HG3	1:A:265:ARG:HG3	1.97	0.46
1:D:155:ARG:O	1:D:156:ALA:HB2	2.16	0.46
1:B:122:ARG:HG3	1:B:141:HIS:CD2	2.52	0.45
1:A:172:GLN:HG3	1:A:173:HIS:N	2.32	0.45
1:A:268:GLN:HG2	1:A:271:MET:CE	2.45	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:B:250:SER:HG	1:B:253:VAL:HG23	1.82	0.45
1:C:103:ASN:HD22	1:C:106:ARG:NH2	2.09	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:B:302:ARG:HD3	2:B:344:HOH:O	2.16	0.44
1:D:125:LEU:C	1:D:125:LEU:HD23	2.38	0.44
1:C:135:LEU:HD23	1:C:135:LEU:N	2.32	0.44
1:B:238:ARG:CZ	1:B:241:ALA:HA	2.48	0.44
1:D:253:VAL:HG11	1:D:280:ILE:HG23	2.00	0.44
1:C:308:LEU:HA	1:D:214:GLY:O	2.18	0.43
1:B:208:PRO:HG3	1:B:219:ARG:HB2	2.00	0.43
1:D:113:TRP:HE3	1:D:135:LEU:HD11	1.82	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:221:LEU:HD23	1:A:230:TRP:N	2.33	0.43
1:A:303:THR:HA	1:B:302:ARG:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:138:THR:HG22	1:B:140:LEU:HG	2.02	0.42
1:C:128:ARG:HB3	1:C:128:ARG:NH2	2.34	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:A:243:ASP:OD1	1:A:300:HIS:NE2	2.54	0.41
1:A:321:ILE:HD13	1:B:217:TYR:CZ	2.55	0.41
1:B:156:ALA:O	1:B:160:ARG:HG3	2.21	0.41
1:C:142:VAL:HG13	1:C:142:VAL:O	2.20	0.41
1:D:146:ARG:N	1:D:146:ARG:NE	2.68	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:177:GLN:N	1:D:178:PRO:CD	2.84	0.40
1:D:221:LEU:HB2	1:D:229:GLY:HA3	2.02	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:N	1:A:221:LEU:HD22	2.37	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	238/246 (97%)	226 (95%)	9 (4%)	3 (1%)	12	6
1	B	238/246 (97%)	223 (94%)	11 (5%)	4 (2%)	9	4
1	C	238/246 (97%)	217 (91%)	14 (6%)	7 (3%)	4	1
1	D	237/246 (96%)	216 (91%)	18 (8%)	3 (1%)	12	6
All	All	951/984 (97%)	882 (93%)	52 (6%)	17 (2%)	8	3

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 [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	208/212 (98%)	200 (96%)	8 (4%)	33	31
1	B	208/212 (98%)	200 (96%)	8 (4%)	33	31
1	C	208/212 (98%)	203 (98%)	5 (2%)	49	51
1	D	207/212 (98%)	200 (97%)	7 (3%)	37	36
All	All	831/848 (98%)	803 (97%)	28 (3%)	37	36

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
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 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	242/246 (98%)	0.40	17 (7%) 16 15	12, 30, 59, 81	0
1	B	242/246 (98%)	0.42	17 (7%) 16 15	12, 30, 62, 75	0
1	C	242/246 (98%)	0.47	18 (7%) 14 13	13, 28, 65, 86	0
1	D	241/246 (97%)	0.73	26 (10%) 5 5	13, 39, 75, 88	0
All	All	967/984 (98%)	0.51	78 (8%) 12 11	12, 31, 67, 88	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ALA	11.3
1	C	314	TYR	10.9
1	C	173	HIS	10.5
1	D	176	ALA	9.9
1	D	269	PRO	9.6
1	D	268	GLN	9.2
1	A	175	ARG	8.2
1	B	267	SER	7.9
1	D	173	HIS	7.7
1	C	315	HIS	7.1
1	D	267	SER	6.8
1	C	265	ARG	6.4
1	C	267	SER	6.3
1	B	314	TYR	6.3
1	B	265	ARG	6.2
1	C	176	ALA	6.2
1	A	269	PRO	6.1
1	D	230	TRP	5.3
1	D	174	GLN	5.3
1	C	316	LEU	5.3
1	D	280	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	234	TRP	5.0
1	A	173	HIS	4.8
1	C	175	ARG	4.8
1	A	265	ARG	4.1
1	B	176	ALA	4.0
1	B	309	ALA	3.8
1	A	267	SER	3.8
1	B	316	LEU	3.7
1	B	315	HIS	3.7
1	A	154	PRO	3.7
1	D	175	ARG	3.6
1	A	266	GLY	3.6
1	B	268	GLN	3.5
1	B	172	GLN	3.5
1	D	228	VAL	3.4
1	C	317	ASP	3.4
1	D	172	GLN	3.4
1	A	174	GLN	3.4
1	C	269	PRO	3.4
1	C	268	GLN	3.3
1	A	146	ARG	3.2
1	A	234	TRP	3.2
1	D	222	VAL	3.2
1	A	235	ARG	3.2
1	A	172	GLN	3.1
1	D	265	ARG	2.8
1	C	313	LYS	2.8
1	D	155	ARG	2.7
1	C	174	GLN	2.7
1	A	153	LEU	2.7
1	D	227	VAL	2.7
1	D	153	LEU	2.7
1	B	173	HIS	2.6
1	D	224	ASN	2.6
1	B	146	ARG	2.6
1	C	312	PRO	2.6
1	B	264	ARG	2.6
1	B	153	LEU	2.6
1	C	318	THR	2.5
1	D	284	GLU	2.5
1	D	146	ARG	2.5
1	B	145	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	177	GLN	2.4
1	D	152	GLY	2.4
1	D	223	GLU	2.4
1	D	177	GLN	2.4
1	B	266	GLY	2.3
1	D	285	GLU	2.2
1	D	302	ARG	2.2
1	A	270	GLY	2.2
1	C	172	GLN	2.2
1	D	300	HIS	2.2
1	B	143	PRO	2.2
1	C	177	GLN	2.1
1	C	321	ILE	2.1
1	A	268	GLN	2.1
1	A	78	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.