



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2025 – 01:09 pm BST

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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

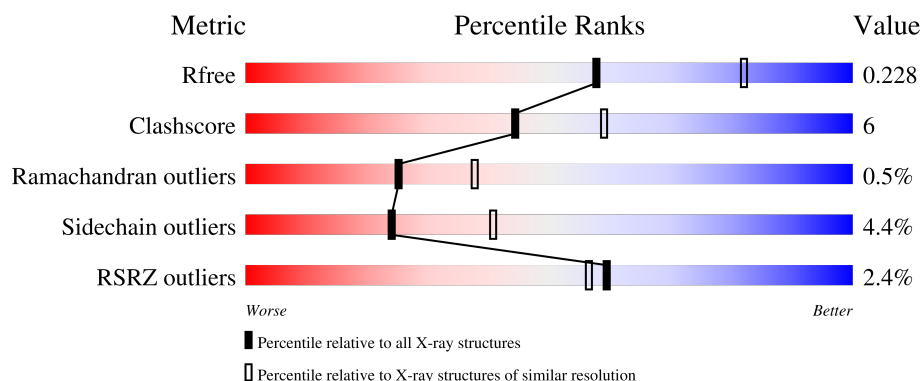
# 1 Overall quality at a glance

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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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  $\geq 3$ , 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	337	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	337	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	337	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	D	337	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>

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	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11202 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.

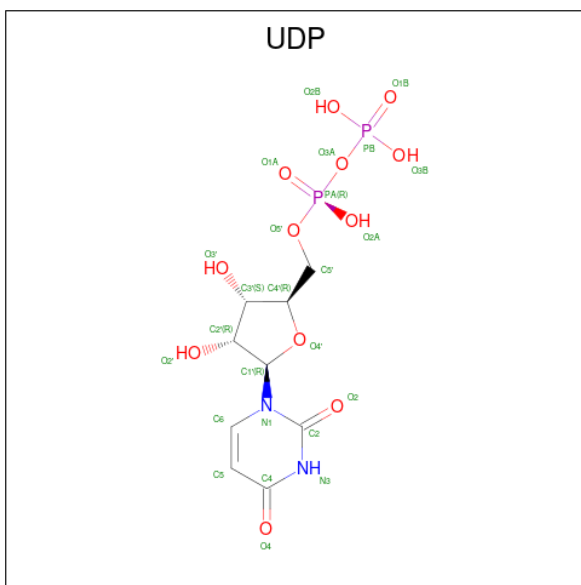
- Molecule 1 is a protein called Glucosyltransferase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2704	1747	447	503	7			
1	B	335	Total	C	N	O	S	0	0	0
			2710	1750	449	504	7			
1	C	336	Total	C	N	O	S	0	0	0
			2720	1756	451	506	7			
1	D	335	Total	C	N	O	S	0	0	0
			2714	1753	450	504	7			

There are 16 discrepancies between the modelled and reference sequences:

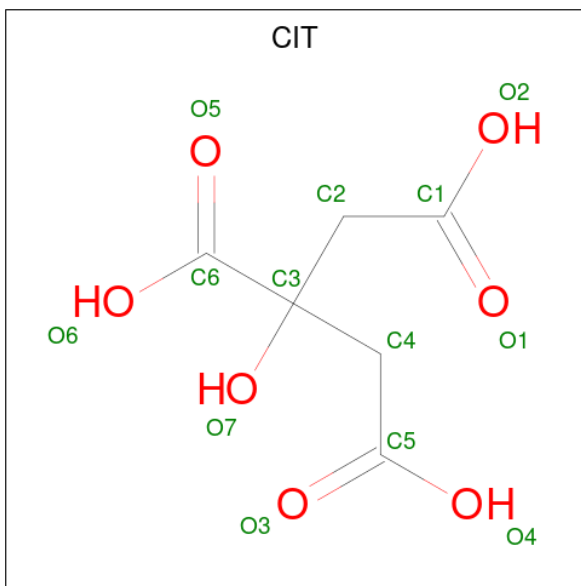
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP B3XPQ7
A	-1	SER	-	expression tag	UNP B3XPQ7
A	0	HIS	-	expression tag	UNP B3XPQ7
A	1	LEU	-	expression tag	UNP B3XPQ7
B	-2	GLY	-	expression tag	UNP B3XPQ7
B	-1	SER	-	expression tag	UNP B3XPQ7
B	0	HIS	-	expression tag	UNP B3XPQ7
B	1	LEU	-	expression tag	UNP B3XPQ7
C	-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
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).



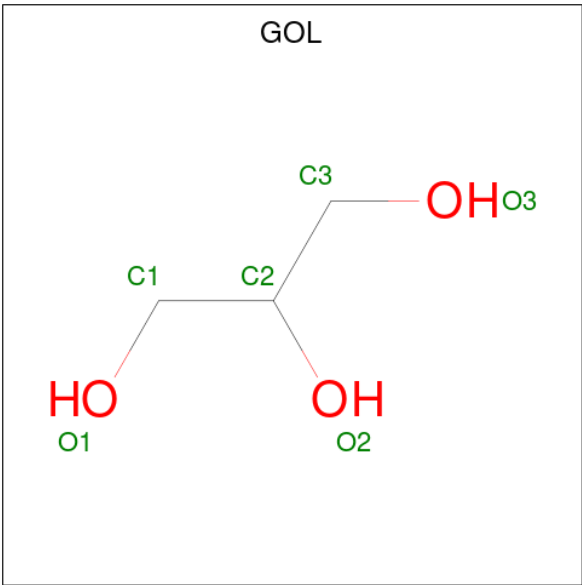
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula:  $\text{C}_6\text{H}_8\text{O}_7$ ).



