



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:06 PM UTC

PDB ID : 1FR8 / pdb_00001fr8
Title : CRYSTAL STRUCTURE OF THE BOVINE BETA 1,4 GALACTOSYLTRANSFERASE (B4GALT1) CATALYTIC DOMAIN COMPLEXED WITH URIDINE DIPHOSPHOGALACTOSE
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Deposited on : 2000-09-07
Resolution : 2.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

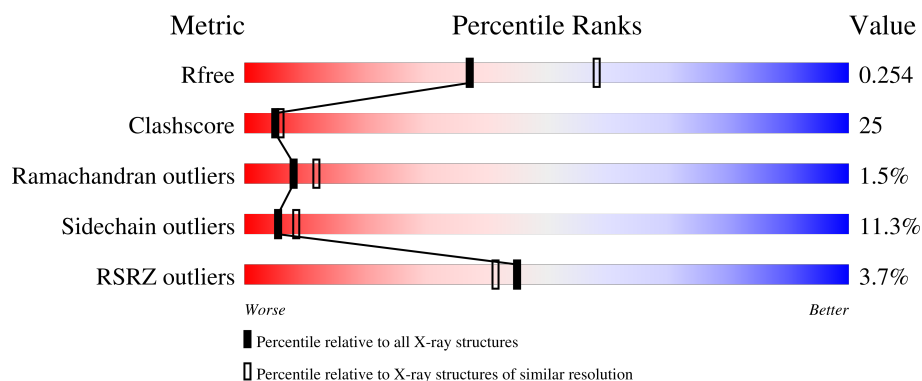
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	288	3% 46% 36% 11% 6%
1	B	288	3% 53% 32% 7% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4549 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.

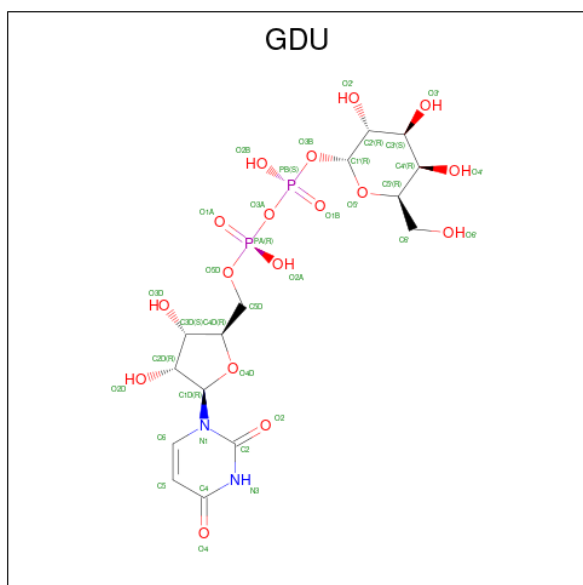
- Molecule 1 is a protein called BETA 1,4 GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2210	1418	381	397	14			
1	B	271	Total	C	N	O	S	0	0	0
			2210	1418	381	397	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	VAL	ILE	conflict	UNP P08037
A	187	PRO	LEU	SEE REMARK 999	UNP P08037
B	158	VAL	ILE	conflict	UNP P08037
B	187	PRO	LEU	SEE REMARK 999	UNP P08037

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

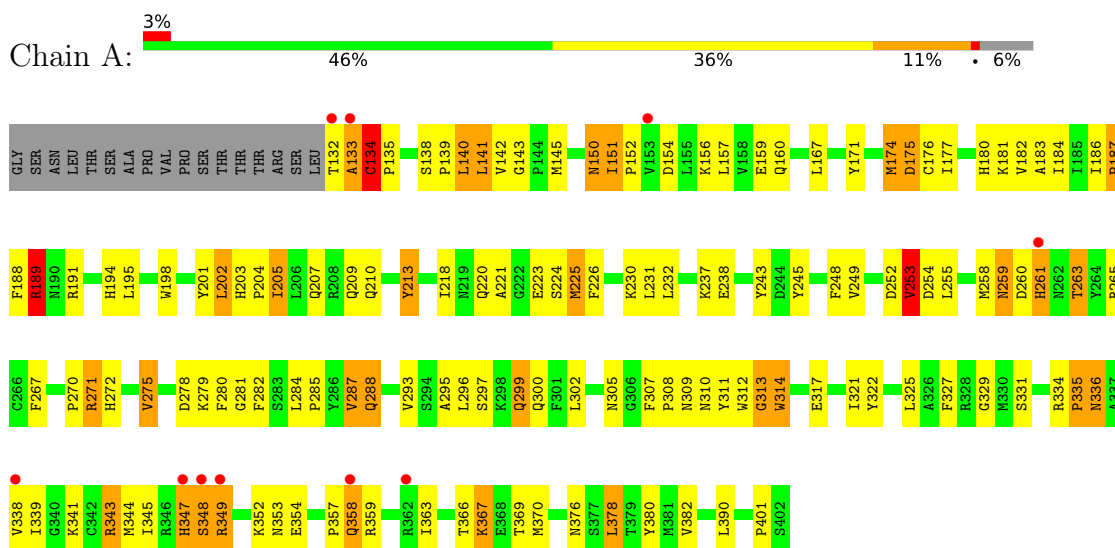
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	47	Total	O	0	0
			47	47		

