



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:55 PM UTC

PDB ID : 9HUA / pdb_00009hua
Title : Glycosyltransferase C from the *Limosilactobacillus reuteri* accessory secretion system. Complex with UDP.
Authors : Asworth, G.J.; Griffiths, R.; Juge, N.; Dong, C.J.; Hemmings, A.M.
Deposited on : 2024-12-21
Resolution : 2.60 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

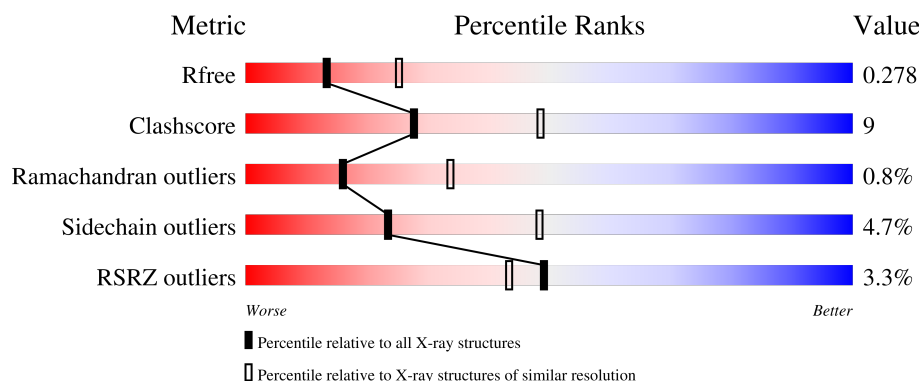
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

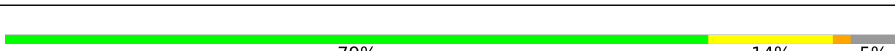
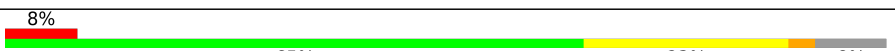
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	354	
1	B	354	
1	C	354	
1	D	354	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20683 atoms, of which 9973 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 Glucosyltransferase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	3	0
			5292	1758	2568	454	505	7			
1	B	320	Total	C	H	N	O	S	0	0	0
			4912	1639	2366	422	479	6			
1	C	335	Total	C	H	N	O	S	0	0	0
			5256	1744	2552	449	504	7			
1	D	326	Total	C	H	N	O	S	0	0	0
			5073	1685	2460	435	486	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B3XPQ7
A	-18	GLY	-	expression tag	UNP B3XPQ7
A	-17	SER	-	expression tag	UNP B3XPQ7
A	-16	SER	-	expression tag	UNP B3XPQ7
A	-15	HIS	-	expression tag	UNP B3XPQ7
A	-14	HIS	-	expression tag	UNP B3XPQ7
A	-13	HIS	-	expression tag	UNP B3XPQ7
A	-12	HIS	-	expression tag	UNP B3XPQ7
A	-11	HIS	-	expression tag	UNP B3XPQ7
A	-10	HIS	-	expression tag	UNP B3XPQ7
A	-9	SER	-	expression tag	UNP B3XPQ7
A	-8	SER	-	expression tag	UNP B3XPQ7
A	-7	GLY	-	expression tag	UNP B3XPQ7
A	-6	LEU	-	expression tag	UNP B3XPQ7
A	-5	VAL	-	expression tag	UNP B3XPQ7
A	-4	PRO	-	expression tag	UNP B3XPQ7
A	-3	ARG	-	expression tag	UNP B3XPQ7
A	-2	GLY	-	expression tag	UNP B3XPQ7
A	-1	SER	-	expression tag	UNP B3XPQ7
A	0	HIS	-	expression tag	UNP B3XPQ7
A	1	LEU	-	expression tag	UNP B3XPQ7

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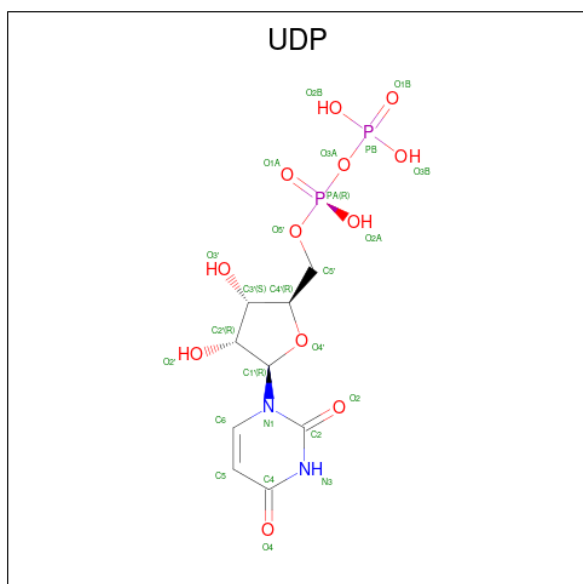
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP B3XPQ7
B	-18	GLY	-	expression tag	UNP B3XPQ7
B	-17	SER	-	expression tag	UNP B3XPQ7
B	-16	SER	-	expression tag	UNP B3XPQ7
B	-15	HIS	-	expression tag	UNP B3XPQ7
B	-14	HIS	-	expression tag	UNP B3XPQ7
B	-13	HIS	-	expression tag	UNP B3XPQ7
B	-12	HIS	-	expression tag	UNP B3XPQ7
B	-11	HIS	-	expression tag	UNP B3XPQ7
B	-10	HIS	-	expression tag	UNP B3XPQ7
B	-9	SER	-	expression tag	UNP B3XPQ7
B	-8	SER	-	expression tag	UNP B3XPQ7
B	-7	GLY	-	expression tag	UNP B3XPQ7
B	-6	LEU	-	expression tag	UNP B3XPQ7
B	-5	VAL	-	expression tag	UNP B3XPQ7
B	-4	PRO	-	expression tag	UNP B3XPQ7
B	-3	ARG	-	expression tag	UNP B3XPQ7
B	-2	GLY	-	expression tag	UNP B3XPQ7
B	-1	SER	-	expression tag	UNP B3XPQ7
B	0	HIS	-	expression tag	UNP B3XPQ7
B	1	LEU	-	expression tag	UNP B3XPQ7
C	-19	MET	-	initiating methionine	UNP B3XPQ7
C	-18	GLY	-	expression tag	UNP B3XPQ7
C	-17	SER	-	expression tag	UNP B3XPQ7
C	-16	SER	-	expression tag	UNP B3XPQ7
C	-15	HIS	-	expression tag	UNP B3XPQ7
C	-14	HIS	-	expression tag	UNP B3XPQ7
C	-13	HIS	-	expression tag	UNP B3XPQ7
C	-12	HIS	-	expression tag	UNP B3XPQ7
C	-11	HIS	-	expression tag	UNP B3XPQ7
C	-10	HIS	-	expression tag	UNP B3XPQ7
C	-9	SER	-	expression tag	UNP B3XPQ7
C	-8	SER	-	expression tag	UNP B3XPQ7
C	-7	GLY	-	expression tag	UNP B3XPQ7
C	-6	LEU	-	expression tag	UNP B3XPQ7
C	-5	VAL	-	expression tag	UNP B3XPQ7
C	-4	PRO	-	expression tag	UNP B3XPQ7
C	-3	ARG	-	expression tag	UNP B3XPQ7
C	-2	GLY	-	expression tag	UNP B3XPQ7
C	-1	SER	-	expression tag	UNP B3XPQ7
C	0	HIS	-	expression tag	UNP B3XPQ7
C	1	LEU	-	expression tag	UNP B3XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP B3XPQ7
D	-18	GLY	-	expression tag	UNP B3XPQ7
D	-17	SER	-	expression tag	UNP B3XPQ7
D	-16	SER	-	expression tag	UNP B3XPQ7
D	-15	HIS	-	expression tag	UNP B3XPQ7
D	-14	HIS	-	expression tag	UNP B3XPQ7
D	-13	HIS	-	expression tag	UNP B3XPQ7
D	-12	HIS	-	expression tag	UNP B3XPQ7
D	-11	HIS	-	expression tag	UNP B3XPQ7
D	-10	HIS	-	expression tag	UNP B3XPQ7
D	-9	SER	-	expression tag	UNP B3XPQ7
D	-8	SER	-	expression tag	UNP B3XPQ7
D	-7	GLY	-	expression tag	UNP B3XPQ7
D	-6	LEU	-	expression tag	UNP B3XPQ7
D	-5	VAL	-	expression tag	UNP B3XPQ7
D	-4	PRO	-	expression tag	UNP B3XPQ7
D	-3	ARG	-	expression tag	UNP B3XPQ7
D	-2	GLY	-	expression tag	UNP B3XPQ7
D	-1	SER	-	expression tag	UNP B3XPQ7
D	0	HIS	-	expression tag	UNP B3XPQ7
D	1	LEU	-	expression tag	UNP B3XPQ7