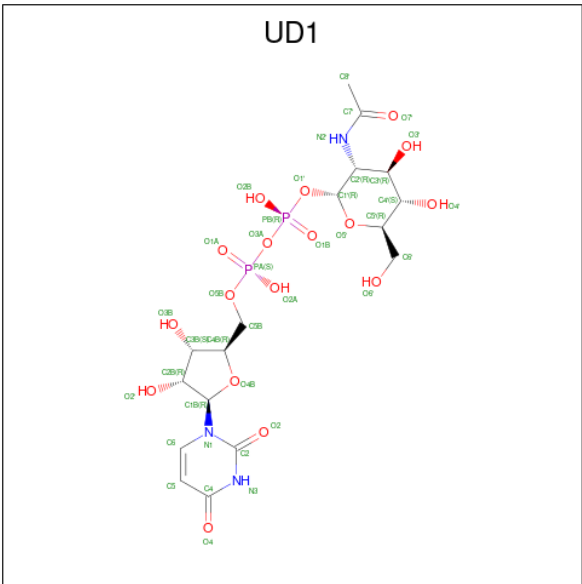
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



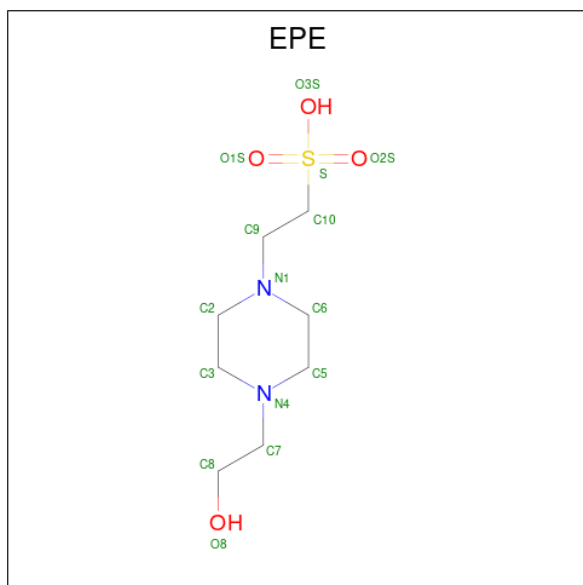
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

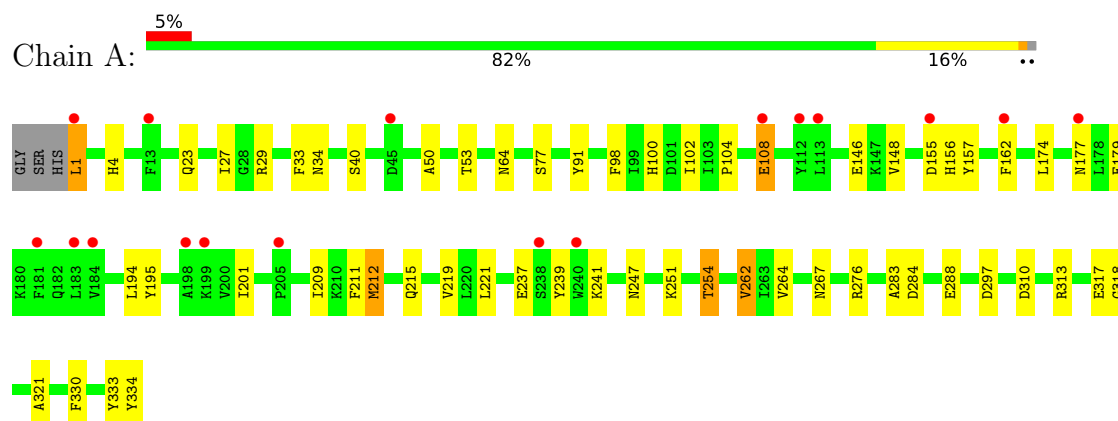
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	B	63	Total	O	0	0
			63	63		
7	C	42	Total	O	0	0
			42	42		
7	D	52	Total	O	0	0
			52	52		

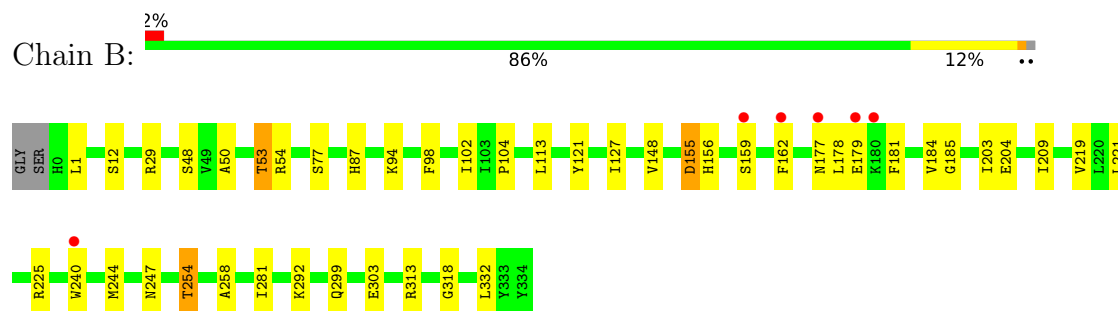
### 3 Residue-property plots [i](#)

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.