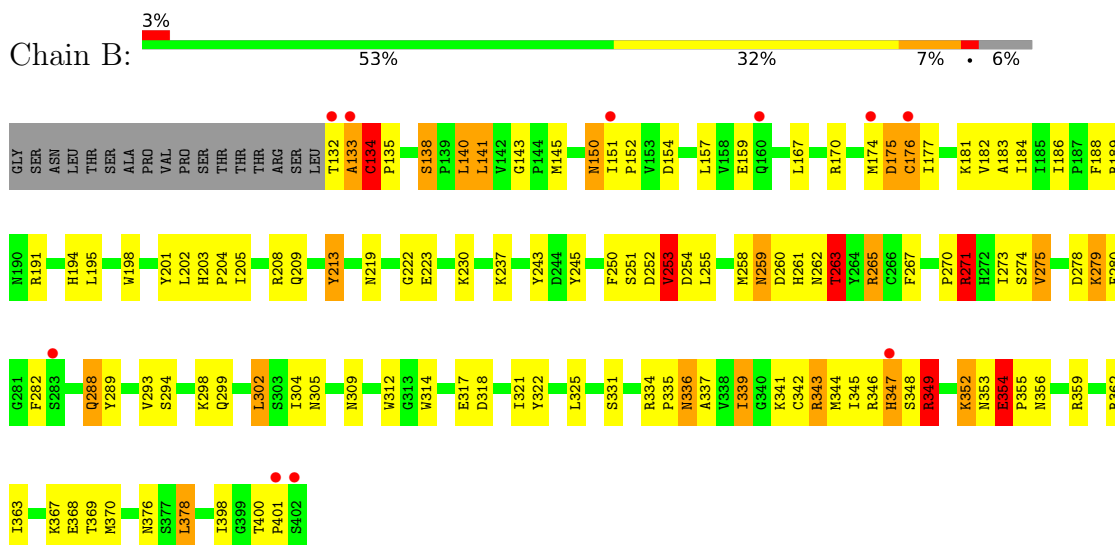
3 Residue-property plots [i](#)

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: BETA 1,4 GALACTOSYLTRANSFERASE



• Molecule 1: BETA 1,4 GALACTOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.72Å 161.37Å 106.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.40) 91.8 (30.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.31Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.262 0.229 , 0.254	Depositor DCC
R_{free} test set	1000 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4549	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: GDU

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	0.74	0/2270	1.20	29/3074 (0.9%)
1	B	0.80	0/2270	1.19	20/3074 (0.7%)
All	All	0.77	0/4540	1.19	49/6148 (0.8%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	VAL	N-CA-C	7.97	118.77	110.72
1	B	335	PRO	N-CA-C	-7.80	99.50	111.13
1	B	275	VAL	N-CA-C	7.65	119.34	111.00
1	B	182	VAL	N-CA-C	7.58	119.19	108.36
1	A	221	ALA	N-CA-C	7.55	120.58	111.82
1	B	253	VAL	CB-CA-C	-7.55	101.95	112.14
1	A	213	TYR	N-CA-C	7.50	120.81	109.41
1	B	134	CYS	N-CA-C	7.22	120.48	110.01
1	A	313	GLY	N-CA-C	-6.97	105.19	115.72
1	B	378	LEU	N-CA-C	6.97	119.18	109.15
1	A	202	LEU	N-CA-C	6.63	118.59	111.36
1	A	134	CYS	N-CA-C	6.48	118.05	109.83
1	B	271	ARG	N-CA-C	6.47	119.50	109.07
1	A	253	VAL	CB-CA-C	-6.46	101.79	112.26
1	A	287	VAL	N-CA-C	6.46	119.12	111.05
1	B	213	TYR	N-CA-C	6.41	118.92	109.69
1	A	271	ARG	N-CA-C	6.29	119.49	109.24
1	A	378	LEU	N-CA-C	6.26	118.79	109.59
1	B	159	GLU	N-CA-C	-6.25	104.15	110.97
1	B	280	PHE	N-CA-C	-6.12	103.24	111.87
1	A	314	TRP	N-CA-C	-6.09	105.88	113.38
1	B	368	GLU	N-CA-C	6.07	117.58	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	THR	N-CA-C	5.96	120.55	113.28
1	B	309	ASN	N-CA-C	-5.83	106.02	114.12
1	B	188	PHE	N-CA-C	5.80	118.23	109.23
1	B	219	ASN	N-CA-C	5.79	118.09	108.20
1	A	263	THR	N-CA-C	5.73	118.66	110.24
1	A	223	GLU	N-CA-C	-5.70	104.07	111.71
1	B	138	SER	CA-C-N	5.68	125.21	119.19
1	B	138	SER	C-N-CA	5.68	125.21	119.19
1	A	182	VAL	N-CA-C	5.58	116.34	108.36
1	B	223	GLU	N-CA-C	-5.58	104.02	112.99
1	B	354	GLU	N-CA-C	5.52	118.30	110.24
1	A	156	LYS	N-CA-C	-5.50	105.28	111.28
1	A	311	TYR	N-CA-C	-5.42	100.95	109.25
1	A	348	SER	N-CA-C	-5.40	99.29	110.80
1	A	390	LEU	N-CA-C	5.37	119.99	113.38
1	A	205	ILE	N-CA-C	5.33	115.96	110.36
1	A	188	PHE	N-CA-C	5.31	117.46	109.23
1	A	369	THR	N-CA-C	5.31	120.03	113.50
1	A	335	PRO	N-CA-C	-5.27	103.55	111.57
1	A	310	ASN	N-CA-C	5.26	119.70	113.28
1	A	221	ALA	CA-C-N	-5.24	114.50	122.04
1	A	221	ALA	C-N-CA	-5.24	114.50	122.04
1	B	263	THR	N-CA-C	5.20	117.85	110.10
1	A	159	GLU	N-CA-C	-5.11	105.61	111.07
1	A	261	HIS	N-CA-C	-5.09	106.58	112.89
1	A	187	PRO	N-CA-C	-5.01	103.32	111.19
1	A	382	VAL	CB-CA-C	-5.00	106.50	111.80

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	2210	0	2174	115	0
1	B	2210	0	2174	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	11	2	0
2	B	25	0	11	3	0
3	A	32	0	0	2	0
3	B	47	0	0	12	0
All	All	4549	0	4370	219	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 25.

