



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 2D0J / pdb_00002d0j
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

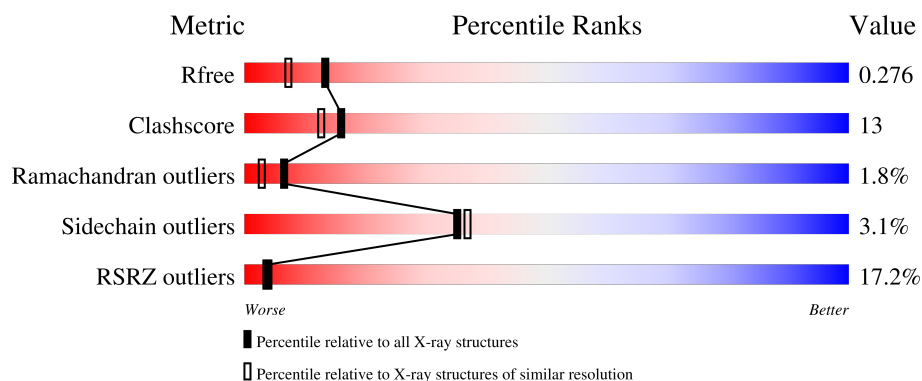
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of 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	
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 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			

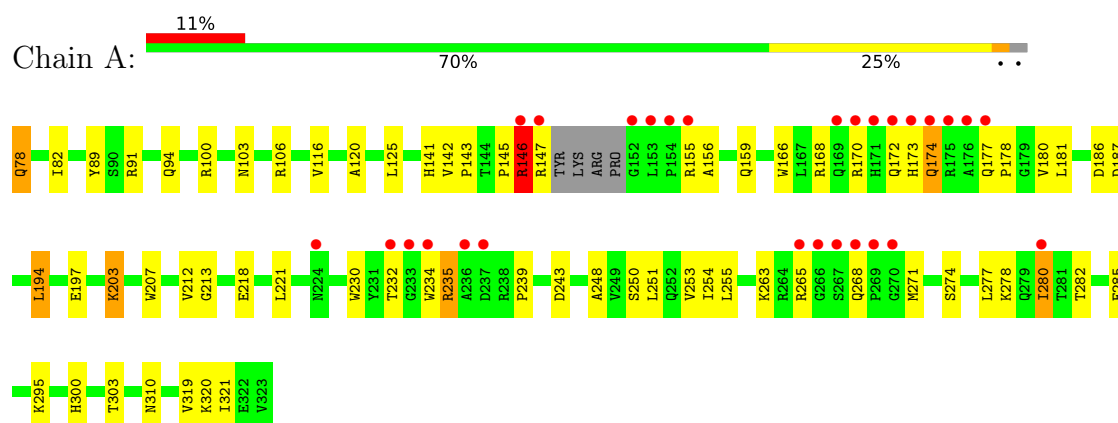
- Molecule 2 is water.

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		

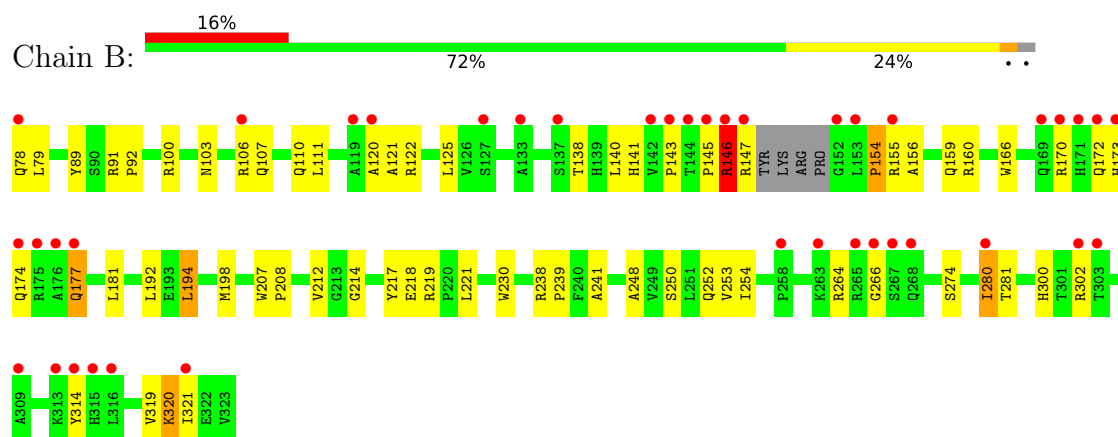
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

