



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:50 AM UTC

PDB ID : 9HU9 / pdb_00009hu9
Title : Glycosyltransferase C from the *Limosilactobacillus reuteri* accessory secretion system. Complex with UDP-GlcNAc.
Authors : Pfalzgraf, H.E.; Griffiths, R.; Juge, N.; Hemmings, A.M.
Deposited on : 2024-12-21
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

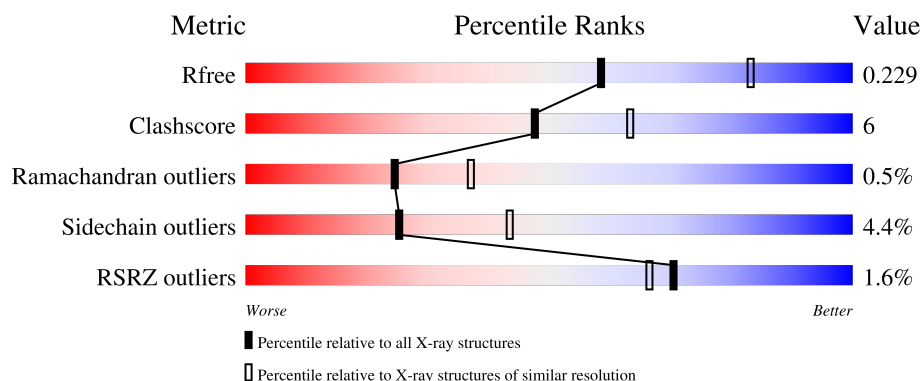
1 Overall quality at a glance

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	336	4% 77% 18% ...
1	B	336	% 83% 14% .
1	C	336	% 81% 15% ..
1	D	336	% 82% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	402	-	X	-	-
3	CIT	D	401	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21576 atoms, of which 10358 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.

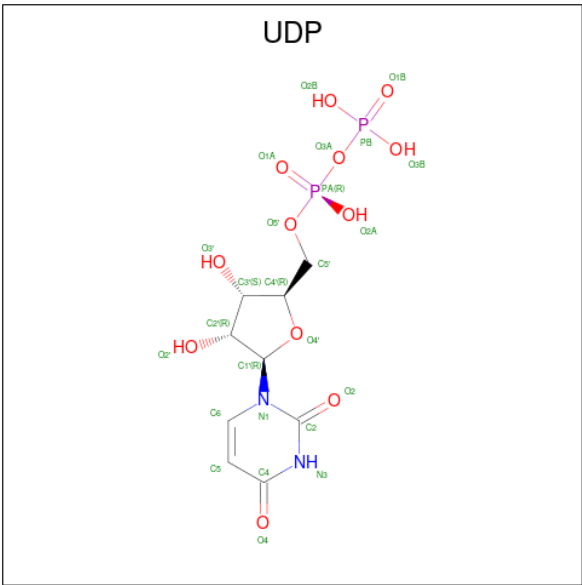
- Molecule 1 is a protein called Glucosyltransferase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	2	0
			5285	1753	2571	450	504	7			
1	B	335	Total	C	H	N	O	S	0	0	0
			5269	1750	2559	449	504	7			
1	C	336	Total	C	H	N	O	S	0	0	0
			5296	1756	2576	451	506	7			
1	D	335	Total	C	H	N	O	S	0	0	0
			5269	1750	2559	449	504	7			

There are 12 discrepancies between the modelled and reference sequences:

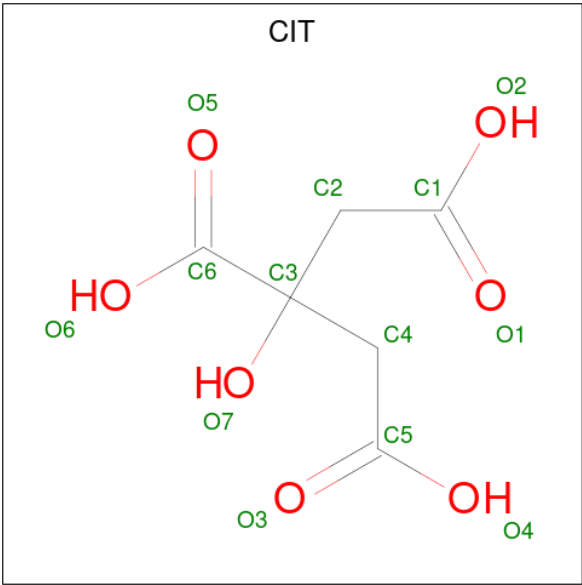
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B3XPQ7
A	0	HIS	-	expression tag	UNP B3XPQ7
A	1	LEU	-	expression tag	UNP B3XPQ7
B	-1	SER	-	expression tag	UNP B3XPQ7
B	0	HIS	-	expression tag	UNP B3XPQ7
B	1	LEU	-	expression tag	UNP B3XPQ7
C	-1	SER	-	expression tag	UNP B3XPQ7
C	0	HIS	-	expression tag	UNP B3XPQ7
C	1	LEU	-	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	C	H	N	O	P	0	0
			34	9	9	2	12	2		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



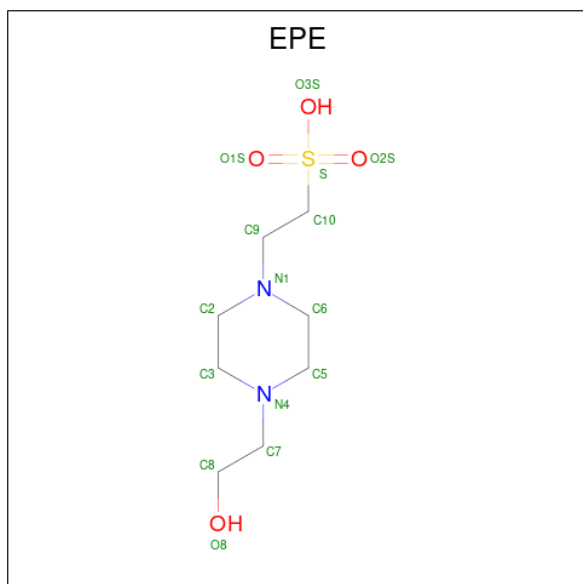
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	6	4	7		
3	D	1	Total	C	H	O	0	0
			17	6	4	7		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			11	3	5	3		
4	C	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	0	0
			31	8	16	2	4	1		

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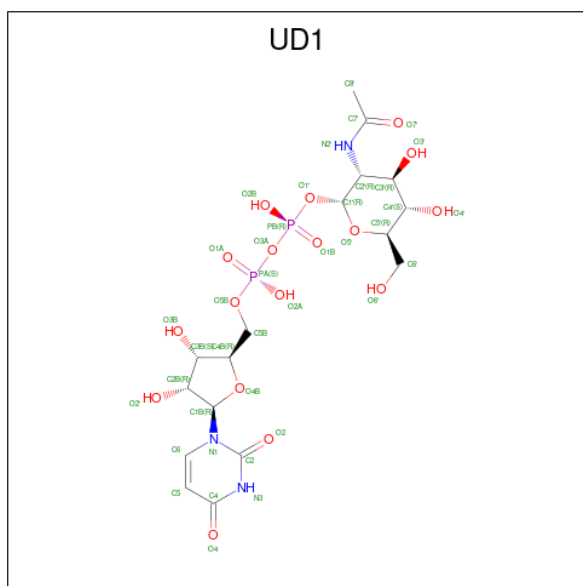
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	H	N	O	S	0
			31	8	16	2	4	1	

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	P	0
			56	17	17	3	17	2	
7	C	1	Total	C	H	N	O	P	0
			56	17	17	3	17	2	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	37	Total	O	0	0
			37	37		
8	B	63	Total	O	0	0
			63	63		