All (219) 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:258:MET:HE2	1:B:341:LYS:HB3	1.42	0.98
1:B:362:ARG:HD3	3:B:55:HOH:O	1.63	0.98
1:B:336:ASN:HD21	1:B:339:ILE:HG23	1.31	0.93
1:B:349:ARG:NE	1:B:349:ARG:HA	1.83	0.91
1:A:349:ARG:CZ	1:A:349:ARG:HA	2.05	0.85
1:B:250:PHE:HB2	3:B:35:HOH:O	1.75	0.84
1:A:267:PHE:CD1	1:A:271:ARG:HG3	2.11	0.84
1:A:174:MET:HE2	1:A:174:MET:H	1.43	0.83
1:B:258:MET:HE2	1:B:341:LYS:CB	2.09	0.82
1:A:258:MET:HE2	1:A:341:LYS:HB3	1.61	0.81
1:B:134:CYS:SG	1:B:135:PRO:HD2	2.20	0.80
1:B:151:ILE:HD12	1:B:151:ILE:O	1.82	0.80
1:A:336:ASN:C	1:A:336:ASN:HD22	1.91	0.79
1:A:191:ARG:HD2	1:A:194:HIS:HD2	1.47	0.79
1:B:259:ASN:C	1:B:259:ASN:HD22	1.90	0.79
1:B:140:LEU:N	1:B:140:LEU:HD23	1.99	0.78
1:B:349:ARG:HA	1:B:349:ARG:CZ	2.12	0.78
1:A:349:ARG:HA	1:A:349:ARG:NE	2.01	0.76
1:B:336:ASN:HD21	1:B:339:ILE:H	1.31	0.74
1:B:230:LYS:HE2	1:B:398:ILE:HB	1.69	0.74
1:B:132:THR:HB	1:B:177:ILE:HG12	1.70	0.74
1:A:259:ASN:HD22	1:A:261:HIS:H	1.36	0.72
1:A:134:CYS:SG	1:A:135:PRO:HD2	2.31	0.71
1:A:279:LYS:HD3	1:A:344:MET:SD	2.31	0.71
1:B:336:ASN:ND2	1:B:339:ILE:HG23	2.03	0.71
1:A:278:ASP:OD2	1:A:343:ARG:HA	1.92	0.70
1:B:258:MET:HE1	1:B:341:LYS:HE2	1.72	0.70
1:B:305:ASN:HD21	1:B:376:ASN:H	1.38	0.70
1:A:225:MET:SD	1:A:312:TRP:O	2.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HE2	1:A:341:LYS:CB	2.22	0.69
1:A:132:THR:HB	1:A:177:ILE:HG12	1.74	0.69
1:A:174:MET:H	1:A:174:MET:CE	2.05	0.69
1:B:259:ASN:ND2	1:B:261:HIS:H	1.92	0.68
1:B:336:ASN:ND2	1:B:339:ILE:H	1.93	0.67
1:A:140:LEU:HD23	1:A:140:LEU:N	2.08	0.67
1:B:344:MET:HE2	1:B:346:ARG:HB3	1.76	0.67
1:A:252:ASP:HB3	2:A:100:GDU:H3D	1.76	0.66
1:B:259:ASN:HD22	1:B:261:HIS:H	1.42	0.66
1:A:151:ILE:O	1:A:151:ILE:HD12	1.95	0.66
1:A:259:ASN:HD22	1:A:259:ASN:C	2.04	0.66
1:A:259:ASN:ND2	1:A:261:HIS:H	1.95	0.65
1:B:258:MET:CE	1:B:341:LYS:HB3	2.22	0.65
1:B:198:TRP:CZ2	1:B:202:LEU:HG	2.32	0.65
1:B:278:ASP:HA	1:B:282:PHE:CE1	2.32	0.65
1:B:344:MET:CE	1:B:346:ARG:HB3	2.27	0.65
1:B:253:VAL:HG22	2:B:403:GDU:O2D	1.98	0.64
1:A:186:ILE:HG21	1:A:253:VAL:HG13	1.79	0.64
1:B:294:SER:OG	3:B:35:HOH:O	2.15	0.64
1:B:288:GLN:HG3	1:B:359:ARG:CZ	2.28	0.63
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.81	0.62
1:A:279:LYS:HD2	1:A:354:GLU:OE2	1.98	0.62
1:A:313:GLY:N	3:A:75:HOH:O	2.33	0.62
1:B:279:LYS:HB3	1:B:346:ARG:NH1	2.13	0.62
1:B:352:LYS:HE2	1:B:353:ASN:H	1.65	0.61
1:B:354:GLU:HG2	1:B:355:PRO:HD2	1.83	0.61
1:B:362:ARG:NH1	3:B:55:HOH:O	2.26	0.61
1:A:145:MET:HE2	1:A:260:ASP:N	2.16	0.60
1:B:336:ASN:C	1:B:336:ASN:HD22	2.08	0.60
1:B:198:TRP:HZ2	3:B:40:HOH:O	1.83	0.60
1:A:218:ILE:HG22	1:A:231:LEU:HD22	1.84	0.60
1:A:255:LEU:HD12	1:A:293:VAL:HG23	1.82	0.60
1:A:275:VAL:HG22	1:A:334:ARG:HD3	1.82	0.59
1:B:237:LYS:HD2	1:B:378:LEU:HD23	1.84	0.59
1:B:255:LEU:HD12	1:B:293:VAL:HG23	1.82	0.59
1:B:312:TRP:CD2	1:B:401:PRO:HG3	2.38	0.59
1:A:275:VAL:HG21	1:A:335:PRO:HD2	1.85	0.59
1:B:344:MET:HE3	3:B:71:HOH:O	2.01	0.59
1:A:189:ARG:HB3	1:A:226:PHE:CE1	2.38	0.58
1:A:305:ASN:HD21	1:A:376:ASN:H	1.50	0.58
1:A:203:HIS:O	1:A:207:GLN:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD22	1:B:151:ILE:N	2.02	0.58
1:B:344:MET:O	1:B:346:ARG:HG2	2.03	0.58
1:B:186:ILE:HG21	1:B:253:VAL:HG13	1.86	0.57
1:A:154:ASP:O	1:A:157:LEU:HB3	2.04	0.57