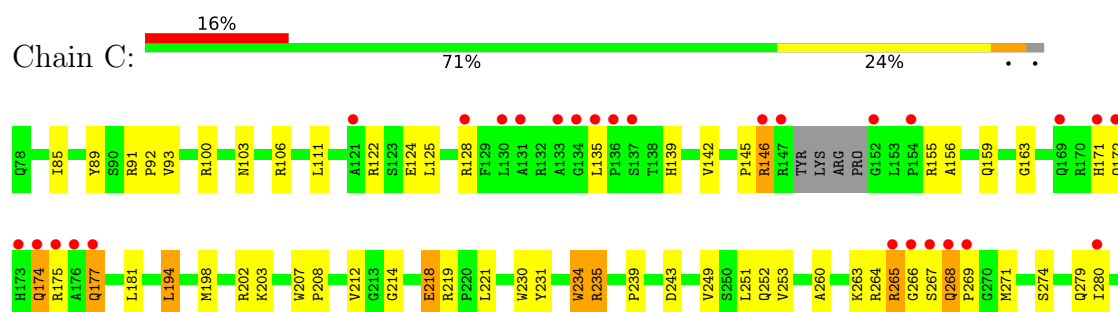
- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2

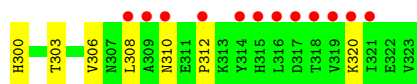


- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2

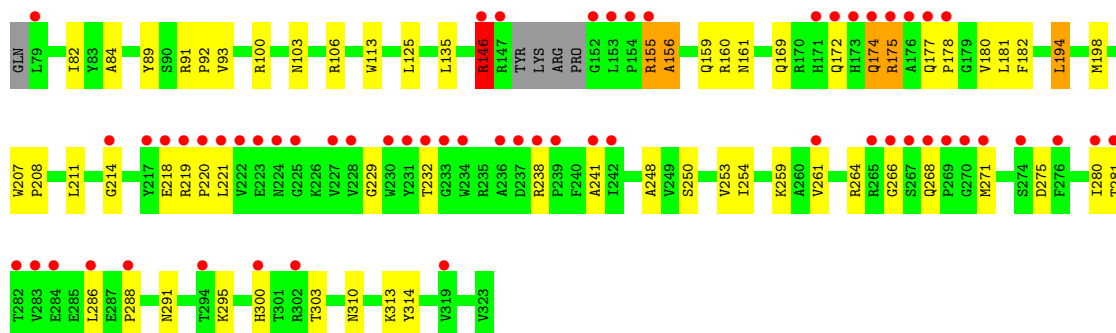
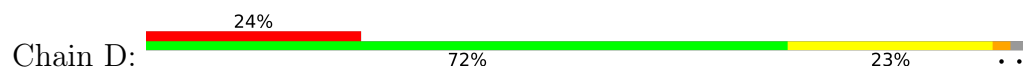


- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2





- Molecule 1: Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.40Å 122.59Å 92.98Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-2.00) 96.0 (40.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	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)	0.35 , 45.0	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 ⓘ