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 34	C 9	H 9	N 2	O 12	P 2	0	0
2	B	1	Total 34	C 9	H 9	N 2	O 12	P 2	0	0
2	C	1	Total 34	C 9	H 9	N 2	O 12	P 2	0	0

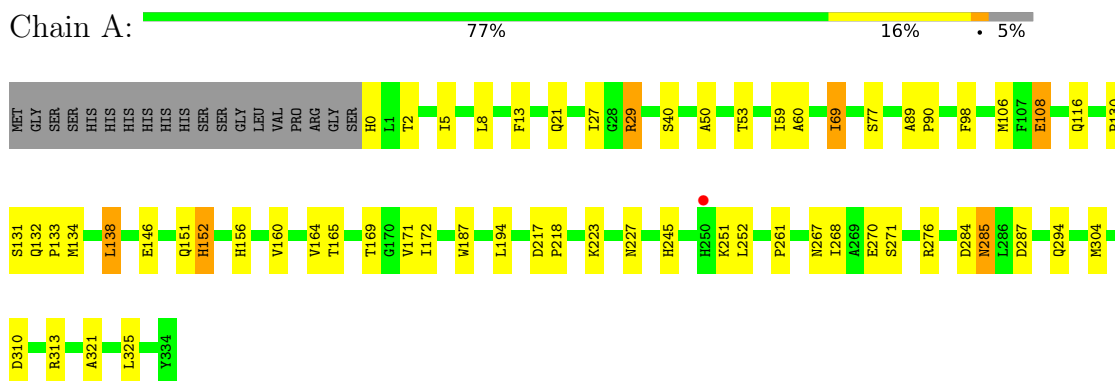
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	9	Total 9	O 9	0	0
3	C	26	Total 26	O 26	0	0
3	D	3	Total 3	O 3	0	0

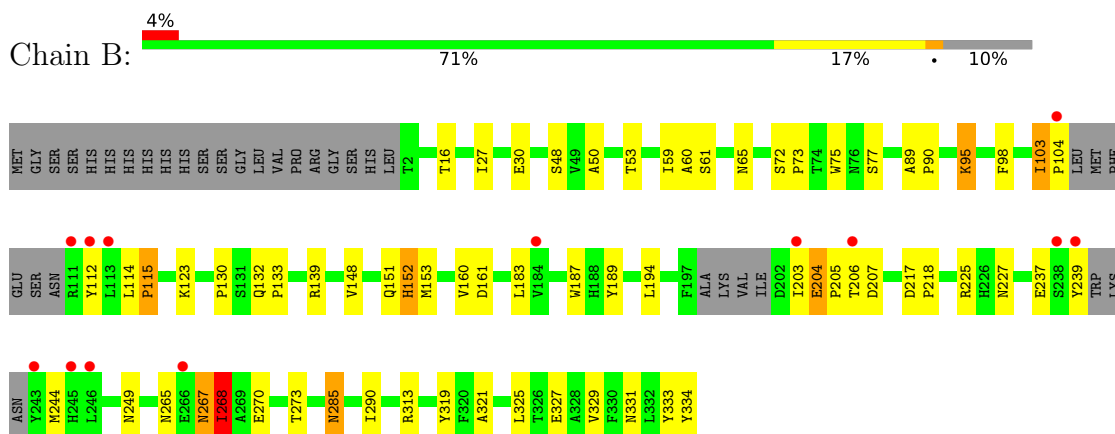
3 Residue-property plots [i](#)

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.

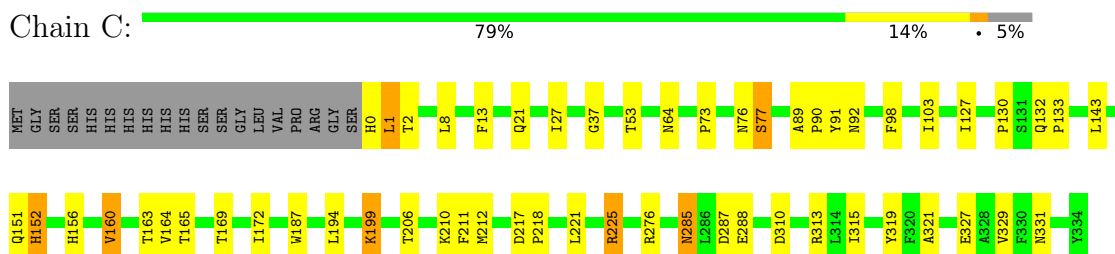
• Molecule 1: Glucosyltransferase 3



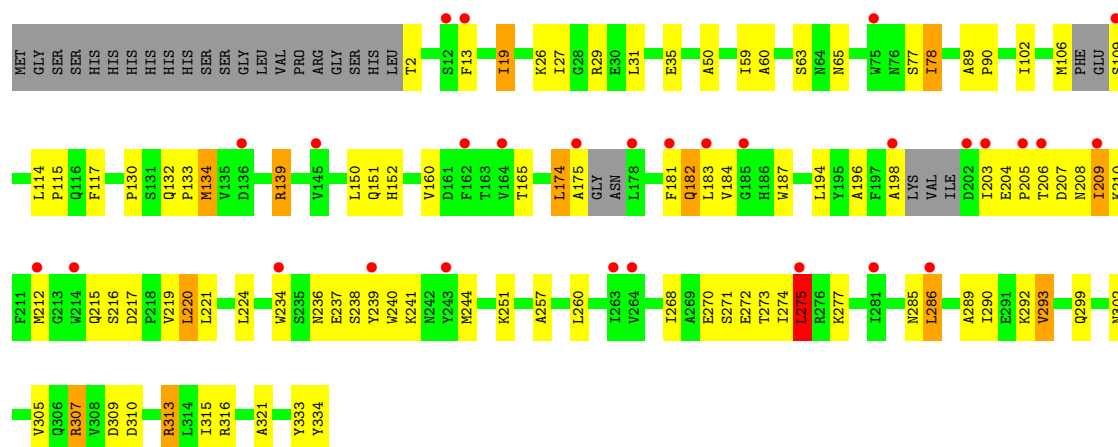
• Molecule 1: Glucosyltransferase 3



• Molecule 1: Glucosyltransferase 3



• Molecule 1: Glucosyltransferase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.41Å 70.69Å 140.31Å 90.00° 91.37° 90.00°	Depositor
Resolution (Å)	70.23 – 2.60 70.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.23-2.60) 87.0 (70.23-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.226 , 0.276 0.225 , 0.278	Depositor DCC
R_{free} test set	2153 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.960	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20683	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: UDP