1:A:336:ASN:C	1:A:336:ASN:ND2	2.63	0.57
1:A:327:PHE:CD1	1:A:370:MET:HE1	2.40	0.56
1:A:150:ASN:O	1:A:152:PRO:HD3	2.05	0.56
1:A:285:PRO:HB3	1:A:357:PRO:HG2	1.87	0.56
1:B:175:ASP:OD1	1:B:175:ASP:N	2.37	0.56
1:B:138:SER:HB3	1:B:141:LEU:HD13	1.87	0.56
1:A:175:ASP:OD1	1:A:175:ASP:N	2.39	0.56
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.41	0.56
1:B:279:LYS:HB2	1:B:354:GLU:HB2	1.87	0.56
1:A:336:ASN:ND2	1:A:339:ILE:H	2.04	0.55
1:A:259:ASN:ND2	1:A:261:HIS:HB2	2.22	0.55
1:B:317:GLU:O	1:B:321:ILE:HG13	2.06	0.55
1:A:347:HIS:C	1:A:348:SER:O	2.45	0.54
1:B:150:ASN:O	1:B:152:PRO:HD3	2.08	0.54
1:A:205:ILE:O	1:A:209:GLN:HG3	2.08	0.54
1:A:358:GLN:HG2	1:A:359:ARG:N	2.22	0.54
1:B:258:MET:CE	1:B:341:LYS:HE2	2.38	0.54
1:B:279:LYS:HB3	1:B:346:ARG:CZ	2.37	0.54
1:A:201:TYR:O	1:A:204:PRO:HD2	2.08	0.54
1:B:267:PHE:CD1	1:B:271:ARG:HG3	2.43	0.54
1:A:271:ARG:HH12	1:A:335:PRO:HB3	1.73	0.53
1:A:272:HIS:HB3	1:A:334:ARG:HG2	1.90	0.53
1:B:254:ASP:HA	1:B:345:ILE:HD12	1.90	0.53
1:B:181:LYS:HD3	1:B:243:TYR:CE2	2.44	0.53
1:A:132:THR:O	1:A:133:ALA:CB	2.56	0.53
1:A:288:GLN:HG3	1:A:359:ARG:HD2	1.91	0.53
1:A:336:ASN:ND2	1:A:338:VAL:H	2.07	0.52
1:A:258:MET:HE1	1:A:341:LYS:HE2	1.90	0.52
1:A:307:PHE:HB3	1:A:308:PRO:HD2	1.91	0.52
1:B:132:THR:O	1:B:133:ALA:CB	2.57	0.52
1:A:132:THR:HB	1:A:177:ILE:CG1	2.40	0.52
1:B:134:CYS:HA	1:B:176:CYS:HB2	1.91	0.52
1:B:312:TRP:CG	1:B:401:PRO:HG3	2.45	0.52
1:A:282:PHE:HE2	1:A:341:LYS:HB3	1.74	0.51
1:B:259:ASN:HB2	3:B:36:HOH:O	2.10	0.51
1:A:189:ARG:HG3	1:A:189:ARG:O	2.09	0.51
1:B:354:GLU:CG	1:B:355:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ALA:H	1:A:177:ILE:H	1.58	0.51
1:B:263:THR:HB	1:B:265:ARG:HG2	1.92	0.51
1:B:154:ASP:O	1:B:157:LEU:HB3	2.11	0.51
1:B:273:ILE:HB	1:B:293:VAL:HG12	1.92	0.50
1:B:145:MET:HE2	1:B:260:ASP:N	2.26	0.50
1:A:336:ASN:HD22	1:A:338:VAL:H	1.58	0.50
1:A:347:HIS:O	1:A:348:SER:HB2	2.12	0.50
1:B:278:ASP:OD2	1:B:343:ARG:HD3	2.12	0.50
1:B:204:PRO:O	1:B:208:ARG:HG3	2.11	0.50
1:B:278:ASP:OD1	1:B:279:LYS:N	2.43	0.50
1:B:134:CYS:HB2	1:B:177:ILE:O	2.12	0.49
1:B:262:ASN:HB2	1:B:339:ILE:HD12	1.94	0.49
1:A:134:CYS:HA	1:A:176:CYS:HB2	1.94	0.49
1:A:150:ASN:HD22	1:A:151:ILE:N	2.11	0.49
1:A:363:ILE:HD13	1:B:314:TRP:CG	2.48	0.49
1:B:261:HIS:C	1:B:339:ILE:HD13	2.37	0.49
1:A:143:GLY:O	1:A:145:MET:HG3	2.13	0.49
1:A:275:VAL:CG2	1:A:334:ARG:HD3	2.43	0.49
1:A:181:LYS:HD3	1:A:243:TYR:CE2	2.48	0.49
1:A:189:ARG:HB3	1:A:226:PHE:HE1	1.77	0.49
1:A:280:PHE:CE2	1:A:357:PRO:HD3	2.48	0.49
2:A:100:GDU:H2D	2:A:100:GDU:O5D	2.12	0.49
1:B:253:VAL:CG2	2:B:403:GDU:O2D	2.60	0.48
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.94	0.48
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.78	0.48
1:A:174:MET:HE2	1:A:174:MET:N	2.21	0.48
1:B:252:ASP:HA	2:B:403:GDU:O3D	2.14	0.48
1:A:191:ARG:HD2	1:A:194:HIS:CD2	2.38	0.48
1:A:270:PRO:HD2	1:A:331:SER:O	2.14	0.47
1:A:184:ILE:HG13	1:A:249:VAL:HB	1.96	0.47
1:A:270:PRO:HG2	1:A:325:LEU:HD22	1.96	0.47
1:B:251:SER:CB	1:B:293:VAL:HG22	2.44	0.47
1:B:304:ILE:HG21	1:B:325:LEU:HD23	1.95	0.47
1:A:336:ASN:HD21	1:A:339:ILE:H	1.61	0.47
1:A:151:ILE:H	1:A:151:ILE:HG13	1.62	0.47
1:B:317:GLU:HG2	1:B:318:ASP:N	2.31	0.46
1:A:281:GLY:N	1:A:353:ASN:HD21	2.13	0.46
1:A:297:SER:OG	1:A:300:GLN:HG3	2.16	0.46
1:A:186:ILE:CG2	1:A:253:VAL:HG13	2.45	0.46