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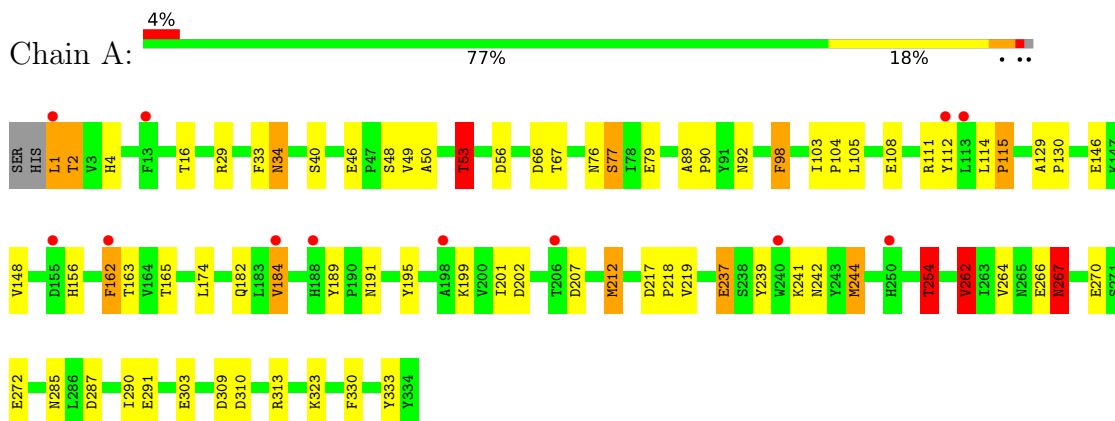
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	41	Total 41	O 41	0	0
8	D	51	Total 51	O 51	0	0

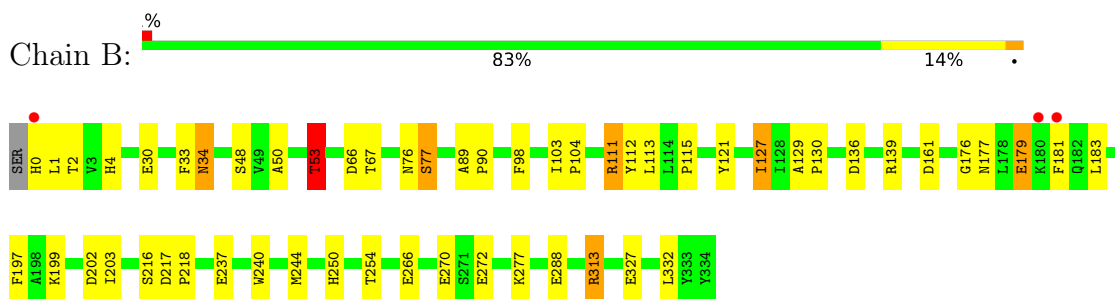
3 Residue-property plots [i](#)

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.

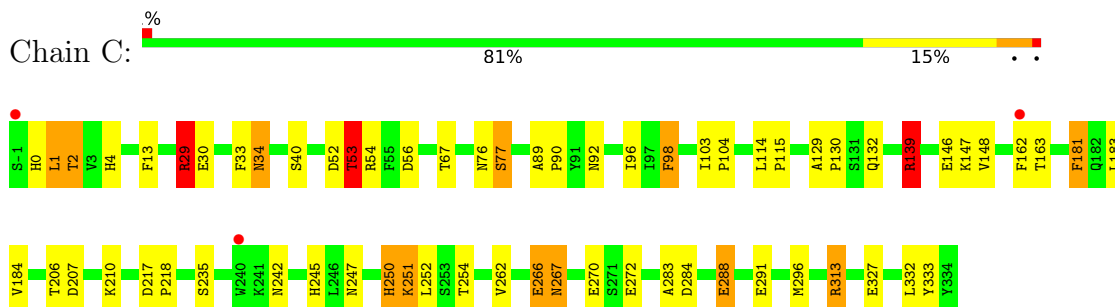
• Molecule 1: Glucosyltransferase 3



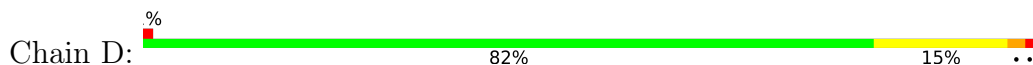
• Molecule 1: Glucosyltransferase 3

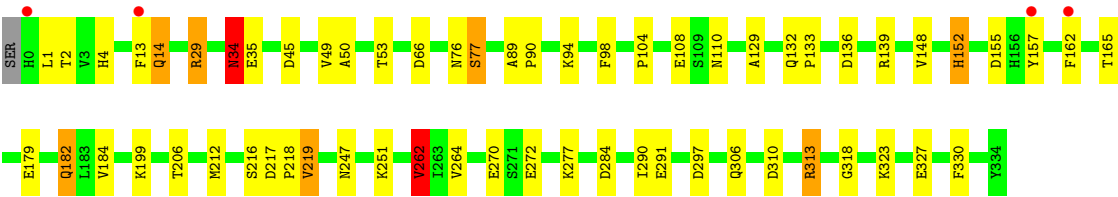


• Molecule 1: Glucosyltransferase 3



• Molecule 1: Glucosyltransferase 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.64Å 121.39Å 174.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.70 – 2.40 60.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.70-2.40) 94.0 (60.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.189 , 0.231 0.183 , 0.229	Depositor DCC
R_{free} test set	3204 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21576	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, UD1, EPE, GOL, CIT, CL

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	0.97	0/2797	1.53	30/3809 (0.8%)
1	B	1.01	1/2784 (0.0%)	1.46	28/3794 (0.7%)
1	C	1.02	3/2794 (0.1%)	1.47	32/3806 (0.8%)
1	D	1.00	2/2784 (0.1%)	1.50	25/3794 (0.7%)
All	All	1.00	6/11159 (0.1%)	1.49	115/15203 (0.8%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	ALA	CA-CB	-5.52	1.47	1.54
1	D	272	GLU	CD-OE1	5.46	1.35	1.25
1	C	148	VAL	C-O	-5.38	1.18	1.23
1	C	250	HIS	CB-CG	5.14	1.57	1.50
1	B	216	SER	CA-CB	-5.12	1.45	1.53
1	C	147	LYS	C-O	-5.05	1.17	1.24