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	0.66	0/2811	1.19	10/3830 (0.3%)
1	B	0.69	0/2611	1.18	8/3558 (0.2%)
1	C	0.72	0/2777	1.27	15/3785 (0.4%)
1	D	0.65	0/2680	1.19	8/3649 (0.2%)
All	All	0.68	0/10879	1.21	41/14822 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	LYS	CB-CA-C	11.04	130.01	110.36
1	C	225	ARG	CA-CB-CG	7.93	129.97	114.10
1	C	91	TYR	CA-C-O	-7.16	112.84	121.28
1	C	169	THR	N-CA-C	-6.80	102.04	110.41
1	D	181	PHE	N-CA-CB	6.75	121.37	110.77
1	C	91	TYR	N-CA-C	-6.59	99.56	110.17
1	D	309	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	265	ASN	CA-CB-CG	6.46	119.06	112.60
1	B	237	GLU	CB-CA-C	6.38	122.45	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	MET	CG-SD-CE	-6.34	86.95	100.90
1	D	2	THR	OG1-CB-CG2	-6.18	96.93	109.30
1	A	13	PHE	CA-CB-CG	6.16	119.96	113.80
1	B	265	ASN	CB-CA-C	-6.06	98.39	109.54
1	C	1	LEU	N-CA-CB	5.92	119.30	109.60
1	D	275	LEU	N-CA-CB	5.77	118.33	109.91
1	B	237	GLU	N-CA-CB	-5.68	101.82	110.45
1	A	106	MET	CG-SD-CE	5.67	113.37	100.90
1	D	206	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	108	GLU	CB-CG-CD	-5.61	103.06	112.60
1	D	198	ALA	CA-C-O	-5.58	111.31	120.80
1	D	292	LYS	CB-CA-C	5.56	121.61	109.99
1	B	30	GLU	CB-CA-C	5.54	121.58	109.99
1	B	103	ILE	N-CA-CB	5.52	114.22	110.52
1	A	284	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	227	ASN	CB-CA-C	-5.43	101.45	110.68
1	C	160	VAL	N-CA-CB	-5.41	102.88	110.13
1	A	287	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	163	THR	N-CA-CB	5.27	119.91	110.32
1	A	2	THR	OG1-CB-CG2	-5.20	98.91	109.30
1	C	199	LYS	CB-CG-CD	5.19	123.24	111.30
1	A	223	LYS	CB-CG-CD	5.18	123.22	111.30
1	C	2	THR	OG1-CB-CG2	-5.13	99.04	109.30
1	C	64	ASN	CA-CB-CG	-5.12	107.48	112.60
1	D	139	ARG	CB-CG-CD	5.07	122.97	111.30
1	A	146	GLU	CB-CG-CD	5.06	121.20	112.60
1	B	98	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	251[A]	LYS	CB-CG-CD	5.03	122.87	111.30
1	A	251[B]	LYS	CB-CG-CD	5.03	122.87	111.30
1	C	98	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	37	GLY	O-C-N	5.02	126.18	122.62
1	C	287	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29[A]	ARG	Sidechain
1	A	29[B]	ARG	Sidechain
1	C	211	PHE	Peptide
1	D	210	LYS	Peptide
1	D	307	ARG	Sidechain

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	2724	2568	2617	34	1
1	B	2546	2366	2418	54	0
1	C	2704	2552	2614	37	0
1	D	2613	2460	2513	78	0
2	A	25	9	11	1	0
2	B	25	9	11	0	0
2	C	25	9	11	0	0
3	A	10	0	0	2	0
3	B	9	0	0	0	0
3	C	26	0	0	4	0
3	D	3	0	0	0	0
All	All	10710	9973	10195	187	1