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	0.38	0/2002	0.87	4/2718 (0.1%)
1	B	0.39	0/2002	0.83	1/2718 (0.0%)
1	C	0.40	0/2002	0.85	5/2718 (0.2%)
1	D	0.36	0/1993	0.82	0/2706
All	All	0.38	0/7999	0.84	10/10860 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	GLU	N-CA-C	-6.06	100.12	109.52
1	C	268	GLN	CA-C-N	5.93	125.55	119.56
1	C	268	GLN	C-N-CA	5.93	125.55	119.56
1	A	94	GLN	N-CA-C	5.91	118.22	111.02
1	C	218	GLU	N-CA-C	-5.60	100.84	109.52
1	C	207	TRP	N-CA-C	5.54	113.00	108.07
1	A	280	ILE	N-CA-C	5.45	116.31	111.90
1	A	116	VAL	N-CA-C	5.24	115.12	107.37
1	C	234	TRP	N-CA-C	5.22	117.42	108.90
1	A	186	ASP	N-CA-C	5.17	119.21	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	59	0
1	B	1955	0	1968	53	0
1	C	1955	0	1968	54	0
1	D	1946	0	1960	53	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	207	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 (207) 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:A:268:GLN:HG2	1:A:271:MET:HE2	1.75	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:D:135:LEU:O	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:125:LEU:HD23	1:B:125:LEU:C	2.26	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
1:A:321:ILE:N	1:A:321:ILE:HD12	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:A:320:LYS:C	1:A:321:ILE:HD12	2.31	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: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:O	1:A:170:ARG:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:CD2	1:B:230:TRP:C	2.81	0.53
1:A:235:ARG:HG2	1:A:235:ARG:HH21	1.73	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:C:320:LYS:HD3	1:C:320:LYS:C	2.34	0.52
1:A:251:LEU:O	1:A:255:LEU:HG	2.09	0.52
1:C:194:LEU:HD13	1:C:198:MET:HE3	1.90	0.52
1:D:156:ALA:O	1:D:160:ARG:HG3	2.10	0.52
1:B:155:ARG:O	1:B:156:ALA:HB3	2.09	0.52
1:A:155:ARG:O	1:A:156:ALA:HB3	2.10	0.52
1:D:221:LEU:HD23	1:D:229:GLY:C	2.35	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:111:LEU:HD23	1:C:111:LEU:C	2.36	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:172:GLN:C	1:A:174:GLN:H	2.19	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
1:A:146:ARG:HD3	1:A:146:ARG:N	2.24	0.50
1:C:203:LYS:HZ3	1:C:252:GLN:HE22	1.58	0.50
1:A:218:GLU:HG3	1:A:232:THR:HB	1.94	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: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:125:LEU:C	1:D:125:LEU:HD23	2.38	0.48
1:D:219:ARG:HD2	1:D:219:ARG:O	2.13	0.48
1:D:194:LEU:HD13	1:D:198:MET:CE	2.44	0.48
1:B:170:ARG:HG2	1:B:170:ARG:HH21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:PRO:HB2	1:C:306:VAL:HG21	1.96	0.47
1:A:78:GLN:N	1:A:78:GLN:OE1	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:145:PRO:O	1:B:146:ARG:C	2.56	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:D:264:ARG:C	1:D:266:GLY:H	2.24	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: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
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:A:268:GLN:CG	1:A:271:MET:HE2	2.45	0.45
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: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: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:H	1:A:146:ARG:CD	2.26	0.45
1:A:82:ILE:HG12	1:A:180:VAL:CG2	2.47	0.44
1:A:141:HIS:O	1:A:142:VAL:HG23	2.17	0.44
1:A:268:GLN:HG2	1:A:271:MET:CE	2.45	0.44
1:A:125:LEU:C	1:A:125:LEU:HD23	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:MET:HE3	1:D:275:ASP:OD1	2.18	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:C:135:LEU:N	1:C:135:LEU:HD23	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:HB3	1:D:219:ARG:HB3	2.00	0.43
1:D:208:PRO:CB	1:D:219:ARG:HB3	2.47	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
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:B:250:SER:HG	1:B:253:VAL:HG23	1.83	0.42
1:C:235:ARG:HH11	1:C:235:ARG:CG	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:NH2	1:C:128:ARG:HB3	2.34	0.42
1:B:89:TYR:CE1	1:B:91:ARG:HD3	2.54	0.42
1:B:111:LEU:C	1:B:111:LEU:HD23	2.44	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:172:GLN:C	1:D:174:GLN:H	2.28	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:C:221:LEU:HD13	1:C:230:TRP:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HD23	1:B:230:TRP:C	2.45	0.41
1:C:142:VAL:HG13	1:C:142:VAL:O	2.20	0.41
1:D:146:ARG:NE	1:D:146:ARG:N	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:C:125:LEU:C	1:C:125:LEU:HD23	2.46	0.41
1:A:181:LEU:HD21	1:A:254:ILE:CG1	2.46	0.41
1:A:141:HIS:C	1:A:142:VAL:HG23	2.46	0.40
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:194:LEU:HD13	1:D:198:MET:HE2	2.02	0.40
1:D:221:LEU:HB2	1:D:229:GLY:HA3	2.02	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
1:A:319:VAL:HG12	1:A:320:LYS:N	2.36	0.40
1:A:268:GLN:CB	1:A:271:MET:HE2	2.51	0.40
1:C:159:GLN:H	1:C:159:GLN:CD	2.29	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%)	9	5
1	B	238/246 (97%)	223 (94%)	11 (5%)	4 (2%)	7	3
1	C	238/246 (97%)	217 (91%)	14 (6%)	7 (3%)	3	1
1	D	237/246 (96%)	216 (91%)	18 (8%)	3 (1%)	9	5
All	All	951/984 (97%)	882 (93%)	52 (6%)	17 (2%)	6	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 ⓘ