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASN	CB-CA-C	-16.30	83.14	110.85
1	A	262	VAL	N-CA-CB	-13.26	87.41	111.93
1	D	13	PHE	CA-CB-CG	11.37	125.17	113.80
1	D	162	PHE	CA-CB-CG	9.18	122.98	113.80
1	A	212	MET	CG-SD-CE	-9.02	81.05	100.90
1	A	2	THR	CB-CA-C	8.64	124.10	109.50
1	C	53	THR	N-CA-CB	-8.41	97.25	110.28
1	C	13	PHE	CA-CB-CG	8.32	122.12	113.80
1	A	53	THR	N-CA-CB	-8.30	97.42	110.28
1	B	177	ASN	CB-CA-C	8.22	123.40	109.50
1	D	157	TYR	N-CA-CB	8.22	122.22	109.48
1	B	53	THR	N-CA-CB	-8.10	97.72	110.28
1	C	2	THR	CB-CA-C	8.01	122.94	109.48
1	C	327	GLU	CB-CG-CD	7.83	125.91	112.60
1	D	262	VAL	N-CA-CB	-7.73	97.62	111.93
1	B	2	THR	CB-CA-C	7.59	122.23	109.48
1	D	2	THR	CB-CA-C	7.41	121.92	109.48
1	B	161	ASP	CA-CB-CG	7.39	119.99	112.60
1	D	152	HIS	CA-CB-CG	7.36	121.16	113.80
1	C	272	GLU	CB-CG-CD	7.22	124.87	112.60
1	C	132	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	C	162	PHE	CA-CB-CG	6.99	120.79	113.80
1	C	291	GLU	CG-CD-OE2	-6.88	102.58	118.40
1	D	66	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	108	GLU	N-CA-CB	6.72	120.00	110.12
1	B	266	GLU	N-CA-CB	6.71	121.73	110.32
1	B	272	GLU	CB-CG-CD	6.69	123.98	112.60
1	D	108	GLU	CB-CA-C	6.69	121.89	110.79
1	B	111	ARG	CA-CB-CG	-6.66	100.78	114.10
1	D	284	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	254	THR	CA-CB-OG1	-6.51	99.84	109.60
1	B	199	LYS	CB-CA-C	6.50	120.76	109.65
1	C	184	VAL	N-CA-CB	-6.46	100.57	111.23
1	B	202	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	2	THR	N-CA-C	-6.35	99.95	110.17
1	D	29	ARG	CB-CA-C	6.28	121.53	110.85
1	D	2	THR	OG1-CB-CG2	-6.28	96.75	109.30
1	C	163	THR	CA-CB-OG1	6.27	119.00	109.60
1	B	176	GLY	CA-C-N	-6.25	112.01	122.64
1	B	176	GLY	C-N-CA	-6.25	112.01	122.64
1	A	163	THR	CA-CB-OG1	6.25	118.97	109.60
1	A	162	PHE	CB-CA-C	6.23	121.68	109.72
1	B	0	HIS	CA-C-N	6.18	130.15	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	0	HIS	C-N-CA	6.18	130.15	121.24
1	D	34	ASN	CB-CA-C	6.17	119.84	109.48
1	A	92	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	199	LYS	CB-CA-C	6.06	119.78	109.72
1	D	104	PRO	CB-CA-C	-6.03	103.29	111.85
1	A	237	GLU	CB-CG-CD	6.00	122.81	112.60
1	C	53	THR	OG1-CB-CG2	5.92	121.14	109.30
1	A	291	GLU	N-CA-CB	5.87	118.68	109.94
1	C	288	GLU	N-CA-CB	5.86	118.84	110.16
1	D	1	LEU	CA-C-O	5.86	126.63	120.36
1	C	207	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	146	GLU	N-CA-CB	5.82	119.27	110.30
1	A	270	GLU	CB-CG-CD	5.80	122.46	112.60
1	A	66	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	34	ASN	CB-CA-C	5.76	119.17	109.48
1	C	29	ARG	CB-CA-C	5.76	120.64	110.85
1	A	48	SER	CB-CA-C	-5.73	101.23	110.74
1	D	110	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	303	GLU	CB-CG-CD	5.69	122.27	112.60
1	C	242	ASN	CB-CA-C	-5.69	99.75	110.67
1	C	296	MET	CG-SD-CE	-5.63	88.50	100.90
1	A	53	THR	CA-CB-OG1	5.61	118.02	109.60
1	C	34	ASN	CB-CA-C	5.58	118.86	109.48
1	C	146	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	242	ASN	CB-CA-C	-5.57	99.97	110.67
1	C	254	THR	CA-CB-OG1	-5.57	101.24	109.60
1	B	33	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	66	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	33	PHE	CA-CB-CG	5.54	119.34	113.80
1	C	139	ARG	CD-NE-CZ	5.54	132.15	124.40
1	B	270	GLU	CB-CG-CD	5.51	121.96	112.60
1	A	242	ASN	N-CA-CB	5.51	118.81	110.28
1	A	254	THR	CA-CB-OG1	5.48	117.81	109.60
1	B	136	ASP	CB-CA-C	5.47	119.47	110.88
1	D	297	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	313	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	D	35	GLU	CB-CG-CD	5.44	121.85	112.60
1	C	0	HIS	CA-C-N	5.37	129.57	122.42
1	C	0	HIS	C-N-CA	5.37	129.57	122.42
1	B	179	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	112	TYR	N-CA-CB	-5.34	101.04	110.39
1	B	244	MET	CG-SD-CE	-5.34	89.16	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	ASN	N-CA-CB	5.29	118.48	110.28
1	D	270	GLU	CB-CG-CD	5.29	121.59	112.60
1	B	197	PHE	CA-CB-CG	-5.29	108.51	113.80
1	D	165	THR	OG1-CB-CG2	-5.28	98.73	109.30
1	D	45	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	1	LEU	CA-C-O	5.27	126.22	120.58
1	A	33	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	98	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	29	ARG	CB-CA-C	5.20	119.70	110.85
1	D	165	THR	CA-CB-OG1	-5.20	101.81	109.60
1	C	210	LYS	CB-CA-C	5.19	119.22	109.71
1	B	288	GLU	CB-CG-CD	5.19	121.43	112.60
1	D	110	ASN	CB-CA-C	-5.18	101.97	110.72
1	B	34	ASN	CB-CA-C	5.17	118.17	109.48
1	C	270	GLU	CB-CG-CD	5.16	121.38	112.60
1	C	30	GLU	CG-CD-OE2	-5.16	106.53	118.40
1	D	136	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	327	GLU	CG-CD-OE1	-5.15	106.55	118.40
1	A	162	PHE	N-CA-C	-5.14	107.01	113.28
1	C	313	ARG	CB-CG-CD	5.14	123.11	111.30
1	B	2	THR	N-CA-C	-5.11	101.38	109.76
1	D	199	LYS	CB-CA-C	5.10	118.19	109.72
1	A	79	GLU	CB-CG-CD	5.08	121.23	112.60
1	B	30	GLU	CG-CD-OE2	-5.07	106.75	118.40
1	B	237	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	1	LEU	N-CA-CB	5.04	119.06	110.50
1	D	291	GLU	CB-CA-C	5.04	119.15	110.79
1	C	313	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	244	MET	CB-CG-SD	5.03	127.78	112.70
1	A	98	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	B	111	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	313	ARG	Sidechain
1	D	139	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	2714	2571	2619	45	0
1	B	2710	2559	2621	35	0
1	C	2720	2576	2637	32	0
1	D	2710	2559	2621	26	0
2	A	25	9	11	3	0
3	A	13	4	5	0	0
3	D	13	4	5	0	0
4	A	6	5	8	2	0
4	C	6	5	8	2	0
5	A	15	16	18	1	0
5	C	15	16	18	3	0
6	A	1	0	0	1	0
7	B	39	17	25	5	0
7	C	39	17	25	2	0
8	A	37	0	0	3	0
8	B	63	0	0	2	0
8	C	41	0	0	4	0
8	D	51	0	0	1	0
All	All	11218	10358	10621	121	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 6.