1:A:259:ASN:HD21	1:A:261:HIS:HB2	1.81	0.45
1:A:138:SER:HA	1:A:139:PRO:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ILE:O	1:B:275:VAL:N	2.50	0.45
1:A:366:THR:HG22	1:A:370:MET:HE2	1.98	0.45
1:B:209:GLN:NE2	1:B:263:THR:HA	2.32	0.45
1:A:198:TRP:CZ2	1:A:202:LEU:HG	2.53	0.44
1:B:259:ASN:HD22	1:B:260:ASP:N	2.15	0.44
1:A:248:PHE:O	1:A:295:ALA:HA	2.17	0.44
1:A:363:ILE:HD13	1:B:314:TRP:HB2	1.99	0.44
1:A:312:TRP:CG	1:A:401:PRO:HB3	2.52	0.44
1:A:317:GLU:O	1:A:321:ILE:HG13	2.18	0.44
1:A:329:GLY:HA2	3:B:22:HOH:O	2.18	0.44
1:B:151:ILE:O	1:B:151:ILE:CD1	2.59	0.44
1:B:258:MET:SD	1:B:343:ARG:HG2	2.58	0.44
1:B:289:TYR:O	1:B:334:ARG:NH2	2.49	0.44
1:A:259:ASN:C	1:A:259:ASN:ND2	2.75	0.44
1:B:288:GLN:HB3	1:B:322:TYR:CE2	2.53	0.43
1:B:344:MET:HE2	1:B:346:ARG:HD3	2.00	0.43
1:A:254:ASP:HA	1:A:345:ILE:HD12	2.00	0.43
1:A:299:GLN:HB2	3:A:17:HOH:O	2.18	0.43
1:B:288:GLN:HB3	1:B:288:GLN:HE21	1.55	0.43
1:B:336:ASN:ND2	1:B:336:ASN:C	2.73	0.43
1:B:143:GLY:O	1:B:145:MET:HG3	2.18	0.43
1:B:209:GLN:HG2	3:B:37:HOH:O	2.17	0.43
1:A:230:LYS:HD2	1:A:309:ASN:HB3	1.99	0.43
1:A:312:TRP:HB2	1:A:314:TRP:CZ3	2.53	0.43
1:A:237:LYS:HD2	1:A:378:LEU:HD23	2.01	0.43
1:A:275:VAL:CG2	1:A:335:PRO:HD2	2.47	0.43
1:B:337:ALA:O	1:B:341:LYS:HG3	2.18	0.43
1:A:238:GLU:OE2	1:A:380:TYR:OH	2.33	0.43
1:B:202:LEU:O	1:B:203:HIS:C	2.60	0.42
1:A:142:VAL:O	1:A:142:VAL:HG12	2.18	0.42
1:A:145:MET:HE2	1:A:259:ASN:C	2.45	0.42
1:A:278:ASP:OD2	1:A:343:ARG:HD3	2.19	0.42
1:B:259:ASN:C	1:B:259:ASN:ND2	2.62	0.42
1:A:220:GLN:HB2	1:A:231:LEU:HD11	2.02	0.42
1:A:295:ALA:C	1:A:296:LEU:HD12	2.44	0.42
1:A:142:VAL:O	1:A:142:VAL:CG1	2.68	0.42
1:A:327:PHE:CZ	1:A:367:LYS:HB2	2.55	0.42
1:A:336:ASN:HD21	1:A:339:ILE:HG23	1.85	0.42
1:A:183:ALA:HB2	1:A:245:TYR:CD1	2.55	0.42
1:B:151:ILE:H	1:B:151:ILE:HG13	1.64	0.42
1:A:135:PRO:HG2	1:A:210:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:HD22	1:A:150:ASN:C	2.28	0.41
1:B:170:ARG:NH1	1:B:213:TYR:O	2.43	0.41
1:B:342:CYS:SG	3:B:60:HOH:O	2.34	0.41
1:B:370:MET:HE3	1:B:370:MET:HB3	1.81	0.41
1:A:171:TYR:HD2	1:A:213:TYR:CE2	2.39	0.41
1:A:278:ASP:OD1	1:A:279:LYS:N	2.54	0.41
1:B:288:GLN:H	1:B:288:GLN:HG2	1.57	0.41
1:B:150:ASN:HD22	1:B:150:ASN:C	2.28	0.41
1:B:271:ARG:NH1	3:B:39:HOH:O	2.39	0.41
1:A:157:LEU:O	1:A:160:GLN:HB3	2.20	0.41
1:A:258:MET:SD	1:A:343:ARG:HG2	2.61	0.41
1:A:284:LEU:HD21	1:A:334:ARG:CZ	2.50	0.41
1:A:359:ARG:HH12	1:B:314:TRP:CA	2.34	0.41
1:B:191:ARG:HD2	1:B:194:HIS:HD2	1.85	0.41
1:B:198:TRP:CE2	1:B:202:LEU:HG	2.56	0.41
1:B:222:GLY:HA3	3:B:32:HOH:O	2.20	0.41
1:B:339:ILE:HD12	1:B:339:ILE:O	2.21	0.41
1:B:201:TYR:O	1:B:205:ILE:HG13	2.21	0.41
1:B:349:ARG:NE	1:B:349:ARG:CA	2.67	0.41
1:B:305:ASN:ND2	1:B:376:ASN:H	2.14	0.40
1:A:189:ARG:NH2	1:A:224:SER:O	2.47	0.40
1:A:258:MET:CE	1:A:341:LYS:HE2	2.51	0.40
1:A:288:GLN:HB3	1:A:322:TYR:CZ	2.55	0.40
1:B:183:ALA:HB2	1:B:245:TYR:CD1	2.56	0.40
1:B:270:PRO:HD2	1:B:331:SER:O	2.21	0.40
1:B:298:LYS:HG2	1:B:302:LEU:HD22	2.04	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	269/288 (93%)	248 (92%)	19 (7%)	2 (1%)	18	28
1	B	269/288 (93%)	244 (91%)	19 (7%)	6 (2%)	5	6
All	All	538/576 (93%)	492 (91%)	38 (7%)	8 (2%)	8	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ALA
1	B	133	ALA
1	B	274	SER
1	B	349	ARG
1	A	189	ARG
1	B	348	SER
1	B	347	HIS
1	B	363	ILE