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%)	203 (98%)	5 (2%)	43	47
1	B	208/212 (98%)	197 (95%)	11 (5%)	20	18
1	C	208/212 (98%)	204 (98%)	4 (2%)	50	56
1	D	207/212 (98%)	201 (97%)	6 (3%)	37	40
All	All	831/848 (98%)	805 (97%)	26 (3%)	35	37

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	146	ARG
1	A	194	LEU
1	A	203	LYS
1	A	234	TRP

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Mol	Chain	Res	Type
1	B	146	ARG
1	B	172	GLN
1	B	173	HIS
1	B	177	GLN
1	B	181	LEU
1	B	192	LEU
1	B	194	LEU
1	B	252	GLN
1	B	254	ILE
1	B	280	ILE
1	B	320	LYS
1	C	177	GLN
1	C	194	LEU
1	C	235	ARG
1	C	279	GLN
1	D	146	ARG
1	D	155	ARG
1	D	169	GLN
1	D	175	ARG
1	D	194	LEU
1	D	300	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	141	HIS
1	A	174	GLN
1	A	177	GLN
1	A	279	GLN
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	307	ASN

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Mol	Chain	Res	Type
1	B	310	ASN
1	B	315	HIS
1	C	103	ASN
1	C	107	GLN
1	C	188	ASN
1	C	196	GLN
1	C	252	GLN
1	C	279	GLN
1	C	300	HIS
1	D	103	ASN
1	D	107	GLN
1	D	110	GLN
1	D	141	HIS
1	D	172	GLN
1	D	177	GLN
1	D	188	ASN
1	D	196	GLN
1	D	224	ASN
1	D	279	GLN
1	D	291	ASN
1	D	300	HIS
1	D	310	ASN