All (121) 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:195:TYR:HB3	1:A:212:MET:HE1	1.28	1.12
1:A:56:ASP:HB3	5:A:404:EPE:H81	1.52	0.90
1:A:53:THR:HG22	1:B:53:THR:CG2	2.06	0.85
1:A:53:THR:CG2	1:B:53:THR:HG22	2.06	0.85
1:A:46:GLU:O	6:A:405:CL:CL	2.39	0.78
1:A:148:VAL:HG22	4:A:403:GOL:H2	1.67	0.75
1:C:267:ASN:ND2	8:C:501:HOH:O	2.18	0.75
1:C:54:ARG:HH12	5:C:403:EPE:H22	1.54	0.72
1:C:139:ARG:HD3	8:C:528:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:VAL:HG13	1:D:264:VAL:HG13	1.76	0.68
1:A:53:THR:HG21	1:B:50:ALA:O	1.94	0.66
1:A:244:MET:HG2	8:A:509:HOH:O	1.96	0.66
1:A:53:THR:CG2	1:B:50:ALA:O	2.47	0.63
1:A:53:THR:CG2	1:B:53:THR:CG2	2.71	0.63
1:A:201:ILE:HD12	1:A:202:ASP:O	2.01	0.61
1:C:53:THR:HG21	1:D:50:ALA:O	2.00	0.61
1:A:148:VAL:CG2	4:A:403:GOL:H2	2.32	0.59
1:A:111:ARG:O	1:A:111:ARG:HD2	2.02	0.58
1:B:203:ILE:N	8:B:501:HOH:O	2.26	0.58
1:A:50:ALA:O	1:B:53:THR:HG21	2.03	0.58
1:C:53:THR:CG2	1:D:50:ALA:O	2.52	0.58
1:D:323:LYS:NZ	1:D:327:GLU:OE2	2.36	0.58
1:C:250:HIS:HB2	7:C:401:UD1:O5'	2.05	0.57
1:B:250:HIS:HB2	7:B:401:UD1:C6'	2.35	0.57
1:C:181:PHE:HB3	1:C:235:SER:HA	1.86	0.56
1:A:1:LEU:HD11	1:A:67:THR:OG1	2.06	0.56
1:B:181:PHE:HB2	1:B:183:LEU:HD13	1.86	0.56
1:C:247:ASN:HB2	8:C:539:HOH:O	2.05	0.56
1:D:216:SER:OG	1:D:219:VAL:HG13	2.07	0.55
1:C:251:LYS:HG3	7:C:401:UD1:H5'2	1.88	0.55
1:D:14:GLN:HE21	1:D:14:GLN:N	2.05	0.55
1:B:240:TRP:CE3	7:B:401:UD1:H8'1	2.41	0.54
1:B:112:TYR:CE1	1:B:113:LEU:CD2	2.91	0.54
1:A:156:HIS:CE1	1:A:254:THR:HB	2.43	0.53
1:A:241:LYS:HG3	1:A:267:ASN:OD1	2.08	0.53
1:D:217:ASP:HB3	1:D:218:PRO:HD3	1.91	0.53
1:A:50:ALA:O	1:B:53:THR:CG2	2.56	0.53
1:C:1:LEU:HD11	1:C:67:THR:OG1	2.08	0.53
1:B:121:TYR:HB3	1:B:127:ILE:HD11	1.92	0.51
1:C:76:ASN:O	1:C:77:SER:CB	2.58	0.51
1:C:266:GLU:OE2	1:C:267:ASN:HB3	2.10	0.51
1:D:262:VAL:HG13	1:D:264:VAL:CG1	2.39	0.51
1:A:105:LEU:O	1:A:239:TYR:CE2	2.64	0.51
1:B:217:ASP:HB3	1:B:218:PRO:HD3	1.93	0.51
1:C:129:ALA:HB1	1:C:130:PRO:HD2	1.93	0.51
1:C:54:ARG:HH22	5:C:403:EPE:H22	1.77	0.50
1:A:191:ASN:ND2	8:A:504:HOH:O	2.43	0.50
1:B:1:LEU:HD11	1:B:67:THR:OG1	2.12	0.49
1:B:250:HIS:HB2	7:B:401:UD1:C5'	2.42	0.49
1:A:262:VAL:HG13	1:A:264:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:O	1:A:207:ASP:OD2	2.30	0.49
1:A:323:LYS:HD2	1:D:330:PHE:CG	2.48	0.49
1:A:89:ALA:N	1:A:90:PRO:CD	2.76	0.49
1:B:181:PHE:HB2	1:B:183:LEU:CD1	2.43	0.48
1:C:89:ALA:N	1:C:90:PRO:CD	2.76	0.48
1:A:76:ASN:O	1:A:77:SER:CB	2.62	0.48
1:C:76:ASN:O	1:C:77:SER:HB3	2.12	0.48
1:D:89:ALA:N	1:D:90:PRO:CD	2.77	0.48
1:C:54:ARG:NH1	5:C:403:EPE:H22	2.27	0.48
1:A:333:TYR:O	1:D:277:LYS:HE2	2.14	0.48
1:A:182:GLN:HA	1:A:184:VAL:HG23	1.96	0.47
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.27	0.47
1:C:217:ASP:HB3	1:C:218:PRO:HD3	1.96	0.47
1:B:76:ASN:O	1:B:77:SER:CB	2.63	0.47
1:A:237:GLU:OE1	1:A:239:TYR:N	2.44	0.46
1:C:245:HIS:HB2	8:C:501:HOH:O	2.16	0.46
1:B:240:TRP:CZ3	7:B:401:UD1:O7'	2.69	0.45
1:A:212:MET:HB2	1:A:212:MET:HE2	1.42	0.45
2:A:401:UDP:H4'	2:A:401:UDP:O2A	2.16	0.45
1:D:76:ASN:O	1:D:77:SER:CB	2.65	0.45
1:A:129:ALA:HB1	1:A:130:PRO:HD2	1.98	0.45
1:A:4:HIS:HA	1:A:34:ASN:O	2.17	0.45
1:C:283:ALA:HB1	1:C:288:GLU:HG3	1.99	0.44
1:C:4:HIS:HA	1:C:34:ASN:O	2.17	0.44
1:A:285:ASN:ND2	1:A:287:ASP:HB2	2.33	0.44
1:B:181:PHE:C	1:B:183:LEU:HD12	2.43	0.44
1:D:182:GLN:OE1	1:D:182:GLN:HA	2.17	0.43
1:B:89:ALA:N	1:B:90:PRO:CD	2.80	0.43
1:B:250:HIS:HB2	7:B:401:UD1:H5'	2.00	0.43
1:D:184:VAL:HG23	8:D:531:HOH:O	2.19	0.43
1:A:49:VAL:HG23	8:A:531:HOH:O	2.19	0.43
1:A:53:THR:HG21	1:B:50:ALA:CA	2.48	0.43
1:B:76:ASN:O	1:B:77:SER:HB3	2.17	0.43
1:C:96:ILE:HD11	1:C:332:LEU:HD22	1.99	0.43
1:A:53:THR:HG21	1:B:50:ALA:C	2.44	0.42
1:A:217:ASP:HB3	1:A:218:PRO:HD3	2.01	0.42
1:B:277:LYS:NZ	8:B:506:HOH:O	2.51	0.42
1:C:53:THR:HG22	1:D:53:THR:OG1	2.18	0.42
1:C:181:PHE:O	1:C:183:LEU:N	2.52	0.42
1:C:52:ASP:HB3	4:C:402:GOL:H12	2.02	0.42
1:D:4:HIS:HA	1:D:34:ASN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLU:O	1:D:182:GLN:OE1	2.38	0.42
1:D:216:SER:HG	1:D:219:VAL:HG13	1.83	0.42
1:A:330:PHE:CG	1:D:323:LYS:HD2	2.55	0.42
1:C:103:ILE:N	1:C:104:PRO:CD	2.82	0.42
1:C:114:LEU:HB3	1:C:115:PRO:HD3	2.02	0.42
1:B:313:ARG:HB3	1:C:1:LEU:HD22	2.01	0.42
1:B:4:HIS:HA	1:B:34:ASN:O	2.20	0.42
1:A:16:THR:HG21	2:A:401:UDP:O2A	2.19	0.41
1:D:132:GLN:N	1:D:133:PRO:CD	2.84	0.41
1:D:155:ASP:OD1	1:D:318:GLY:HA2	2.20	0.41
1:A:103:ILE:N	1:A:104:PRO:CD	2.82	0.41
1:D:14:GLN:N	1:D:14:GLN:NE2	2.68	0.41
1:A:53:THR:HG23	1:B:50:ALA:O	2.20	0.41
1:A:76:ASN:O	1:A:77:SER:HB3	2.20	0.41
1:B:129:ALA:HB1	1:B:130:PRO:HD2	2.02	0.41
1:A:114:LEU:HB3	1:A:115:PRO:HD3	2.03	0.41
1:B:103:ILE:N	1:B:104:PRO:CD	2.84	0.41
1:B:277:LYS:HE2	1:C:333:TYR:O	2.21	0.41
1:D:155:ASP:CG	1:D:318:GLY:HA2	2.46	0.41
1:B:112:TYR:CE1	1:B:113:LEU:HD21	2.55	0.41
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.77	0.41
1:C:252:LEU:HD12	1:C:262:VAL:HG11	2.02	0.41
1:A:1:LEU:HD22	1:D:313:ARG:HB3	2.02	0.40
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.85	0.40
1:C:56:ASP:OD2	4:C:402:GOL:O1	2.27	0.40
1:D:313:ARG:HH11	1:D:313:ARG:HG3	1.86	0.40
1:A:189:TYR:CE2	1:A:290:ILE:HD12	2.56	0.40
1:D:29:ARG:HH21	1:D:29:ARG:HG3	1.87	0.40
1:B:139:ARG:HH11	1:B:139:ARG:HG2	1.87	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	334/336 (99%)	327 (98%)	5 (2%)	2 (1%)	21	32
1	B	333/336 (99%)	324 (97%)	8 (2%)	1 (0%)	36	50
1	C	334/336 (99%)	326 (98%)	7 (2%)	1 (0%)	36	50
1	D	333/336 (99%)	327 (98%)	4 (1%)	2 (1%)	21	32
All	All	1334/1344 (99%)	1304 (98%)	24 (2%)	6 (0%)	24	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	184	VAL
1	B	77	SER
1	C	77	SER
1	D	77	SER
1	D	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	294/294 (100%)	277 (94%)	17 (6%)	18	32
1	B	292/294 (99%)	286 (98%)	6 (2%)	47	69
1	C	294/294 (100%)	282 (96%)	12 (4%)	27	46
1	D	292/294 (99%)	275 (94%)	17 (6%)	18	32
All	All	1172/1176 (100%)	1120 (96%)	52 (4%)	25	43