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	244/259 (94%)	219 (90%)	25 (10%)	7	11
1	B	244/259 (94%)	214 (88%)	30 (12%)	4	6
All	All	488/518 (94%)	433 (89%)	55 (11%)	5	8

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	CYS
1	A	140	LEU
1	A	141	LEU
1	A	150	ASN
1	A	151	ILE
1	A	167	LEU
1	A	174	MET
1	A	175	ASP

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Mol	Chain	Res	Type
1	A	189	ARG
1	A	195	LEU
1	A	225	MET
1	A	253	VAL
1	A	259	ASN
1	A	263	THR
1	A	287	VAL
1	A	288	GLN
1	A	299	GLN
1	A	302	LEU
1	A	336	ASN
1	A	343	ARG
1	A	347	HIS
1	A	349	ARG
1	A	352	LYS
1	A	358	GLN
1	A	367	LYS
1	B	134	CYS
1	B	140	LEU
1	B	141	LEU
1	B	150	ASN
1	B	167	LEU
1	B	174	MET
1	B	175	ASP
1	B	176	CYS
1	B	184	ILE
1	B	189	ARG
1	B	195	LEU
1	B	253	VAL
1	B	259	ASN
1	B	263	THR
1	B	265	ARG
1	B	271	ARG
1	B	279	LYS
1	B	288	GLN
1	B	299	GLN
1	B	302	LEU
1	B	336	ASN
1	B	339	ILE
1	B	343	ARG
1	B	347	HIS
1	B	349	ARG

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Mol	Chain	Res	Type
1	B	352	LYS
1	B	354	GLU
1	B	356	ASN
1	B	367	LYS
1	B	400	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	160	GLN
1	A	162	ASN
1	A	180	HIS
1	A	190	ASN
1	A	192	GLN
1	A	207	GLN
1	A	210	GLN
1	A	219	ASN
1	A	259	ASN
1	A	288	GLN
1	A	305	ASN
1	A	310	ASN
1	A	336	ASN
1	A	353	ASN
1	A	356	ASN
1	B	150	ASN
1	B	160	GLN
1	B	190	ASN
1	B	192	GLN
1	B	210	GLN
1	B	219	ASN
1	B	259	ASN
1	B	261	HIS
1	B	288	GLN
1	B	305	ASN
1	B	310	ASN
1	B	336	ASN
1	B	356	ASN
1	B	365	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GDU	A	100	-	25,26,38	2.42	3 (12%)	38,40,58	3.13	18 (47%)
2	GDU	B	403	-	25,26,38	2.43	2 (8%)	38,40,58	3.02	14 (36%)

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	GDU	A	100	-	-	2/16/32/59	0/2/2/3
2	GDU	B	403	-	-	2/16/32/59	0/2/2/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	100	GDU	PA-O3A	10.44	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	GDU	PA-O3A	10.41	1.70	1.59
2	B	403	GDU	PB-O1B	4.04	1.63	1.50
2	A	100	GDU	PB-O1B	3.96	1.62	1.50
2	A	100	GDU	C3D-C2D	-2.18	1.47	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	100	GDU	O3B-PB-O2B	-9.28	72.99	107.80
2	B	403	GDU	O3B-PB-O2B	-8.85	74.63	107.80
2	B	403	GDU	O2A-PA-O3A	-8.51	84.27	107.27
2	A	100	GDU	O2A-PA-O3A	-7.35	87.40	107.27
2	A	100	GDU	O3A-PA-O1A	-7.06	89.47	110.70
2	B	403	GDU	O3B-PB-O3A	-6.20	83.85	104.64
2	B	403	GDU	O3A-PA-O1A	-6.05	92.49	110.70
2	B	403	GDU	O2B-PB-O3A	5.54	123.22	104.64
2	A	100	GDU	O3B-PB-O3A	-5.13	87.44	104.64
2	A	100	GDU	O2B-PB-O3A	5.00	121.40	104.64
2	A	100	GDU	O2-C2-N1	-3.98	117.62	122.80
2	A	100	GDU	O4D-C4D-C3D	-3.68	97.85	105.15
2	B	403	GDU	O5D-C5D-C4D	3.58	121.20	108.99
2	B	403	GDU	O2A-PA-O5D	3.55	123.67	107.57
2	A	100	GDU	O2B-PB-O1B	3.47	124.35	110.83
2	A	100	GDU	C2D-C1D-N1	3.25	122.29	113.25
2	A	100	GDU	O3B-PB-O1B	-3.20	98.37	110.83
2	A	100	GDU	O2A-PA-O5D	3.17	121.92	107.57
2	B	403	GDU	C2D-C1D-N1	2.99	121.57	113.25
2	A	100	GDU	O2-C2-N3	2.95	126.92	121.49
2	B	403	GDU	O2B-PB-O1B	2.85	121.95	110.83
2	A	100	GDU	O5D-C5D-C4D	2.69	118.16	108.99
2	B	403	GDU	O3B-PB-O1B	-2.69	100.36	110.83
2	B	403	GDU	O2-C2-N3	2.68	126.42	121.49
2	A	100	GDU	C1D-N1-C2	-2.56	112.99	117.59
2	A	100	GDU	C2D-C3D-C4D	-2.56	97.67	102.61
2	B	403	GDU	O2-C2-N1	-2.46	119.60	122.80
2	A	100	GDU	O5D-PA-O1A	2.41	118.48	108.94
2	A	100	GDU	O2D-C2D-C1D	2.39	118.33	110.10
2	B	403	GDU	C2D-C3D-C4D	2.29	107.04	102.61
2	B	403	GDU	O5D-PA-O1A	2.25	117.84	108.94
2	A	100	GDU	C1D-N1-C6	2.17	125.41	120.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