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 9.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:NH2	1:D:65:ASN:O	1.89	1.06
1:B:65:ASN:O	1:C:313:ARG:NH1	2.00	0.93
1:B:103:ILE:HG13	1:B:104:PRO:HD3	1.55	0.89
1:B:189:TYR:CZ	1:B:290:ILE:HD12	2.16	0.81
1:A:227:ASN:HB3	3:A:508:HOH:O	1.81	0.79
1:D:184:VAL:HG22	1:D:205:PRO:HA	1.62	0.78
1:C:327:GLU:O	1:C:331:ASN:ND2	2.16	0.78
1:D:175:ALA:O	1:D:251:LYS:NZ	2.17	0.77
1:D:183:LEU:HD21	1:D:187:TRP:CE3	2.20	0.76
1:C:143:LEU:O	3:C:501:HOH:O	2.02	0.76
1:A:169:THR:HG22	1:A:171:VAL:HG23	1.67	0.75
1:B:244:MET:HE2	1:B:249:ASN:HD22	1.53	0.74
1:D:215:GLN:HB3	1:D:219:VAL:HG23	1.70	0.73
1:A:156:HIS:NE2	1:A:217:ASP:OD1	2.21	0.73
1:B:161:ASP:OD2	1:D:216:SER:OG	2.04	0.72
1:C:156:HIS:HE2	1:C:217:ASP:CG	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:HIS:NE2	1:C:217:ASP:OD1	2.24	0.71
1:D:220:LEU:HD22	1:D:221:LEU:HD12	1.73	0.70
1:A:134:MET:O	1:A:138:LEU:HD22	1.92	0.70
1:D:290:ILE:HA	1:D:293:VAL:HG13	1.75	0.69
1:A:156:HIS:HE2	1:A:217:ASP:CG	2.00	0.69
1:D:78:ILE:HD13	1:D:117:PHE:CD1	2.26	0.69
1:D:184:VAL:CG2	1:D:205:PRO:HA	2.24	0.68
1:B:103:ILE:CG1	1:B:104:PRO:HD3	2.22	0.66
1:D:286:LEU:O	1:D:290:ILE:HD12	1.96	0.66
1:D:270:GLU:O	1:D:274:ILE:HD12	1.96	0.66
1:A:218:PRO:HB2	1:C:218:PRO:HB2	1.79	0.65
1:B:189:TYR:CE2	1:B:290:ILE:CD1	2.81	0.64
1:A:169:THR:CG2	1:A:171:VAL:HG23	2.28	0.64
1:D:257:ALA:HA	1:D:315:ILE:HD11	1.79	0.63
1:B:189:TYR:CE2	1:B:290:ILE:HD12	2.34	0.63
1:B:75:TRP:CH2	1:B:103:ILE:HG22	2.34	0.63
1:D:102:ILE:O	1:D:106:MET:HE3	1.98	0.62
1:D:272:GLU:O	1:D:275:LEU:HG	2.00	0.62
1:D:220:LEU:HD23	1:D:224:LEU:HD12	1.82	0.61
1:D:184:VAL:O	1:D:207:ASP:CG	2.44	0.61
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.65	0.60
1:D:109:SER:N	1:D:239:TYR:HH	1.99	0.60
1:D:203:ILE:HG22	1:D:204:GLU:H	1.66	0.59
1:C:73:PRO:HG3	1:C:103:ILE:CD1	2.33	0.59
1:A:134:MET:O	1:A:138:LEU:CD2	2.51	0.58
1:C:73:PRO:HG3	1:C:103:ILE:HD13	1.85	0.58
1:B:334:TYR:OXT	1:C:276:ARG:NH1	2.37	0.57
1:B:189:TYR:CD2	1:B:290:ILE:CD1	2.88	0.57
1:D:286:LEU:O	1:D:290:ILE:CD1	2.53	0.57
1:D:302:ASN:O	1:D:305:VAL:HG22	2.05	0.57
1:D:78:ILE:HD13	1:D:117:PHE:CG	2.39	0.56
1:D:272:GLU:HA	1:D:275:LEU:CD2	2.36	0.55
1:A:50:ALA:HB1	1:B:53:THR:HG21	1.87	0.55
1:C:132:GLN:OE1	3:C:502:HOH:O	2.18	0.55
1:B:189:TYR:CG	1:B:290:ILE:HD13	2.42	0.54
1:D:174:LEU:HD13	1:D:175:ALA:C	2.33	0.54
1:D:102:ILE:C	1:D:106:MET:CE	2.80	0.54
1:D:272:GLU:HA	1:D:275:LEU:HD21	1.88	0.54
1:C:187:TRP:CE2	1:C:194:LEU:HB2	2.43	0.54
1:D:78:ILE:CD1	1:D:117:PHE:HA	2.38	0.54
1:A:187:TRP:CE2	1:A:194:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:NH1	1:D:334:TYR:OXT	2.42	0.53
1:D:302:ASN:HA	1:D:305:VAL:HG22	1.89	0.53
1:B:313:ARG:NH1	1:C:1:LEU:HD13	2.23	0.53
1:B:189:TYR:CD2	1:B:290:ILE:HD13	2.44	0.53
1:D:270:GLU:OE1	1:D:273:THR:HG21	2.09	0.52
1:B:187:TRP:CE2	1:B:194:LEU:HB2	2.45	0.52
1:D:187:TRP:HB3	1:D:209:ILE:CG2	2.40	0.52
1:D:187:TRP:CE2	1:D:194:LEU:HB2	2.44	0.52
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.22	0.52
1:D:203:ILE:O	1:D:205:PRO:HD3	2.10	0.52
1:D:289:ALA:O	1:D:293:VAL:HG13	2.10	0.52
1:D:187:TRP:HB3	1:D:209:ILE:HG22	1.92	0.51
1:D:244:MET:HE3	1:D:268:ILE:CG1	2.40	0.51
1:C:53:THR:HG21	1:D:50:ALA:HB1	1.94	0.50
1:D:26:LYS:NZ	1:D:35:GLU:OE1	2.44	0.50
1:D:102:ILE:C	1:D:106:MET:HE3	2.37	0.49
1:D:182:GLN:HA	1:D:182:GLN:OE1	2.12	0.49
1:B:103:ILE:HD12	1:B:104:PRO:N	2.28	0.49
1:D:78:ILE:HD11	1:D:117:PHE:HA	1.93	0.49
1:D:236:ASN:O	1:D:237:GLU:C	2.55	0.49
1:D:174:LEU:CD1	1:D:175:ALA:C	2.86	0.48
1:C:221:LEU:O	1:C:225:ARG:HG2	2.13	0.48
1:B:244:MET:HE3	1:B:268:ILE:CD1	2.44	0.48
1:C:310:ASP:OD1	1:C:313:ARG:NH2	2.46	0.48
1:B:327:GLU:O	1:B:331:ASN:OD1	2.31	0.48
1:D:132:GLN:N	1:D:133:PRO:HD2	2.28	0.48
1:D:27:ILE:HD13	1:D:321:ALA:HB3	1.96	0.48
1:B:313:ARG:NE	1:C:1:LEU:HB2	2.28	0.48
1:B:285:ASN:ND2	1:B:285:ASN:H	2.12	0.47
1:A:0:HIS:N	3:A:503:HOH:O	2.47	0.47
1:D:102:ILE:HG13	1:D:134:MET:HE1	1.96	0.47
1:D:286:LEU:H	1:D:286:LEU:CD2	2.27	0.47
1:A:151:GLN:O	1:A:152:HIS:HB2	2.15	0.47
1:B:132:GLN:N	1:B:133:PRO:HD2	2.29	0.47
1:B:189:TYR:CE1	1:B:290:ILE:HD12	2.49	0.47
1:C:187:TRP:NE1	1:C:194:LEU:HB2	2.29	0.47
1:D:207:ASP:HB3	1:D:208:ASN:H	1.51	0.47
1:A:89:ALA:N	1:A:90:PRO:HD2	2.30	0.47
1:A:268:ILE:O	1:A:271:SER:OG	2.28	0.46
1:D:220:LEU:CD2	1:D:221:LEU:HD12	2.44	0.46
1:C:285:ASN:ND2	1:C:285:ASN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HG13	1:B:270:GLU:OE1	2.15	0.46
1:B:267:ASN:O	1:B:268:ILE:O	2.33	0.46
1:B:187:TRP:NE1	1:B:194:LEU:HB2	2.30	0.46
1:C:127:ILE:HD12	1:C:143:LEU:HD11	1.98	0.46
1:D:183:LEU:HD23	1:D:183:LEU:O	2.15	0.46
1:D:236:ASN:HB3	1:D:240:TRP:HB3	1.98	0.46
1:D:130:PRO:HA	1:D:151:GLN:HB3	1.97	0.46
1:D:286:LEU:H	1:D:286:LEU:HD23	1.81	0.45
1:B:244:MET:HE3	1:B:268:ILE:HD11	1.98	0.45
1:D:184:VAL:HG21	1:D:204:GLU:O	2.16	0.45
1:B:103:ILE:HD12	1:B:104:PRO:CD	2.47	0.45
1:D:187:TRP:NE1	1:D:194:LEU:HB2	2.31	0.45
1:B:206:THR:HG22	1:B:206:THR:O	2.16	0.45
1:B:151:GLN:O	1:B:152:HIS:HB2	2.17	0.45
1:D:151:GLN:O	1:D:152:HIS:HB2	2.17	0.45
1:B:95:LYS:HE2	1:B:123:LYS:O	2.17	0.45
1:B:285:ASN:ND2	1:B:285:ASN:N	2.65	0.45
1:B:333:TYR:CZ	1:C:313:ARG:HD2	2.52	0.45
1:D:132:GLN:HE21	1:D:150:LEU:HD21	1.82	0.45
1:A:5:ILE:HD12	1:A:69:ILE:HD13	1.99	0.44
1:B:203:ILE:HG22	1:B:204:GLU:N	2.32	0.44
1:C:27:ILE:HD13	1:C:321:ALA:HB3	2.00	0.44
1:D:315:ILE:HD12	1:D:316:ARG:N	2.32	0.44
1:C:172:ILE:O	1:C:194:LEU:HA	2.17	0.44
1:A:8:LEU:HB2	1:A:21:GLN:OE1	2.17	0.44
1:B:244:MET:O	1:B:268:ILE:HD12	2.16	0.44
1:C:8:LEU:HB2	1:C:21:GLN:OE1	2.18	0.44
1:D:89:ALA:N	1:D:90:PRO:HD2	2.33	0.44
1:A:285:ASN:ND2	1:A:285:ASN:H	2.16	0.44
1:A:245:HIS:CE1	1:A:267:ASN:HB3	2.52	0.44
1:A:134:MET:HG3	1:A:138:LEU:CD2	2.48	0.44
1:B:103:ILE:CD1	1:B:104:PRO:HD3	2.48	0.44
1:D:132:GLN:NE2	1:D:132:GLN:HA	2.33	0.44
1:B:27:ILE:HD13	1:B:321:ALA:HB3	2.00	0.43
1:B:313:ARG:CD	1:C:1:LEU:HB2	2.47	0.43
1:C:89:ALA:N	1:C:90:PRO:HD2	2.33	0.43
1:D:102:ILE:N	1:D:106:MET:HE1	2.33	0.43
1:B:313:ARG:HD3	1:C:1:LEU:HB2	2.01	0.43
1:A:270:GLU:O	1:A:271:SER:C	2.61	0.43
1:D:270:GLU:C	1:D:274:ILE:HD12	2.43	0.43
1:B:89:ALA:N	1:B:90:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:N	1:B:218:PRO:HD2	2.34	0.43
1:D:217:ASP:O	1:D:221:LEU:HD13	2.18	0.43
1:A:69:ILE:HD11	1:A:98:PHE:HD2	1.83	0.43
1:C:164:VAL:HG22	1:C:165:THR:N	2.34	0.43
1:D:102:ILE:C	1:D:106:MET:HE1	2.44	0.43
1:D:238:SER:HA	1:D:241:LYS:HD2	2.01	0.43
1:A:130:PRO:HA	1:A:151:GLN:HB3	2.01	0.42
1:A:285:ASN:ND2	1:A:285:ASN:N	2.67	0.42
1:B:130:PRO:HA	1:B:151:GLN:HB3	2.01	0.42
1:B:329:VAL:HG11	1:C:319:TYR:CE1	2.54	0.42
1:A:187:TRP:NE1	1:A:194:LEU:HB2	2.35	0.42
1:C:199:LYS:HA	3:C:507:HOH:O	2.20	0.42
1:B:225:ARG:HH11	1:B:225:ARG:HG3	1.83	0.42
1:B:319:TYR:CE2	1:C:329:VAL:HG11	2.54	0.42
1:C:76:ASN:O	1:C:77:SER:CB	2.67	0.42
1:D:59:ILE:O	1:D:60:ALA:C	2.62	0.42
1:D:19:ILE:HD12	1:D:19:ILE:HA	1.75	0.42
1:A:27:ILE:HD13	1:A:321:ALA:HB3	2.02	0.42
1:B:148:VAL:HG23	1:B:148:VAL:O	2.19	0.42
1:D:182:GLN:NE2	1:D:184:VAL:HG12	2.35	0.42
1:D:310:ASP:O	1:D:313:ARG:HD3	2.20	0.42
1:D:196:ALA:O	1:D:212:MET:O	2.37	0.42
1:C:151:GLN:O	1:C:152:HIS:HB2	2.20	0.41
1:A:53:THR:HG21	1:B:50:ALA:HB1	2.01	0.41
1:D:270:GLU:O	1:D:271:SER:C	2.63	0.41
1:C:132:GLN:N	1:C:133:PRO:HD2	2.35	0.41
1:D:114:LEU:HB3	1:D:115:PRO:HD3	2.01	0.41
1:D:184:VAL:O	1:D:207:ASP:OD2	2.38	0.41
1:A:132:GLN:N	1:A:133:PRO:HD2	2.35	0.41
1:B:203:ILE:HG22	1:B:204:GLU:H	1.86	0.41
1:C:0:HIS:CE1	3:C:504:HOH:O	2.73	0.41
1:C:217:ASP:N	1:C:218:PRO:HD2	2.35	0.41
1:C:285:ASN:ND2	1:C:285:ASN:N	2.68	0.41
1:A:164:VAL:HG22	1:A:165:THR:N	2.36	0.41
1:B:205:PRO:HB2	1:B:207:ASP:HB2	2.03	0.41
1:D:220:LEU:CD2	1:D:224:LEU:HD12	2.50	0.41
1:A:172:ILE:O	1:A:194:LEU:HA	2.21	0.41
1:C:130:PRO:HA	1:C:151:GLN:HB3	2.02	0.41
1:D:174:LEU:HD13	1:D:175:ALA:N	2.36	0.41
1:D:299:GLN:HG3	1:D:299:GLN:O	2.21	0.41
1:A:59:ILE:O	1:A:60:ALA:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HB3	1:B:115:PRO:HD3	2.02	0.40
1:A:313:ARG:HD3	1:D:333:TYR:CE1	2.57	0.40
1:A:261:PRO:HB3	1:A:304:MET:HG2	2.02	0.40
1:D:277:LYS:O	1:D:307:ARG:CD	2.70	0.40
1:B:59:ILE:O	1:B:60:ALA:C	2.64	0.40
1:B:72:SER:HA	1:B:73:PRO:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:OE2	1:A:294:GLN:OE1[2_545]	2.13	0.07