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	40	SER
1	A	53	THR
1	A	98	PHE
1	A	115	PRO

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Mol	Chain	Res	Type
1	A	146	GLU
1	A	162	PHE
1	A	165	THR
1	A	174	LEU
1	A	219	VAL
1	A	254	THR
1	A	262	VAL
1	A	266	GLU
1	A	267	ASN
1	A	272	GLU
1	A	309	ASP
1	A	310	ASP
1	B	48	SER
1	B	53	THR
1	B	98	PHE
1	B	115	PRO
1	B	127	ILE
1	B	179	GLU
1	C	2	THR
1	C	29	ARG
1	C	40	SER
1	C	53	THR
1	C	92	ASN
1	C	98	PHE
1	C	181	PHE
1	C	206	THR
1	C	251	LYS
1	C	266	GLU
1	C	267	ASN
1	C	284	ASP
1	D	14	GLN
1	D	34	ASN
1	D	49	VAL
1	D	94	LYS
1	D	98	PHE
1	D	148	VAL
1	D	182	GLN
1	D	206	THR
1	D	212	MET
1	D	219	VAL
1	D	247	ASN
1	D	251	LYS

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Mol	Chain	Res	Type
1	D	262	VAL
1	D	290	ILE
1	D	306	GLN
1	D	310	ASP
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	177	ASN
1	A	191	ASN
1	A	285	ASN
1	B	100	HIS
1	B	177	ASN
1	B	299	GLN
1	C	14	GLN
1	C	23	GLN
1	C	167	GLN
1	C	186	HIS
1	C	192	ASN
1	C	245	HIS
1	C	294	GLN
1	D	14	GLN
1	D	167	GLN
1	D	192	ASN
1	D	267	ASN
1	D	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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
4	GOL	C	402	-	5,5,5	0.21	0	5,5,5	0.59	0
5	EPE	A	404	-	15,15,15	1.64	3 (20%)	19,20,20	2.21	8 (42%)
7	UD1	C	401	-	40,41,41	0.62	0	59,62,62	2.12	16 (27%)
4	GOL	A	403	-	5,5,5	0.70	0	5,5,5	0.87	0
3	CIT	D	401	-	12,12,12	1.52	3 (25%)	17,17,17	1.77	4 (23%)
3	CIT	A	402	-	12,12,12	3.00	5 (41%)	17,17,17	2.04	5 (29%)
5	EPE	C	403	-	15,15,15	1.30	2 (13%)	19,20,20	1.28	1 (5%)
7	UD1	B	401	-	40,41,41	0.87	2 (5%)	59,62,62	1.34	9 (15%)
2	UDP	A	401	-	25,26,26	1.04	2 (8%)	38,40,40	1.66	7 (18%)

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
4	GOL	C	402	-	-	4/4/4/4	-
5	EPE	A	404	-	-	7/9/19/19	0/1/1/1
7	UD1	C	401	-	-	11/26/63/63	0/3/3/3
4	GOL	A	403	-	-	2/4/4/4	-
3	CIT	D	401	-	-	11/16/16/16	-
3	CIT	A	402	-	-	11/16/16/16	-
5	EPE	C	403	-	-	7/9/19/19	0/1/1/1
7	UD1	B	401	-	-	4/26/63/63	0/3/3/3
2	UDP	A	401	-	-	3/16/32/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	CIT	O3-C5	7.20	1.45	1.22
3	A	402	CIT	C4-C3	4.29	1.59	1.54
3	A	402	CIT	C3-C6	3.87	1.57	1.53
5	C	403	EPE	O3S-S	3.39	1.59	1.47
5	A	404	EPE	C9-N1	3.38	1.55	1.47
7	B	401	UD1	PA-O3A	3.37	1.63	1.59
2	A	401	UDP	PA-O3A	3.15	1.62	1.59
5	A	404	EPE	O3S-S	3.10	1.58	1.47
7	B	401	UD1	PB-O3A	2.97	1.62	1.59
3	A	402	CIT	C4-C5	2.62	1.58	1.50
2	A	401	UDP	PB-O3B	-2.61	1.45	1.54
3	A	402	CIT	C2-C3	2.47	1.57	1.54
3	D	401	CIT	C3-C6	2.42	1.56	1.53
5	C	403	EPE	C9-N1	2.36	1.52	1.47
3	D	401	CIT	O4-C5	-2.09	1.23	1.30
5	A	404	EPE	C10-S	2.08	1.80	1.77
3	D	401	CIT	C2-C3	2.04	1.56	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	401	UD1	C3'-C2'-N2'	7.08	123.65	110.62
7	C	401	UD1	C4'-C3'-C2'	-6.44	101.02	110.40
3	A	402	CIT	C3-C4-C5	5.36	128.58	113.92
7	C	401	UD1	O5'-C1'-O1'	5.26	118.24	111.36
2	A	401	UDP	O3A-PB-O1B	-4.70	86.33	111.04
7	C	401	UD1	O3A-PB-O1B	-4.54	97.04	110.70
5	A	404	EPE	C5-N4-C3	4.22	117.93	108.84
2	A	401	UDP	O2B-PB-O3A	4.17	118.63	104.64
5	A	404	EPE	C6-C5-N4	4.15	119.03	110.65
3	D	401	CIT	O5-C6-C3	-4.07	114.20	122.09
7	C	401	UD1	O5'-C5'-C4'	4.01	116.93	109.70
7	B	401	UD1	O5'-C1'-C2'	3.64	117.46	110.59
3	A	402	CIT	O6-C6-C3	3.57	119.98	113.14
7	C	401	UD1	O2B-PB-O1B	3.50	128.75	112.44
7	C	401	UD1	O3'-C3'-C2'	3.43	116.41	109.58
7	C	401	UD1	O3'-C3'-C4'	3.27	118.09	110.38
7	B	401	UD1	O5'-C5'-C4'	-3.22	103.90	109.70
2	A	401	UDP	O2'-C2'-C3'	-3.21	101.54	111.82
7	C	401	UD1	C1'-O5'-C5'	3.18	119.94	113.72
3	D	401	CIT	C3-C2-C1	3.16	122.55	113.92
2	A	401	UDP	O3'-C3'-C2'	-2.91	102.48	111.82
5	A	404	EPE	O3S-S-C10	2.89	111.66	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	EPE	C2-C3-N4	2.89	116.47	110.65
2	A	401	UDP	O3B-PB-O3A	2.79	113.98	104.64
7	B	401	UD1	O3B-C3B-C2B	-2.73	103.06	111.82
7	B	401	UD1	O2B-PB-O3A	2.70	114.57	107.27
3	A	402	CIT	O5-C6-C3	-2.68	116.91	122.09
5	A	404	EPE	C5-C6-N1	2.65	116.00	110.65
5	A	404	EPE	C8-C7-N4	2.65	122.72	113.44
3	D	401	CIT	O6-C6-C3	2.64	118.21	113.14
7	B	401	UD1	C4'-C3'-C2'	-2.56	106.67	110.40
5	A	404	EPE	O3S-S-O2S	-2.41	105.38	111.40
3	A	402	CIT	C3-C2-C1	2.41	120.50	113.92
7	C	401	UD1	C3B-C2B-C1B	2.40	106.00	101.46
5	A	404	EPE	C10-C9-N1	2.34	121.20	112.36
7	B	401	UD1	O3A-PB-O1B	2.28	117.56	110.70
7	C	401	UD1	O2B-PB-O1'	2.28	115.96	106.70
7	C	401	UD1	O2'-C2B-C3B	-2.27	104.53	111.82
7	B	401	UD1	O2A-PA-O1A	2.27	123.00	112.44
5	C	403	EPE	C5-C6-N1	2.23	115.15	110.65
3	A	402	CIT	C2-C3-C6	-2.23	105.10	110.03
7	C	401	UD1	O2A-PA-O3A	2.19	113.18	107.27
2	A	401	UDP	C3'-C2'-C1'	2.18	105.59	101.46
7	C	401	UD1	O2A-PA-O1A	2.15	122.44	112.44
7	B	401	UD1	O5'-C1'-O1'	-2.08	108.65	111.36
3	D	401	CIT	C3-C4-C5	2.04	119.51	113.92
7	B	401	UD1	O3B-C3B-C4B	-2.04	105.24	111.08
7	C	401	UD1	C1'-C2'-C3'	-2.03	104.59	110.19
7	C	401	UD1	O1'-PB-O1B	-2.01	103.37	109.81
2	A	401	UDP	O5'-C5'-C4'	2.00	115.81	108.99