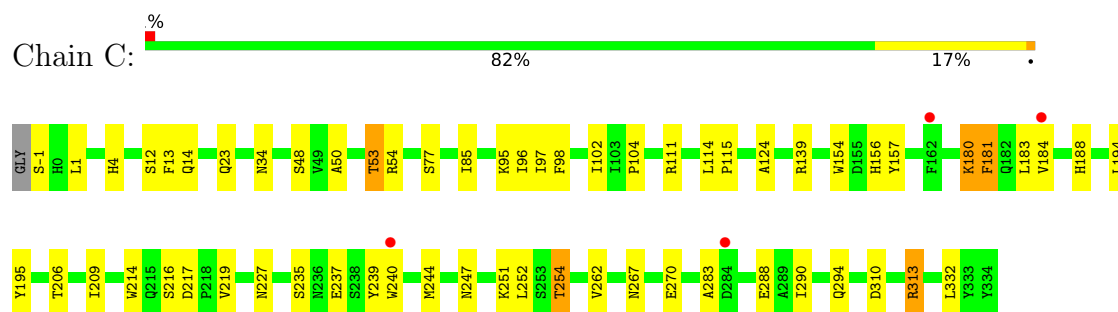
#### • Molecule 1: Glucosyltransferase 3



#### • Molecule 1: Glucosyltransferase 3

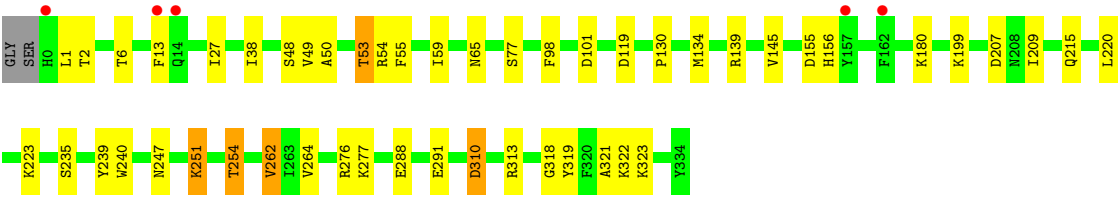
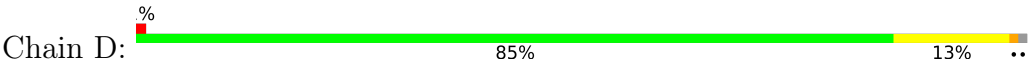


#### • Molecule 1: Glucosyltransferase 3



#### • Molecule 1: Glucosyltransferase 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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)	99.7 (60.70-2.40) 94.0 (60.70-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.55 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.181 , 0.226 0.183 , 0.228	Depositor DCC
$R_{free}$ test set	3217 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, EPE, UDP, GOL, UD1

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	0.47	0/2777	0.60	0/3783
1	B	0.45	0/2784	0.59	0/3794
1	C	0.45	0/2794	0.59	0/3806
1	D	0.45	0/2788	0.61	0/3798
All	All	0.46	0/11143	0.60	0/15181