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	336/354 (95%)	326 (97%)	8 (2%)	2 (1%)	21	42
1	B	312/354 (88%)	301 (96%)	8 (3%)	3 (1%)	12	28
1	C	333/354 (94%)	323 (97%)	7 (2%)	3 (1%)	14	30
1	D	318/354 (90%)	305 (96%)	10 (3%)	3 (1%)	14	30
All	All	1299/1416 (92%)	1255 (97%)	33 (2%)	11 (1%)	16	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	B	77	SER
1	C	13	PHE
1	C	77	SER

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Mol	Chain	Res	Type
1	D	77	SER
1	A	152	HIS
1	B	268	ILE
1	D	13	PHE
1	D	182	GLN
1	B	152	HIS
1	C	152	HIS

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	294/309 (95%)	282 (96%)	12 (4%)	27	54
1	B	268/309 (87%)	252 (94%)	16 (6%)	17	37
1	C	291/309 (94%)	284 (98%)	7 (2%)	43	70
1	D	278/309 (90%)	259 (93%)	19 (7%)	14	32
All	All	1131/1236 (92%)	1077 (95%)	54 (5%)	23	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29[A]	ARG
1	A	29[B]	ARG
1	A	40	SER
1	A	69	ILE
1	A	116	GLN
1	A	131	SER
1	A	138	LEU
1	A	160	VAL
1	A	252	LEU
1	A	285	ASN
1	A	310	ASP
1	A	325	LEU
1	B	16	THR
1	B	48	SER