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 oligosaccharides 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%)	0.58	28 (11%) 9 8	12, 30, 59, 81	0
1	B	242/246 (98%)	0.78	40 (16%) 4 4	12, 30, 62, 75	0
1	C	242/246 (98%)	0.79	39 (16%) 4 4	13, 28, 65, 86	0
1	D	241/246 (97%)	1.26	59 (24%) 2 1	13, 39, 75, 88	0
All	All	967/984 (98%)	0.85	166 (17%) 4 3	12, 31, 67, 88	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	ALA	8.7
1	A	176	ALA	7.7
1	D	269	PRO	7.5
1	C	314	TYR	7.4
1	C	173	HIS	7.0
1	B	316	LEU	6.9
1	C	316	LEU	6.7
1	C	176	ALA	6.4
1	D	152	GLY	6.2
1	B	314	TYR	6.2
1	D	280	ILE	6.0
1	C	175	ARG	5.8
1	D	234	TRP	5.8
1	D	268	GLN	5.7
1	D	230	TRP	5.6
1	C	315	HIS	5.6
1	C	266	GLY	5.5
1	A	269	PRO	5.3
1	C	174	GLN	5.2
1	C	268	GLN	5.2
1	B	315	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	145	PRO	5.0
1	B	267	SER	4.8
1	D	233	GLY	4.7
1	B	266	GLY	4.7
1	A	146	ARG	4.4
1	C	265	ARG	4.4
1	D	173	HIS	4.3
1	D	267	SER	4.3
1	C	267	SER	4.3
1	D	154	PRO	4.2
1	D	221	LEU	4.2
1	A	175	ARG	4.2
1	B	265	ARG	4.1
1	C	269	PRO	4.1
1	B	280	ILE	4.1
1	B	176	ALA	4.1
1	B	268	GLN	4.1
1	A	154	PRO	4.1
1	A	266	GLY	4.0
1	A	267	SER	4.0
1	D	147	ARG	3.9
1	C	308	LEU	3.8
1	A	177	GLN	3.8
1	C	133	ALA	3.7
1	A	270	GLY	3.7
1	D	155	ARG	3.7
1	D	300	HIS	3.6
1	B	146	ARG	3.6
1	D	153	LEU	3.6
1	C	312	PRO	3.6
1	C	172	GLN	3.5
1	B	142	VAL	3.5
1	A	234	TRP	3.5
1	D	231	TYR	3.5
1	D	302	ARG	3.5
1	C	319	VAL	3.5
1	C	131	ALA	3.4
1	C	134	GLY	3.4
1	D	283	VAL	3.4
1	D	177	GLN	3.4
1	A	268	GLN	3.4
1	D	174	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	3.4
1	B	173	HIS	3.3
1	C	177	GLN	3.3
1	A	173	HIS	3.3
1	C	146	ARG	3.3
1	D	227	VAL	3.2
1	D	172	GLN	3.2
1	C	321	ILE	3.2
1	B	175	ARG	3.2
1	C	280	ILE	3.1
1	A	233	GLY	3.1
1	D	175	ARG	3.1
1	B	309	ALA	3.1
1	D	218	GLU	3.1
1	B	147	ARG	3.0
1	D	239	PRO	3.0
1	D	219	ARG	3.0
1	D	270	GLY	3.0
1	C	318	THR	3.0
1	D	171	HIS	3.0
1	A	155	ARG	2.9
1	A	280	ILE	2.9
1	A	172	GLN	2.9
1	D	220	PRO	2.8
1	D	222	VAL	2.8
1	D	261	VAL	2.8
1	A	265	ARG	2.8
1	D	271	MET	2.8
1	A	153	LEU	2.8
1	B	144	THR	2.8
1	D	178	PRO	2.8
1	A	174	GLN	2.7
1	D	286	LEU	2.7
1	C	152	GLY	2.7
1	A	171	HIS	2.7
1	B	133	ALA	2.6
1	D	281	THR	2.6
1	C	154	PRO	2.6
1	B	321	ILE	2.6
1	B	172	GLN	2.6
1	D	232	THR	2.6
1	B	313	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	238	ARG	2.6
1	D	274	SER	2.5
1	D	217	TYR	2.5
1	D	237	ASP	2.5
1	D	241	ALA	2.5
1	B	155	ARG	2.5
1	B	143	PRO	2.5
1	D	236	ALA	2.5
1	A	170	ARG	2.4
1	D	242	ILE	2.4
1	D	284	GLU	2.4
1	C	136	PRO	2.4
1	A	147	ARG	2.4
1	B	171	HIS	2.4
1	C	171	HIS	2.4
1	A	224	ASN	2.4
1	C	320	LYS	2.4
1	D	79	LEU	2.4
1	D	228	VAL	2.4
1	B	152	GLY	2.3
1	C	147	ARG	2.3
1	B	120	ALA	2.3
1	D	266	GLY	2.3
1	B	263	LYS	2.3
1	A	169	GLN	2.3
1	D	294	THR	2.3
1	D	146	ARG	2.3
1	D	276	PHE	2.3
1	D	224	ASN	2.3
1	B	170	ARG	2.3
1	A	237	ASP	2.3
1	B	302	ARG	2.2
1	C	128	ARG	2.2
1	D	288	PRO	2.2
1	C	317	ASP	2.2
1	C	135	LEU	2.2
1	B	169	GLN	2.1
1	C	309	ALA	2.1
1	C	169	GLN	2.1
1	D	214	GLY	2.1
1	D	319	VAL	2.1
1	D	265	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	153	LEU	2.1
1	C	130	LEU	2.1
1	D	223	GLU	2.1
1	B	177	GLN	2.1
1	B	303	THR	2.1
1	B	127	SER	2.1
1	B	137	SER	2.1
1	B	78	GLN	2.1
1	B	258	PRO	2.1
1	D	282	THR	2.1
1	B	174	GLN	2.0
1	B	106	ARG	2.0
1	A	232	THR	2.0
1	C	137	SER	2.0
1	A	236	ALA	2.0
1	B	119	ALA	2.0
1	C	121	ALA	2.0
1	C	310	ASN	2.0
1	D	225	GLY	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 oligosaccharides 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.