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	UDP	C4'-C5'-O5'-PA
3	A	402	CIT	O7-C3-C4-C5
3	A	402	CIT	C6-C3-C4-C5
3	A	402	CIT	C2-C3-C6-O5
3	A	402	CIT	C2-C3-C6-O6
3	A	402	CIT	O7-C3-C6-O5
3	A	402	CIT	O7-C3-C6-O6
3	D	401	CIT	C2-C3-C4-C5
3	D	401	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	401	CIT	C2-C3-C6-O5
3	D	401	CIT	C2-C3-C6-O6
3	D	401	CIT	O7-C3-C6-O5
3	D	401	CIT	O7-C3-C6-O6
4	C	402	GOL	C1-C2-C3-O3
5	A	404	EPE	C10-C9-N1-C2
5	A	404	EPE	S-C10-C9-N1
5	A	404	EPE	C9-C10-S-O1S
5	A	404	EPE	C9-C10-S-O2S
5	A	404	EPE	C9-C10-S-O3S
5	C	403	EPE	C8-C7-N4-C5
5	C	403	EPE	C9-C10-S-O2S
7	B	401	UD1	C5B-O5B-PA-O2A
7	C	401	UD1	C1'-O1'-PB-O3A
5	C	403	EPE	N4-C7-C8-O8
7	C	401	UD1	C3B-C4B-C5B-O5B
3	A	402	CIT	C1-C2-C3-O7
7	C	401	UD1	C8'-C7'-N2'-C2'
7	C	401	UD1	O7'-C7'-N2'-C2'
7	C	401	UD1	O4B-C4B-C5B-O5B
5	C	403	EPE	C9-C10-S-O3S
3	A	402	CIT	C1-C2-C3-C6
3	A	402	CIT	C2-C3-C4-C5
4	A	403	GOL	O1-C1-C2-C3
4	C	402	GOL	O1-C1-C2-C3
4	A	403	GOL	O1-C1-C2-O2
4	C	402	GOL	O1-C1-C2-O2
7	B	401	UD1	C3B-C4B-C5B-O5B
3	D	401	CIT	O7-C3-C4-C5
3	A	402	CIT	C1-C2-C3-C4
7	B	401	UD1	C4'-C5'-C6'-O6'
5	C	403	EPE	C10-C9-N1-C6
7	C	401	UD1	O5'-C5'-C6'-O6'
3	D	401	CIT	C1-C2-C3-C6
5	C	403	EPE	C9-C10-S-O1S
7	C	401	UD1	C1'-O1'-PB-O1B
7	C	401	UD1	PA-O3A-PB-O2B
4	C	402	GOL	O2-C2-C3-O3
5	A	404	EPE	C10-C9-N1-C6
5	C	403	EPE	C10-C9-N1-C2
7	C	401	UD1	PA-O3A-PB-O1B
7	C	401	UD1	O5'-C1'-O1'-PB

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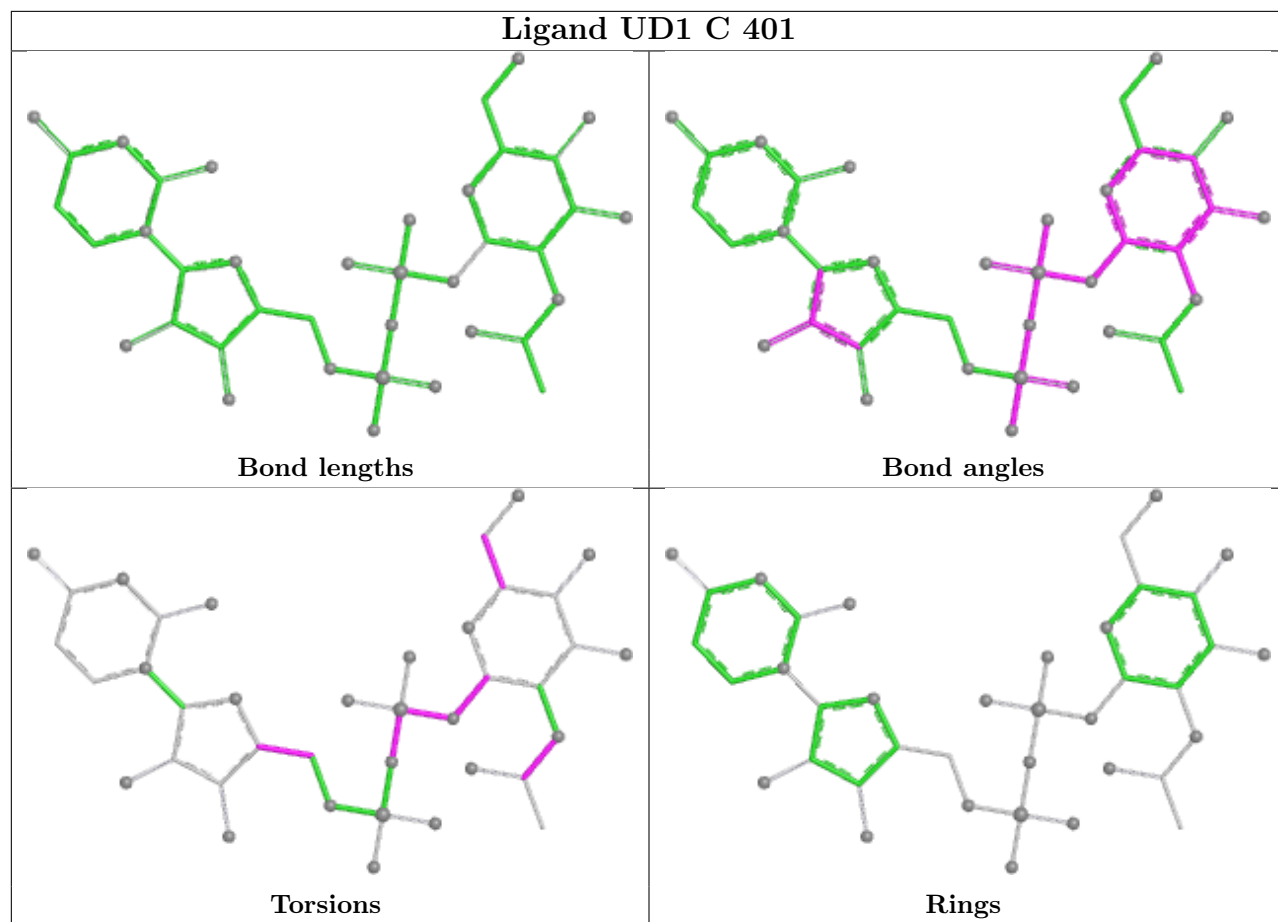
Mol	Chain	Res	Type	Atoms
3	D	401	CIT	C1-C2-C3-O7
7	C	401	UD1	C4'-C5'-C6'-O6'
2	A	401	UDP	PB-O3A-PA-O1A
5	A	404	EPE	C8-C7-N4-C5
2	A	401	UDP	PB-O3A-PA-O2A
7	B	401	UD1	PB-O3A-PA-O2A
3	D	401	CIT	C3-C4-C5-O3
3	A	402	CIT	C3-C4-C5-O3
3	D	401	CIT	C3-C4-C5-O4