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2704	0	2625	40	0
1	B	2710	0	2621	28	0
1	C	2720	0	2637	39	0
1	D	2714	0	2632	35	0
2	A	25	0	11	1	0
3	A	13	0	5	0	0
4	A	6	0	8	2	0
4	C	6	0	8	0	0
5	B	39	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	39	0	25	8	0
6	B	15	0	17	2	0
6	C	15	0	18	2	0
7	A	39	0	0	1	0
7	B	63	0	0	3	0
7	C	42	0	0	2	0
7	D	52	0	0	3	0
All	All	11202	0	10632	127	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 (127) 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:C:270:GLU:OE1	7:C:501:HOH:O	2.03	0.77
1:D:101:ASP:O	7:D:401:HOH:O	2.04	0.75
1:A:148:VAL:HG22	4:A:403:GOL:H2	1.73	0.70
1:A:313:ARG:NH2	1:D:65:ASN:O	2.25	0.70
1:D:139:ARG:NH1	1:D:145:VAL:O	2.27	0.68
1:C:181:PHE:HB3	1:C:235:SER:HA	1.78	0.66
1:A:195:TYR:HB3	1:A:212:MET:CE	2.25	0.66
1:D:119:ASP:O	7:D:402:HOH:O	2.14	0.65
1:C:251:LYS:HG3	5:C:401:UD1:H5'2	1.79	0.64
1:A:195:TYR:HB3	1:A:212:MET:HE1	1.80	0.62
1:B:177:ASN:HD22	1:B:179:GLU:HG3	1.63	0.62
1:C:180:LYS:NZ	5:C:401:UD1:H8'1	2.15	0.61
1:D:262:VAL:HG13	1:D:264:VAL:HG13	1.85	0.58
1:A:102:ILE:HG22	1:A:104:PRO:HD2	1.85	0.58
1:B:299:GLN:O	1:B:303:GLU:HG3	2.04	0.58
1:C:139:ARG:HD3	7:C:513:HOH:O	2.04	0.57
1:A:174:LEU:HB2	1:A:194:LEU:HD11	1.87	0.56
1:A:241:LYS:HE3	1:A:267:ASN:OD1	2.07	0.55
1:A:156:HIS:CE1	1:A:254:THR:HB	2.42	0.55
1:A:195:TYR:CD2	1:A:212:MET:HE1	2.42	0.55
1:C:154:TRP:CE2	5:C:401:UD1:H6'1	2.42	0.55
1:A:251:LYS:HG3	2:A:401:UDP:H5'2	1.89	0.54
1:C:23:GLN:HE22	1:C:157:TYR:H	1.56	0.53
1:C:53:THR:HG21	1:D:50:ALA:O	2.09	0.53
1:A:23:GLN:HE22	1:A:157:TYR:H	1.55	0.52
1:A:148:VAL:CG2	4:A:403:GOL:H2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:VAL:HG13	1:A:264:VAL:HG13	1.91	0.52
1:C:96:ILE:HD11	1:C:332:LEU:HD22	1.91	0.52
1:C:97:ILE:HD12	1:C:124:ALA:HB2	1.92	0.52
1:D:313:ARG:HH11	1:D:313:ARG:HG3	1.75	0.52
1:D:6:THR:HB	1:D:38:ILE:HD12	1.92	0.52
1:C:240:TRP:O	1:C:244:MET:HG3	2.10	0.51
1:A:334:TYR:OXT	1:D:276:ARG:NH2	2.43	0.51
1:B:313:ARG:HB3	1:C:1:LEU:HD22	1.91	0.51
1:C:111:ARG:HD3	1:C:239:TYR:OH	2.11	0.51
1:C:156:HIS:CE1	1:C:254:THR:HB	2.46	0.51
1:A:237:GLU:OE1	1:A:239:TYR:N	2.43	0.51
1:A:317:GLU:OE2	1:D:1:LEU:HB3	2.11	0.51
1:C:180:LYS:HZ2	5:C:401:UD1:H8'1	1.75	0.51
1:C:53:THR:HG23	1:D:54:ARG:HB2	1.93	0.51
1:A:50:ALA:HB1	1:B:53:THR:HG21	1.93	0.50
1:B:1:LEU:HB2	1:C:313:ARG:HG2	1.94	0.50
1:C:50:ALA:O	1:D:53:THR:HG21	2.11	0.50
1:B:185:GLY:HA2	1:B:204:GLU:HG3	1.94	0.49
1:D:310:ASP:O	1:D:313:ARG:HD2	2.12	0.49
1:D:215:GLN:HB2	1:D:220:LEU:HB2	1.93	0.49
1:D:50:ALA:O	1:D:53:THR:HG22	2.12	0.49
5:C:401:UD1:H8'3	5:C:401:UD1:H1'	1.95	0.49
1:B:155:ASP:HB3	1:B:318:GLY:HA2	1.96	0.48
1:D:55:PHE:O	1:D:59:ILE:HG12	2.14	0.48
1:C:85:ILE:HD11	1:C:95:LYS:HD2	1.95	0.48
1:C:194:LEU:HD23	1:C:209:ILE:HG12	1.95	0.48
1:A:53:THR:HG21	1:B:50:ALA:HB1	1.96	0.48
1:A:195:TYR:HB3	1:A:212:MET:HE2	1.95	0.48
1:B:178:LEU:HD22	1:B:184:VAL:HG23	1.95	0.48
1:C:14:GLN:HG2	1:C:214:TRP:CZ2	2.49	0.48
1:A:247:ASN:HB2	7:A:527:HOH:O	2.14	0.47
1:B:254:THR:HG21	5:B:401:UD1:O3B	2.13	0.47
6:B:402:EPE:H102	6:B:402:EPE:H22	1.63	0.47
1:D:156:HIS:CE1	1:D:254:THR:HB	2.49	0.47
1:C:114:LEU:HB3	1:C:115:PRO:HD3	1.95	0.47
1:A:283:ALA:HB1	1:A:288:GLU:HG3	1.97	0.47
1:C:54:ARG:HH22	6:C:403:EPE:H22	1.80	0.47