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Mol	Chain	Res	Type
1	B	61	SER
1	B	95	LYS
1	B	112	TYR
1	B	115	PRO
1	B	153	MET
1	B	160	VAL
1	B	183	LEU
1	B	204	GLU
1	B	239	TYR
1	B	267	ASN
1	B	268	ILE
1	B	273	THR
1	B	285	ASN
1	B	325	LEU
1	C	92	ASN
1	C	160	VAL
1	C	206	THR
1	C	210	LYS
1	C	285	ASN
1	C	288	GLU
1	C	315	ILE
1	D	19	ILE
1	D	29	ARG
1	D	31	LEU
1	D	63	SER
1	D	78	ILE
1	D	134	MET
1	D	139	ARG
1	D	160	VAL
1	D	165	THR
1	D	174	LEU
1	D	209	ILE
1	D	220	LEU
1	D	234	TRP
1	D	260	LEU
1	D	275	LEU
1	D	285	ASN
1	D	286	LEU
1	D	293	VAL
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	100	HIS
1	A	173	ASN
1	A	186	HIS
1	A	285	ASN
1	A	294	GLN
1	A	299	GLN
1	A	302	ASN
1	B	14	GLN
1	B	92	ASN
1	B	151	GLN
1	B	186	HIS
1	B	227	ASN
1	B	285	ASN
1	B	294	GLN
1	B	306	GLN
1	B	331	ASN
1	C	100	HIS
1	C	141	ASN
1	C	168	ASN
1	C	186	HIS
1	C	192	ASN
1	C	215	GLN
1	C	227	ASN
1	C	236	ASN
1	C	245	HIS
1	C	294	GLN
1	C	299	GLN
1	C	302	ASN
1	D	65	ASN
1	D	132	GLN
1	D	141	ASN
1	D	188	HIS
1	D	245	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	UDP	A	401	-	25,26,26	0.51	0	38,40,40	0.83	2 (5%)
2	UDP	C	401	-	25,26,26	0.78	1 (4%)	38,40,40	0.98	2 (5%)
2	UDP	B	401	-	25,26,26	0.61	0	38,40,40	0.65	0

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	UDP	A	401	-	-	0/16/32/32	0/2/2/2
2	UDP	C	401	-	-	2/16/32/32	0/2/2/2
2	UDP	B	401	-	-	1/16/32/32	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UDP	PA-O3A	2.50	1.62	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	UDP	O2A-PA-O1A	2.66	124.82	112.44
2	A	401	UDP	O3A-PA-O1A	-2.18	104.14	110.70
2	C	401	UDP	O3'-C3'-C4'	2.18	117.34	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UDP	PA-O5'-C5'	-2.11	109.28	121.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

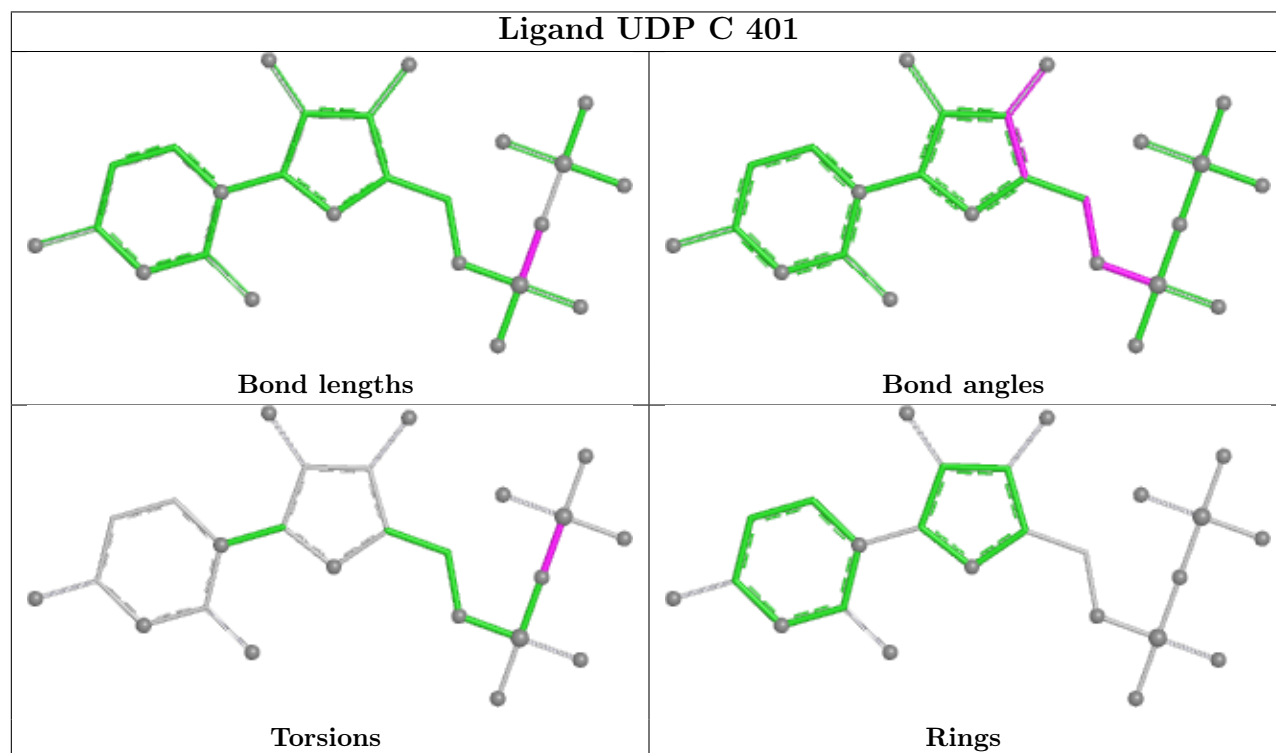
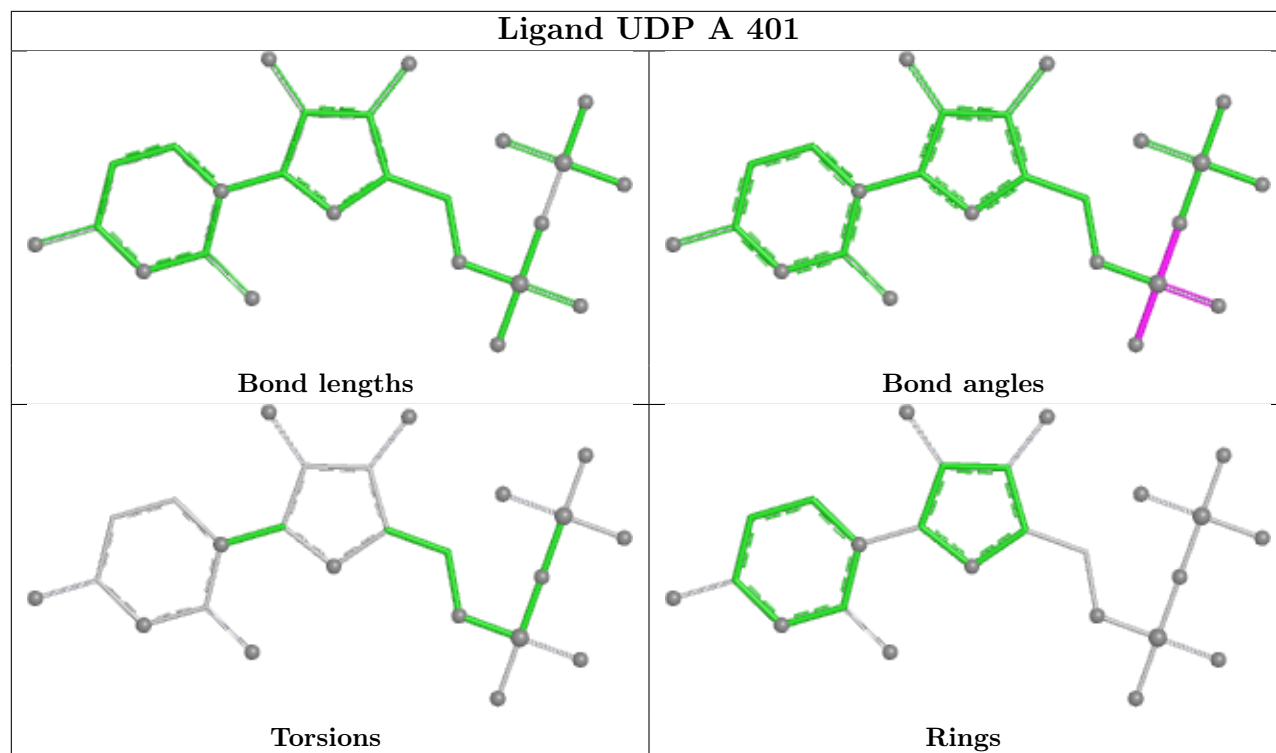
Mol	Chain	Res	Type	Atoms
2	C	401	UDP	PA-O3A-PB-O3B
2	C	401	UDP	PA-O3A-PB-O1B
2	B	401	UDP	PB-O3A-PA-O2A