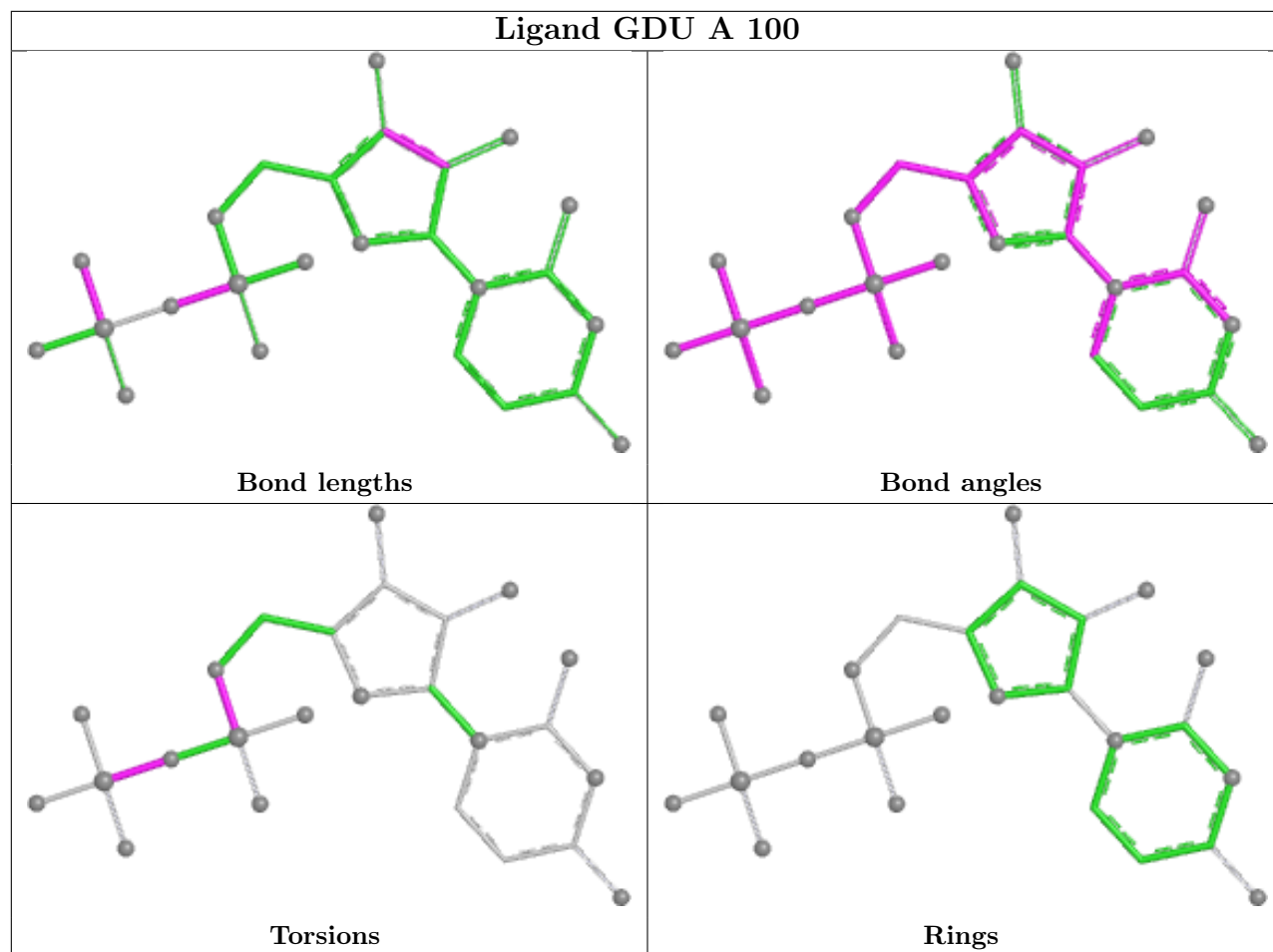
Mol	Chain	Res	Type	Atoms
2	A	100	GDU	C5D-O5D-PA-O2A
2	A	100	GDU	PA-O3A-PB-O2B
2	B	403	GDU	C5D-O5D-PA-O2A
2	B	403	GDU	PA-O3A-PB-O2B

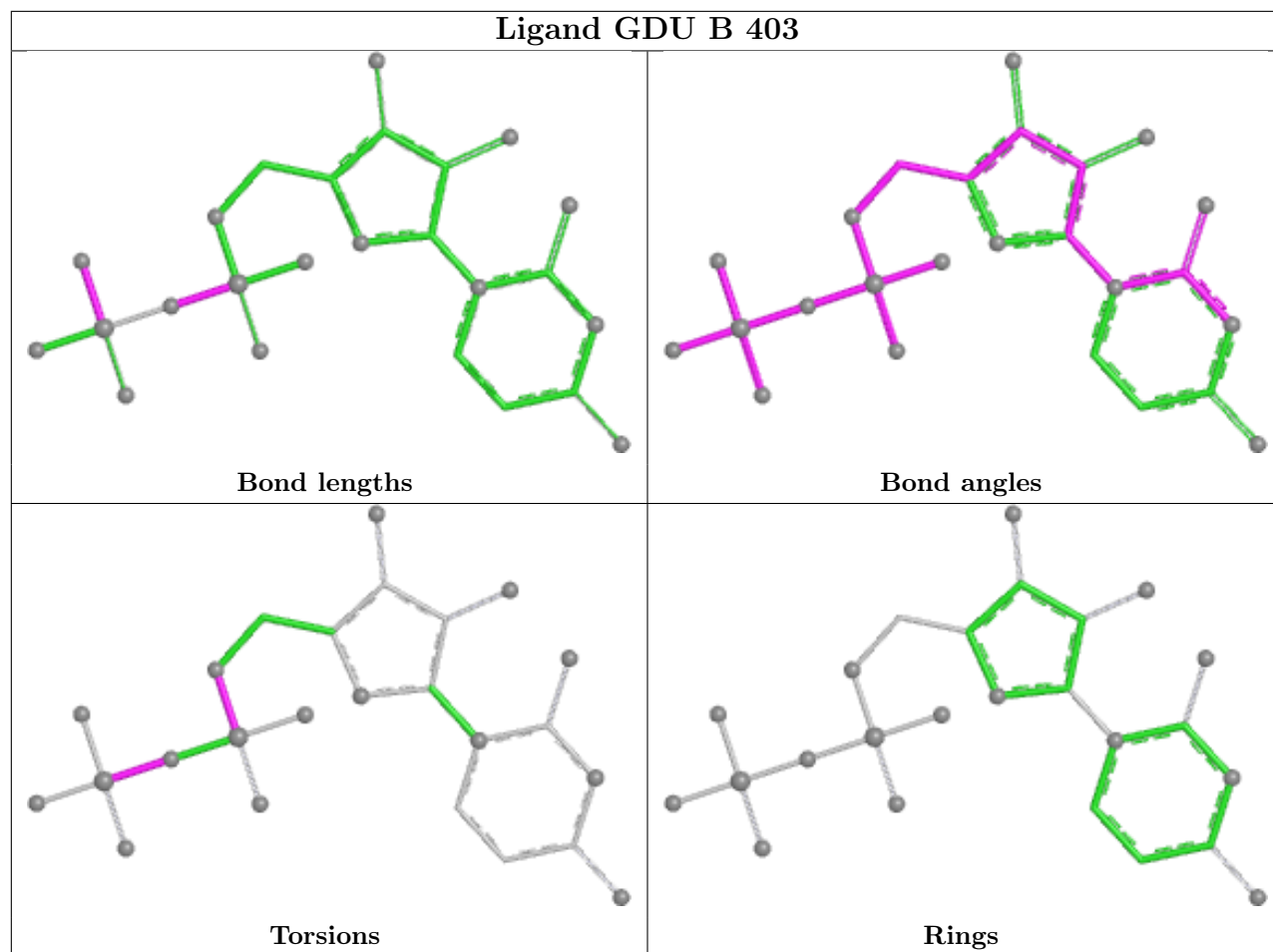
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	100	GDU	2	0
2	B	403	GDU	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	271/288 (94%)	0.14	10 (3%) 45 41	29, 53, 94, 99	0
1	B	271/288 (94%)	0.10	10 (3%) 45 41	25, 49, 83, 99	0
All	All	542/576 (94%)	0.12	20 (3%) 45 41	25, 51, 90, 99	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ILE	3.7
1	B	174	MET	3.0
1	A	261	HIS	2.9
1	B	160	GLN	2.9
1	B	402	SER	2.9
1	A	347	HIS	2.6
1	A	133	ALA	2.5
1	A	358	GLN	2.5
1	B	176	CYS	2.4
1	A	362	ARG	2.4
1	A	338	VAL	2.3
1	B	133	ALA	2.2
1	A	349	ARG	2.2
1	A	153	VAL	2.2
1	A	348	SER	2.1
1	B	283	SER	2.1
1	B	401	PRO	2.1
1	B	132	THR	2.1
1	A	132	THR	2.0
1	B	347	HIS	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](#)