1:D:130:PRO:HD2	1:D:134:MET:HG2	1.96	0.47
1:D:319:TYR:HA	1:D:322:LYS:HB2	1.96	0.47
1:C:195:TYR:HD2	1:C:227:ASN:ND2	2.13	0.46
1:C:252:LEU:HD12	1:C:262:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HB3	1:A:209:ILE:HG12	1.98	0.46
1:A:1:LEU:CB	1:D:313:ARG:HG2	2.46	0.46
1:B:94:LYS:HB3	1:B:332:LEU:HD13	1.98	0.46
1:B:121:TYR:HB3	1:B:127:ILE:HD11	1.98	0.46
1:C:53:THR:CG2	1:D:54:ARG:HB2	2.46	0.46
1:C:283:ALA:HB1	1:C:288:GLU:HG3	1.98	0.46
1:B:156:HIS:CE1	1:B:254:THR:HB	2.51	0.46
1:B:221:LEU:HD22	1:B:258:ALA:HB2	1.98	0.46
1:B:162:PHE:CE1	1:C:-1:SER:HB2	2.51	0.46
1:C:188:HIS:CD2	1:C:188:HIS:H	2.34	0.46
1:D:313:ARG:HG3	1:D:313:ARG:NH1	2.31	0.45
1:A:1:LEU:HB3	1:D:313:ARG:HG2	1.99	0.45
1:A:50:ALA:HA	1:A:53:THR:HG22	1.99	0.45
1:A:4:HIS:HA	1:A:34:ASN:O	2.16	0.45
1:A:27:ILE:HD13	1:A:321:ALA:HB3	1.99	0.45
1:C:216:SER:HB3	1:C:219:VAL:HG12	1.98	0.45
6:C:403:EPE:H82	6:C:403:EPE:H51	1.59	0.45
1:A:64:ASN:HA	1:A:91:TYR:O	2.17	0.45
1:D:1:LEU:HD12	1:D:2:THR:O	2.16	0.45
1:C:240:TRP:CZ3	5:C:401:UD1:O7'	2.71	0.44
1:A:313:ARG:CZ	1:D:1:LEU:HB2	2.46	0.44
1:D:207:ASP:HB3	1:D:209:ILE:HD12	1.99	0.44
1:A:333:TYR:O	1:D:277:LYS:HE2	2.18	0.44
1:C:102:ILE:HG22	1:C:104:PRO:HD2	2.00	0.44
1:D:235:SER:HB3	1:D:240:TRP:CD2	2.53	0.44
1:A:155:ASP:CG	1:A:318:GLY:HA2	2.39	0.44
1:A:33:PHE:O	1:B:29:ARG:NH2	2.50	0.43
1:B:244:MET:HA	1:B:247:ASN:OD1	2.18	0.43
1:C:156:HIS:NE2	1:C:217:ASP:OD1	2.38	0.43
5:C:401:UD1:C7'	5:C:401:UD1:O2B	2.67	0.43
1:D:251:LYS:HA	1:D:254:THR:HG23	1.99	0.43
1:B:203:ILE:HG12	7:B:506:HOH:O	2.19	0.43
1:A:177:ASN:HD21	1:A:179:GLU:HB2	1.83	0.43
1:A:195:TYR:HD2	1:A:212:MET:HE1	1.83	0.43
1:D:223:LYS:NZ	7:D:405:HOH:O	2.51	0.42
1:D:155:ASP:CG	1:D:318:GLY:HA2	2.40	0.42
1:A:201:ILE:HG13	1:A:211:PHE:CZ	2.55	0.42
1:B:102:ILE:HG22	1:B:104:PRO:HD2	2.00	0.42
1:D:288:GLU:HA	1:D:291:GLU:OE1	2.19	0.42
1:B:178:LEU:HD11	1:B:209:ILE:HD13	2.01	0.42
1:B:281:ILE:HG23	1:B:292:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PHE:CD2	1:D:323:LYS:HD3	2.55	0.42
1:C:4:HIS:HA	1:C:34:ASN:O	2.19	0.42
1:C:290:ILE:O	1:C:294:GLN:HG3	2.20	0.42
1:A:1:LEU:HD22	1:D:313:ARG:HG2	2.00	0.42
1:B:54:ARG:NH1	6:B:402:EPE:H71	2.34	0.42
1:A:215:GLN:HB3	1:A:219:VAL:HG22	2.02	0.41
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.92	0.41
1:C:247:ASN:ND2	5:C:401:UD1:HN2'	2.18	0.41
1:C:23:GLN:NE2	1:C:157:TYR:H	2.16	0.41
1:C:181:PHE:O	1:C:183:LEU:N	2.53	0.41
1:B:203:ILE:N	7:B:506:HOH:O	2.44	0.41
1:A:108:GLU:HG2	1:A:239:TYR:CE1	2.56	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.87	0.41
1:D:27:ILE:HD13	1:D:321:ALA:HB3	2.02	0.41
1:B:87:HIS:HB3	7:B:510:HOH:O	2.20	0.41
1:B:240:TRP:CE3	5:B:401:UD1:H8'1	2.56	0.41
1:C:251:LYS:HE3	1:C:251:LYS:HB2	1.88	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.89	0.40
1:B:177:ASN:ND2	1:B:179:GLU:HG3	2.35	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	332/337 (98%)	320 (96%)	11 (3%)	1 (0%)	37	51
1	B	333/337 (99%)	323 (97%)	9 (3%)	1 (0%)	37	51
1	C	334/337 (99%)	326 (98%)	6 (2%)	2 (1%)	22	33
1	D	333/337 (99%)	324 (97%)	7 (2%)	2 (1%)	22	33
All	All	1332/1348 (99%)	1293 (97%)	33 (2%)	6 (0%)	25	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	SER
1	C	77	SER
1	A	77	SER
1	D	77	SER
1	D	180	LYS
1	C	184	VAL