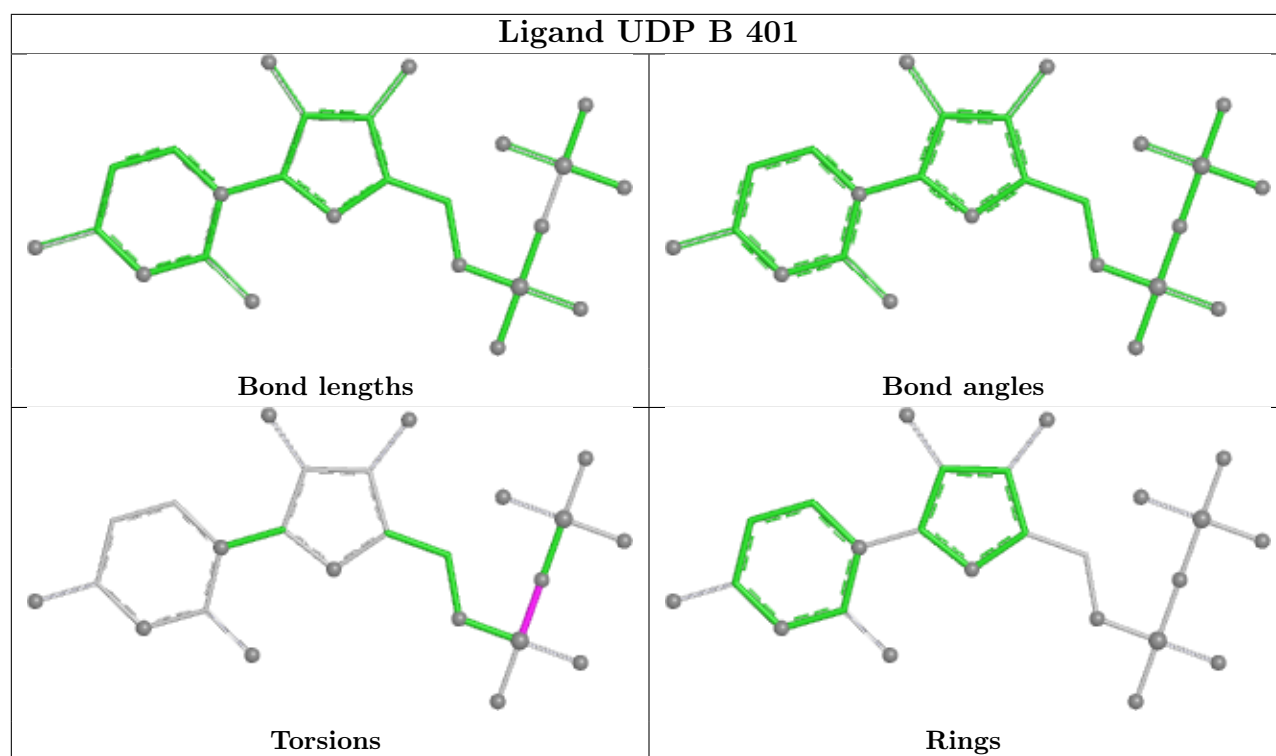
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UDP	1	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	335/354 (94%)	-0.02	1 (0%) 90 88	27, 63, 88, 104	2 (0%)
1	B	320/354 (90%)	0.23	13 (4%) 41 36	42, 63, 120, 156	0
1	C	335/354 (94%)	-0.22	0 100 100	40, 55, 75, 91	0
1	D	326/354 (92%)	0.69	29 (8%) 15 12	51, 91, 148, 170	0
All	All	1316/1416 (92%)	0.16	43 (3%) 49 43	27, 64, 125, 170	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	ARG	5.5
1	B	245	HIS	5.0
1	D	198	ALA	4.2
1	D	175	ALA	3.6
1	D	234	TRP	3.4
1	D	162	PHE	3.2
1	B	239	TYR	3.2
1	B	112	TYR	3.0
1	D	145	VAL	2.9
1	D	183	LEU	2.8
1	B	104	PRO	2.8
1	D	181	PHE	2.8
1	D	12	SER	2.8
1	B	113	LEU	2.8
1	B	184	VAL	2.7
1	D	206	THR	2.7
1	D	286	LEU	2.7
1	D	264	VAL	2.7
1	D	178	LEU	2.7
1	D	281	ILE	2.6
1	D	13	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	250[A]	HIS	2.5
1	D	202	ASP	2.4
1	B	266	GLU	2.4
1	D	243	TYR	2.4
1	B	203	ILE	2.3
1	D	209	ILE	2.3
1	D	214	TRP	2.3
1	B	243	TYR	2.3
1	D	203	ILE	2.3
1	B	206	THR	2.3
1	D	239	TYR	2.2
1	B	238	SER	2.2
1	D	164	VAL	2.2
1	B	246	LEU	2.1
1	D	136	ASP	2.1
1	D	205	PRO	2.1
1	D	212	MET	2.1
1	D	263	ILE	2.1
1	D	109	SER	2.0
1	D	75	TRP	2.0
1	D	275	LEU	2.0
1	D	185	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](#)

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.