There are no ring outliers.

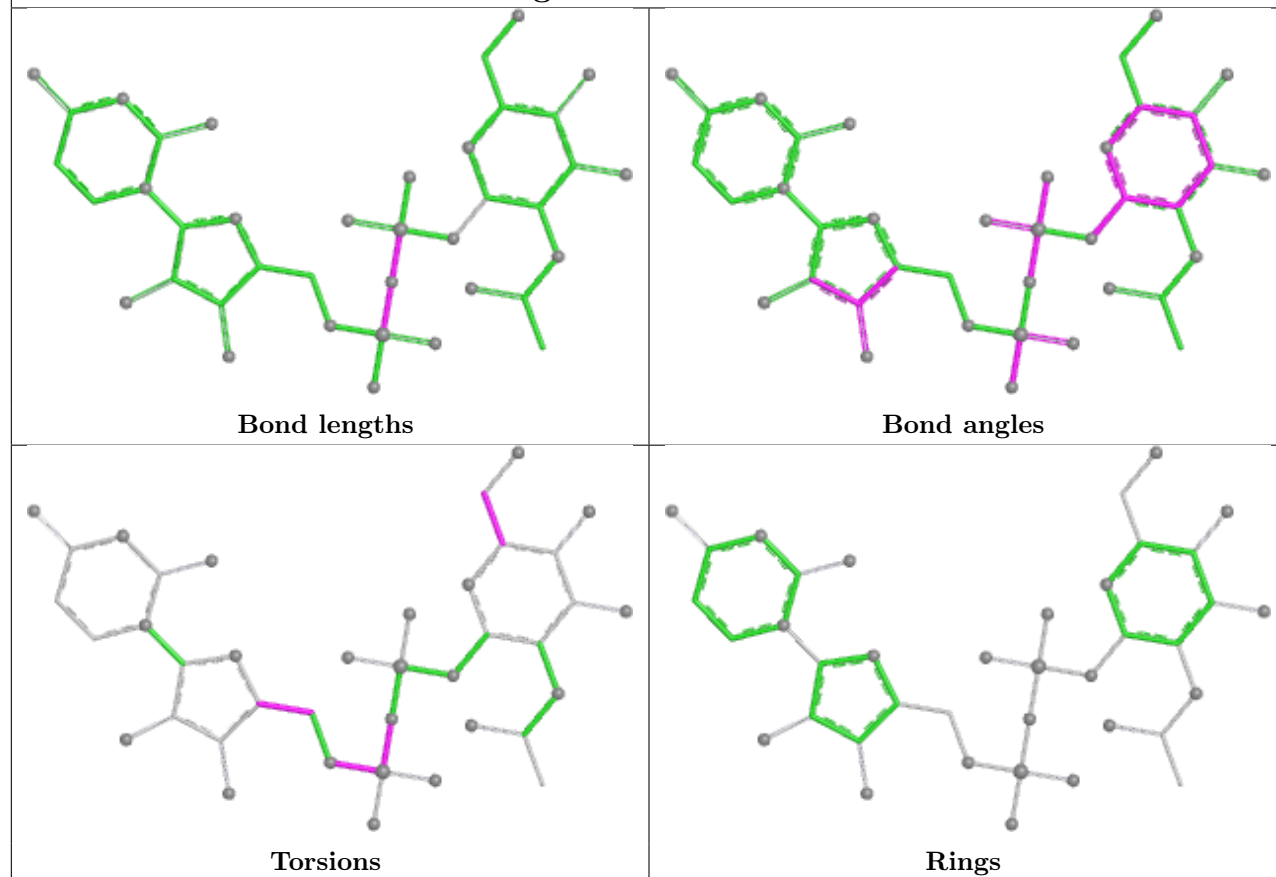
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	GOL	2	0
5	A	404	EPE	1	0
7	C	401	UD1	2	0
4	A	403	GOL	2	0
5	C	403	EPE	3	0
7	B	401	UD1	5	0
2	A	401	UDP	3	0

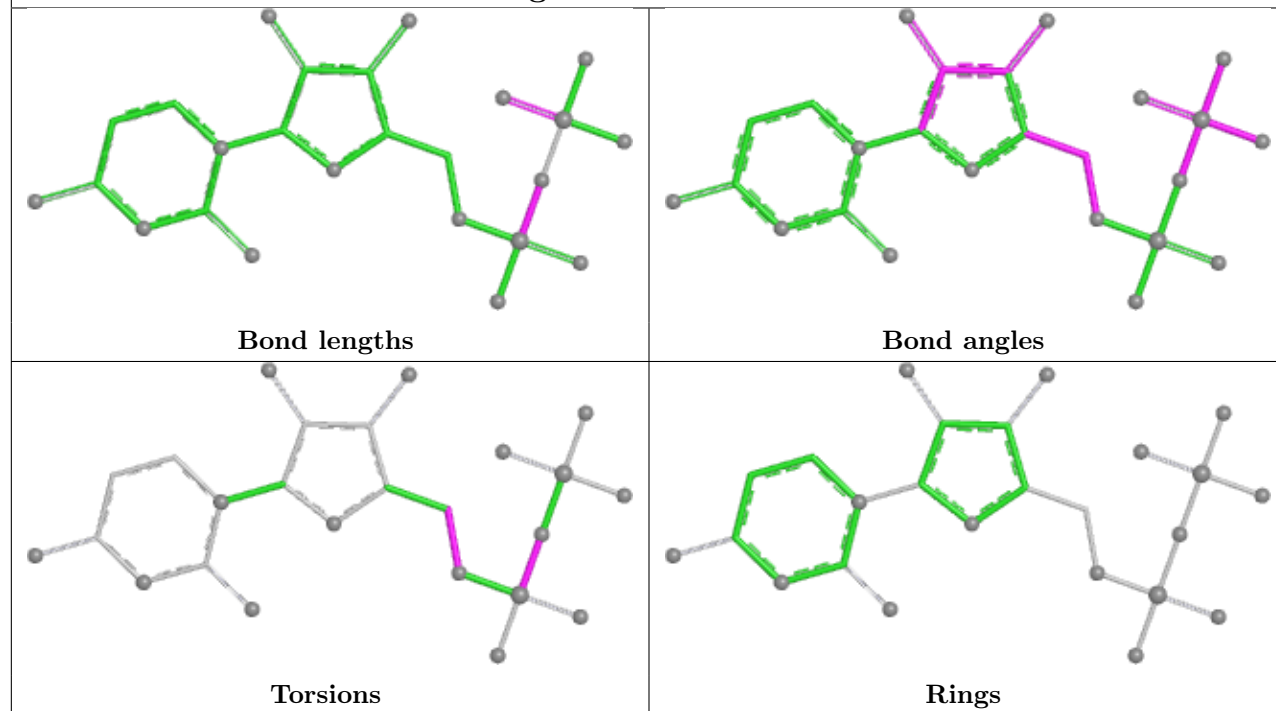
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand UD1 B 401