### 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	292/294 (99%)	277 (95%)	15 (5%)	20	35
1	B	292/294 (99%)	281 (96%)	11 (4%)	28	47
1	C	294/294 (100%)	281 (96%)	13 (4%)	24	41
1	D	293/294 (100%)	281 (96%)	12 (4%)	26	44
All	All	1171/1176 (100%)	1120 (96%)	51 (4%)	24	41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	29	ARG
1	A	40	SER
1	A	98	PHE
1	A	100	HIS
1	A	108	GLU
1	A	146	GLU
1	A	162	PHE
1	A	212	MET
1	A	254	THR
1	A	262	VAL
1	A	276	ARG
1	A	284	ASP
1	A	297	ASP

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Mol	Chain	Res	Type
1	A	310	ASP
1	B	12	SER
1	B	48	SER
1	B	53	THR
1	B	98	PHE
1	B	148	VAL
1	B	155	ASP
1	B	159	SER
1	B	181	PHE
1	B	219	VAL
1	B	225	ARG
1	B	254	THR
1	C	12	SER
1	C	13	PHE
1	C	48	SER
1	C	53	THR
1	C	98	PHE
1	C	180	LYS
1	C	181	PHE
1	C	206	THR
1	C	237	GLU
1	C	254	THR
1	C	267	ASN
1	C	310	ASP
1	C	313	ARG
1	D	13	PHE
1	D	48	SER
1	D	49	VAL
1	D	53	THR
1	D	98	PHE
1	D	199	LYS
1	D	239	TYR
1	D	247	ASN
1	D	251	LYS
1	D	254	THR
1	D	262	VAL
1	D	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN

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Mol	Chain	Res	Type
1	A	177	ASN
1	A	250	HIS
1	B	177	ASN
1	B	182	GLN
1	C	23	GLN
1	C	188	HIS
1	C	245	HIS
1	D	14	GLN
1	D	34	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
4	GOL	C	402	-	5,5,5	0.76	0	5,5,5	1.07	0
5	UD1	B	401	-	38,41,41	0.40	0	57,62,62	0.83	2 (3%)
6	EPE	B	402	-	15,15,15	1.02	1 (6%)	18,20,20	1.96	5 (27%)
6	EPE	C	403	-	15,15,15	1.33	1 (6%)	18,20,20	2.54	9 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UDP	A	401	-	24,26,26	0.47	0	37,40,40	0.85	2 (5%)
4	GOL	A	403	-	5,5,5	1.32	1 (20%)	5,5,5	0.96	0
5	UD1	C	401	-	38,41,41	0.40	0	57,62,62	0.99	4 (7%)
3	CIT	A	402	-	12,12,12	1.37	1 (8%)	17,17,17	1.83	5 (29%)

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	-	-	2/4/4/4	-
5	UD1	B	401	-	-	8/26/63/63	0/3/3/3
6	EPE	B	402	-	-	5/9/19/19	0/1/1/1
6	EPE	C	403	-	-	5/9/19/19	0/1/1/1
2	UDP	A	401	-	-	4/16/32/32	0/2/2/2
4	GOL	A	403	-	-	3/4/4/4	-
5	UD1	C	401	-	-	6/26/63/63	0/3/3/3
3	CIT	A	402	-	-	12/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	EPE	C10-S	4.53	1.83	1.77
6	B	402	EPE	C10-S	3.61	1.82	1.77
4	A	403	GOL	C1-C2	2.58	1.62	1.51
3	A	402	CIT	O3-C5	2.19	1.29	1.22

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	402	EPE	C5-N4-C3	4.95	119.98	108.83
6	C	403	EPE	C6-N1-C2	4.40	118.74	108.83
5	C	401	UD1	O3A-PB-O1'	4.37	111.30	102.48
3	A	402	CIT	O6-C6-C3	4.09	120.15	113.05
6	C	403	EPE	C7-N4-C5	3.88	121.15	111.23
6	C	403	EPE	C5-N4-C3	3.87	117.54	108.83
6	C	403	EPE	C5-C6-N1	3.74	118.31	110.64
6	C	403	EPE	C7-N4-C3	3.65	120.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	UD1	O3A-PB-O1'	3.39	109.32	102.48
6	C	403	EPE	O2S-S-C10	3.28	110.86	106.92
6	B	402	EPE	O3S-S-C10	3.09	110.77	105.77
6	B	402	EPE	C6-C5-N4	2.99	116.78	110.64
5	B	401	UD1	PB-O1'-C1'	-2.96	108.28	119.74
5	C	401	UD1	C1'-C2'-N2'	-2.86	106.07	111.00
6	C	403	EPE	O3S-S-C10	2.83	110.34	105.77
3	A	402	CIT	C4-C3-C6	-2.80	104.08	110.11
5	C	401	UD1	O5'-C1'-C2'	2.61	115.68	110.58
3	A	402	CIT	O2-C1-O1	-2.46	117.17	123.30
2	A	401	UDP	O3B-PB-O3A	2.31	112.39	104.64
3	A	402	CIT	O2-C1-C2	2.31	121.75	114.35
6	C	403	EPE	C6-C5-N4	2.30	115.37	110.64
6	B	402	EPE	O1S-S-C10	2.29	109.67	106.92
5	C	401	UD1	C1'-O5'-C5'	2.19	117.99	113.69
2	A	401	UDP	PA-O3A-PB	-2.15	125.43	132.83
6	C	403	EPE	C3-C2-N1	2.10	114.96	110.64
6	B	402	EPE	C7-N4-C5	2.02	116.41	111.23
3	A	402	CIT	C3-C2-C1	2.01	118.67	113.81