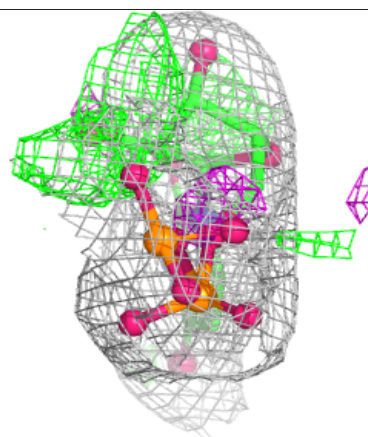
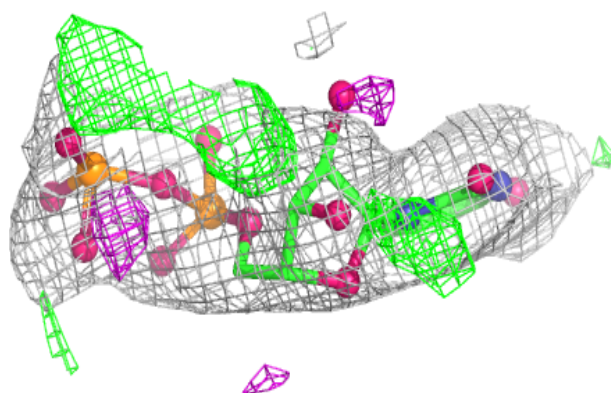
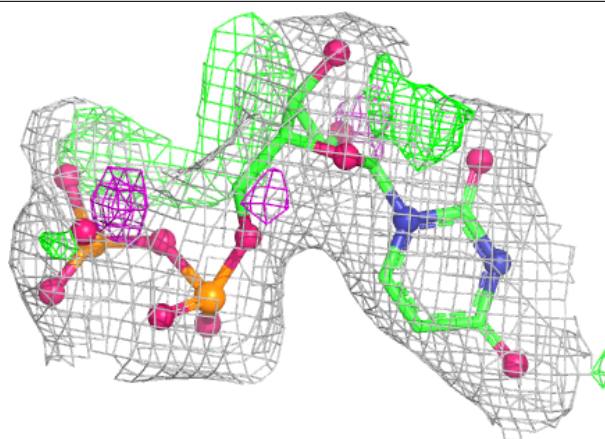
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDU	A	100	25/36	0.87	0.12	40,58,99,99	0
2	GDU	B	403	25/36	0.89	0.10	40,67,99,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

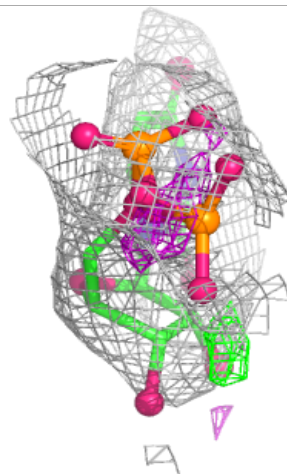
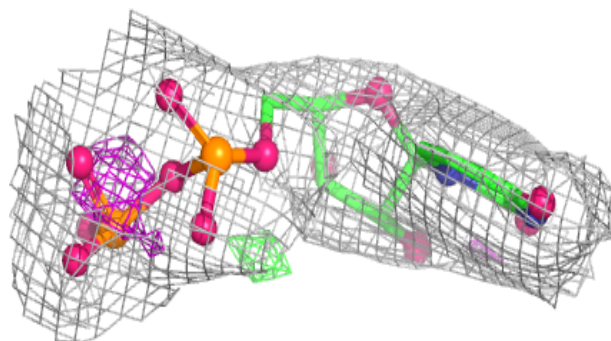
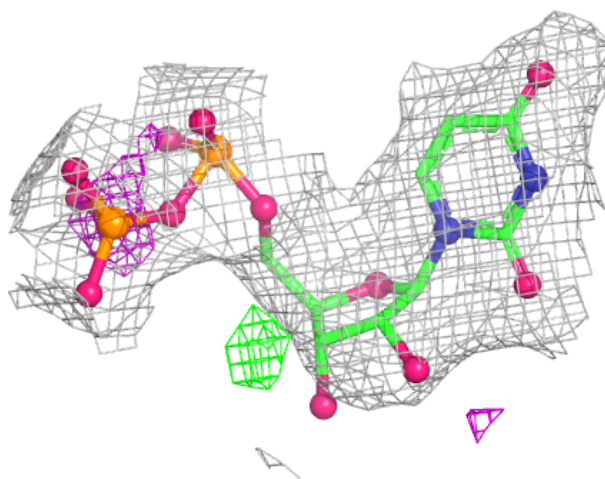
Electron density around GDU A 100:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDU B 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.