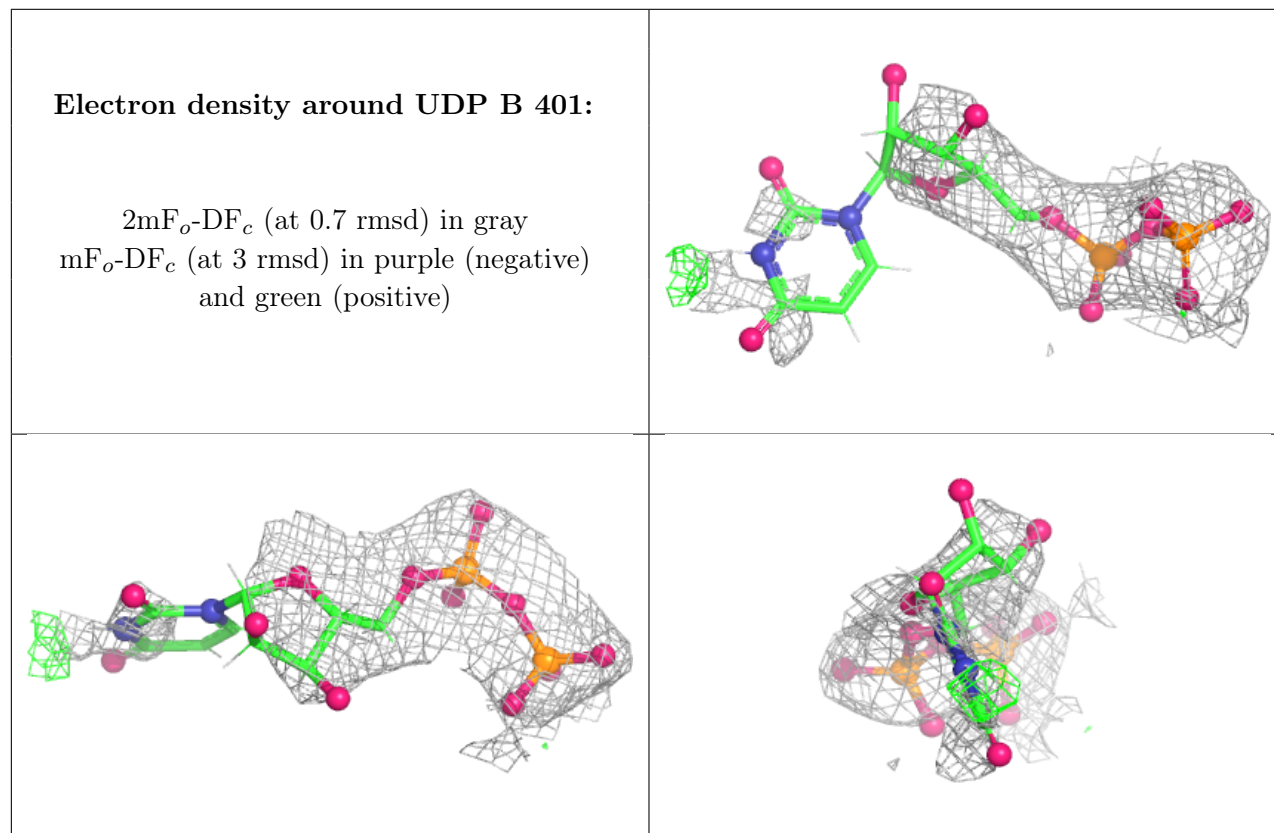
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDP	B	401	25/25	0.81	0.14	70,103,132,137	0

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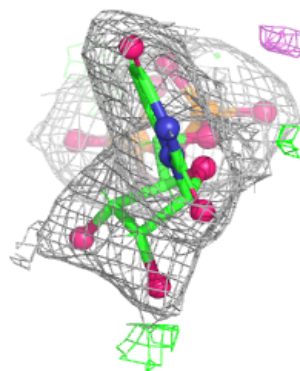
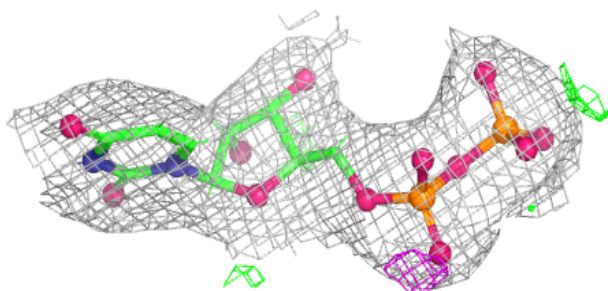
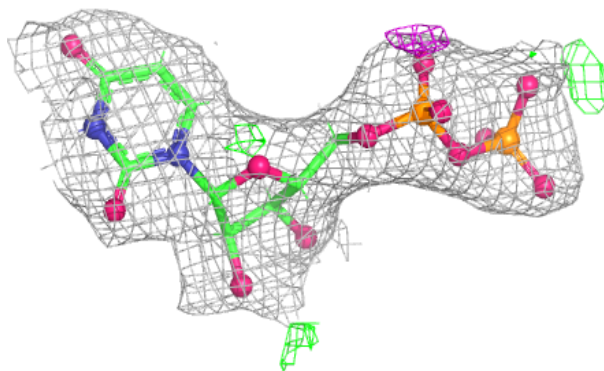
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UDP	A	401	25/25	0.96	0.06	45,53,66,71	0
2	UDP	C	401	25/25	0.96	0.07	34,49,60,68	0

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.

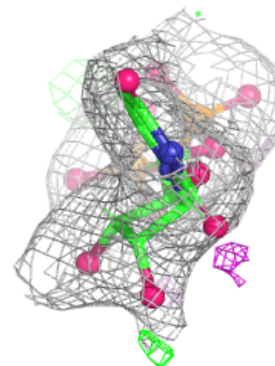
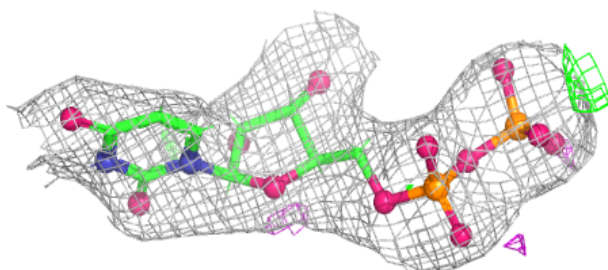
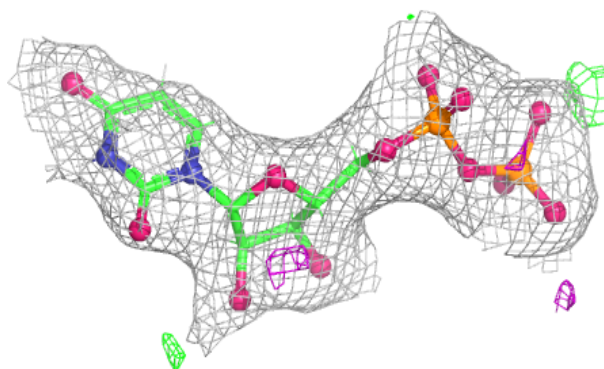


Electron density around UDP A 401:

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

**Electron density around UDP C 401:**

$2mF_o-DF_c$ (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.