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	CIT	C2-C3-C4-C5
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
4	A	403	GOL	O1-C1-C2-C3
5	B	401	UD1	C3B-C4B-C5B-O5B
5	B	401	UD1	C5B-O5B-PA-O2A
5	C	401	UD1	C1'-O1'-PB-O3A
5	C	401	UD1	C3B-C4B-C5B-O5B
6	B	402	EPE	C9-C10-S-O1S
6	B	402	EPE	C9-C10-S-O3S
6	C	403	EPE	C8-C7-N4-C5
6	C	403	EPE	N4-C7-C8-O8
6	C	403	EPE	C9-C10-S-O1S
6	C	403	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
5	C	401	UD1	C8'-C7'-N2'-C2'
5	C	401	UD1	O7'-C7'-N2'-C2'
4	C	402	GOL	O1-C1-C2-C3
4	A	403	GOL	O1-C1-C2-O2
4	C	402	GOL	O1-C1-C2-O2
5	B	401	UD1	O4B-C4B-C5B-O5B
3	A	402	CIT	C1-C2-C3-C6
5	C	401	UD1	O4B-C4B-C5B-O5B
2	A	401	UDP	C4'-C5'-O5'-PA
6	B	402	EPE	C8-C7-N4-C3
3	A	402	CIT	C1-C2-C3-O7
6	B	402	EPE	N4-C7-C8-O8
5	B	401	UD1	C4'-C5'-C6'-O6'
5	B	401	UD1	C5B-O5B-PA-O3A
5	C	401	UD1	PA-O3A-PB-O2B
5	B	401	UD1	C5B-O5B-PA-O1A
6	B	402	EPE	C9-C10-S-O2S
6	C	403	EPE	C9-C10-S-O2S
2	A	401	UDP	PB-O3A-PA-O1A
2	A	401	UDP	PB-O3A-PA-O2A
5	B	401	UD1	C1'-O1'-PB-O3A
3	A	402	CIT	C3-C4-C5-O3
3	A	402	CIT	C3-C4-C5-O4
3	A	402	CIT	C1-C2-C3-C4
4	A	403	GOL	C1-C2-C3-O3
5	B	401	UD1	O5'-C5'-C6'-O6'
2	A	401	UDP	C5'-O5'-PA-O1A

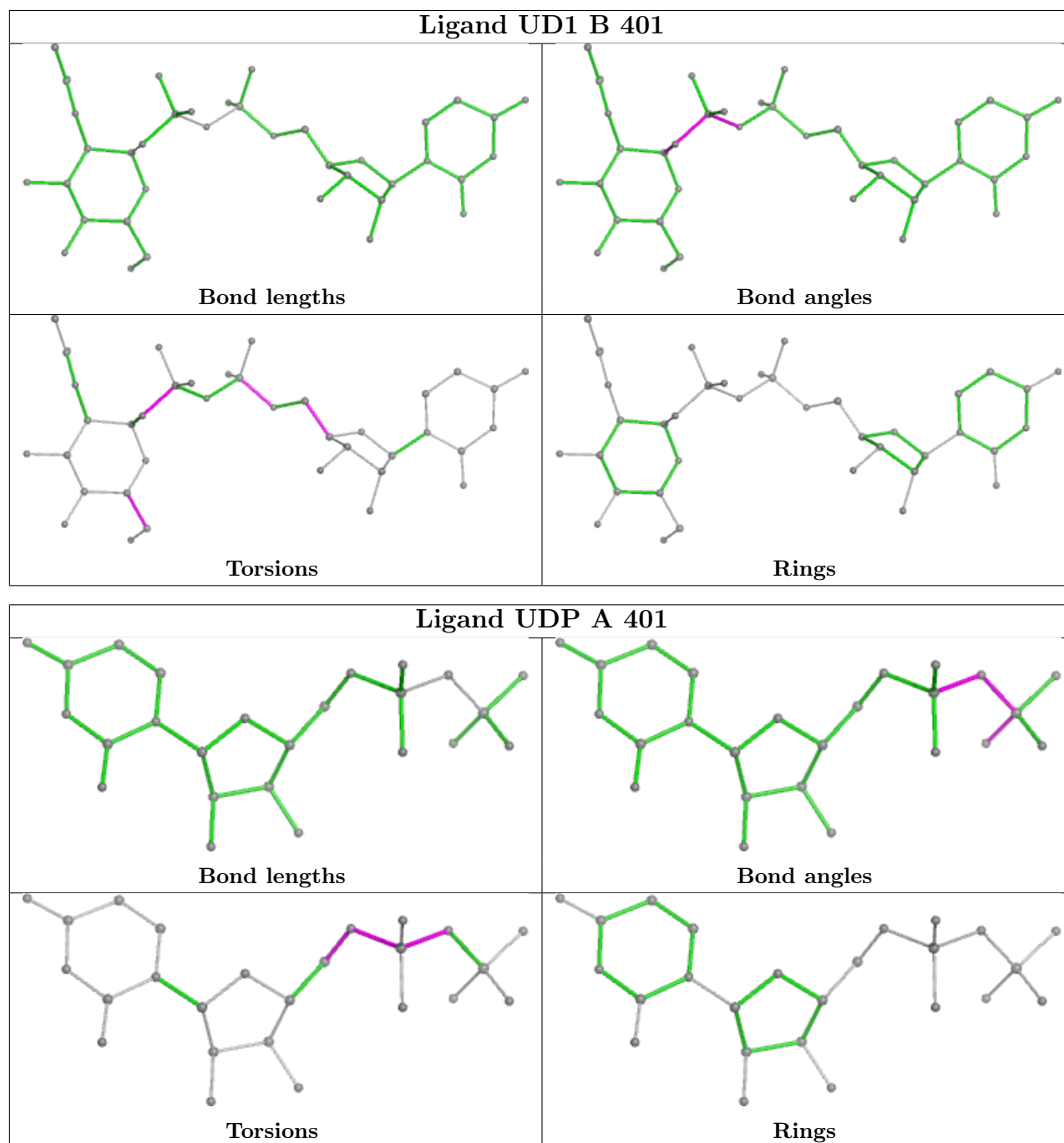
There are no ring outliers.