Ligand UDP A 401



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	334/336 (99%)	-0.07	12 (3%) 46 42	19, 47, 90, 114	1 (0%)
1	B	335/336 (99%)	-0.30	3 (0%) 81 78	29, 44, 76, 102	0
1	C	336/336 (100%)	-0.36	3 (0%) 81 78	27, 43, 72, 99	0
1	D	335/336 (99%)	-0.34	4 (1%) 76 73	29, 45, 69, 110	0
All	All	1340/1344 (99%)	-0.27	22 (1%) 70 66	19, 45, 79, 114	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	PHE	5.4
1	A	112	TYR	5.2
1	A	162	PHE	4.4
1	A	113	LEU	4.3
1	A	184	VAL	4.2
1	A	198	ALA	3.6
1	C	162	PHE	3.5
1	A	240	TRP	3.5
1	D	0	HIS	3.4
1	A	13	PHE	3.3
1	B	181	PHE	3.0
1	C	240	TRP	2.8
1	B	180	LYS	2.7
1	D	162	PHE	2.6
1	A	1	LEU	2.6
1	A	250[A]	HIS	2.4
1	D	157	TYR	2.3
1	A	206	THR	2.2
1	C	-1	SER	2.2
1	A	155	ASP	2.2
1	A	188	HIS	2.2
1	B	0	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

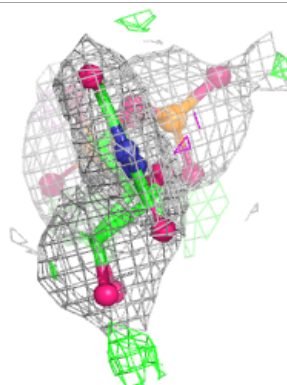
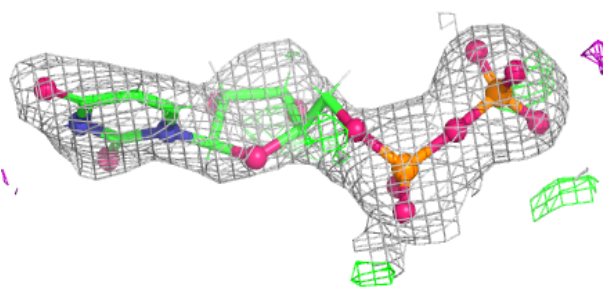
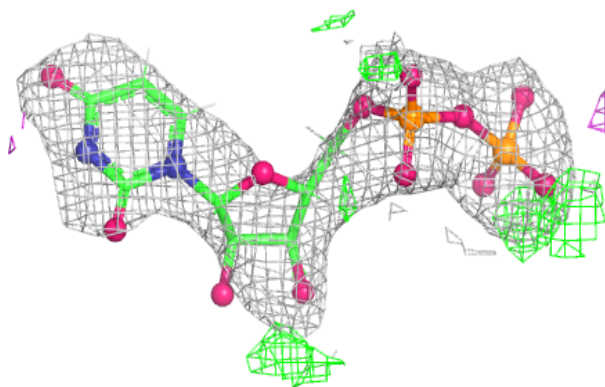
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIT	A	402	13/13	0.73	0.17	49,79,94,98	0
4	GOL	A	403	6/6	0.78	0.16	54,68,79,84	0
4	GOL	C	402	6/6	0.80	0.17	92,101,110,114	0
5	EPE	A	404	15/15	0.80	0.16	58,78,133,181	0
5	EPE	C	403	15/15	0.80	0.18	76,99,153,168	0
3	CIT	D	401	13/13	0.85	0.14	59,85,93,100	0
2	UDP	A	401	25/25	0.89	0.14	47,72,90,102	34
7	UD1	C	401	39/39	0.92	0.14	33,48,105,169	56
6	CL	A	405	1/1	0.93	0.17	67,67,67,67	0
7	UD1	B	401	39/39	0.95	0.10	28,51,70,77	56

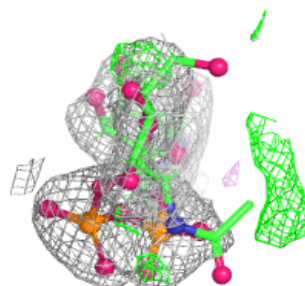
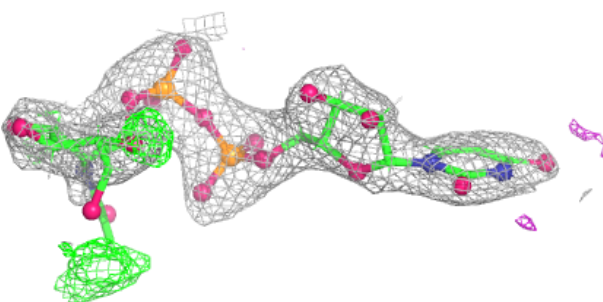
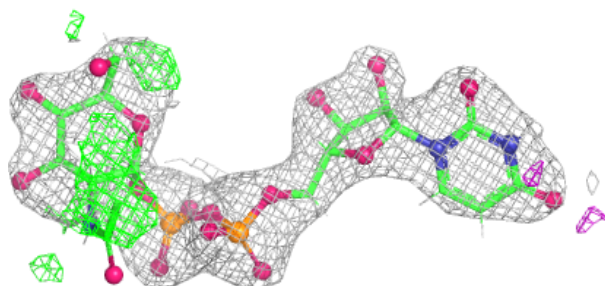
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

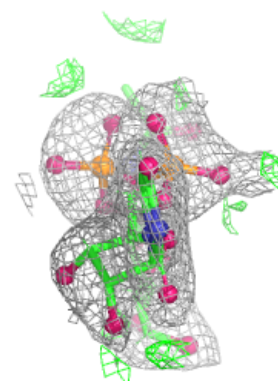
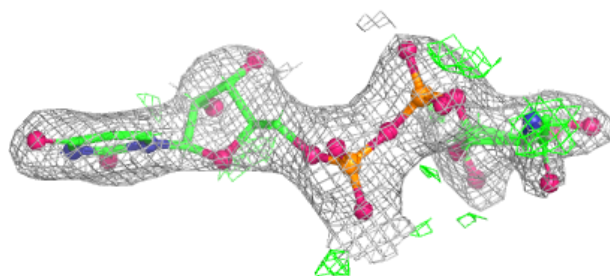
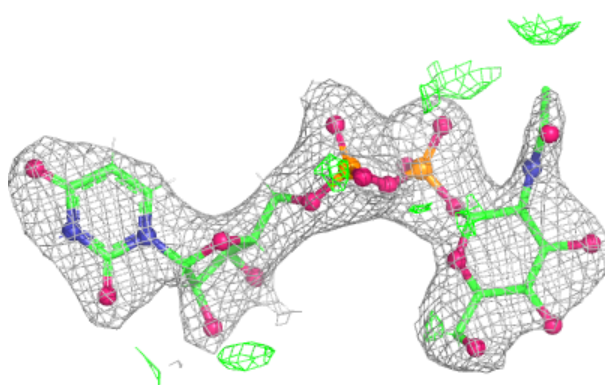
**Electron density around UD1 C 401:**

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



Electron density around UD1 B 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.