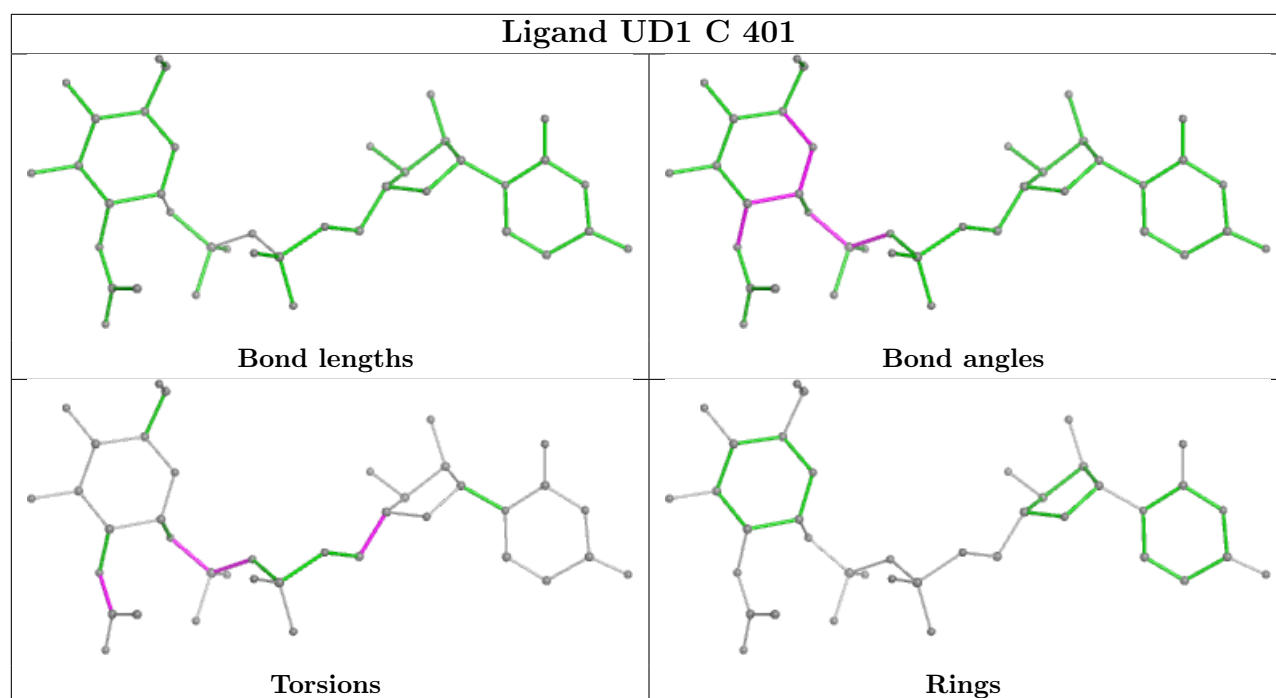
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	UD1	2	0
6	B	402	EPE	2	0
6	C	403	EPE	2	0
2	A	401	UDP	1	0
4	A	403	GOL	2	0
5	C	401	UD1	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/337 (99%)	0.25	17 (5%) 34 32	36, 48, 77, 92	0
1	B	335/337 (99%)	0.02	6 (1%) 67 63	34, 46, 68, 80	0
1	C	336/337 (99%)	-0.00	4 (1%) 76 73	34, 45, 65, 79	0
1	D	335/337 (99%)	-0.03	5 (1%) 71 68	36, 46, 62, 88	0
All	All	1340/1348 (99%)	0.06	32 (2%) 59 56	34, 46, 69, 92	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	PHE	5.1
1	A	184	VAL	4.2
1	A	162	PHE	3.5
1	A	155	ASP	3.3
1	A	198	ALA	3.2
1	A	113	LEU	3.0
1	A	112	TYR	2.9
1	A	13	PHE	2.9
1	A	45	ASP	2.9
1	C	284	ASP	2.9
1	A	1	LEU	2.8
1	C	240	TRP	2.7
1	A	183	LEU	2.6
1	C	162	PHE	2.6
1	A	240	TRP	2.5
1	A	205	PRO	2.3
1	D	14	GLN	2.3
1	D	157	TYR	2.3
1	B	180	LYS	2.2
1	B	240	TRP	2.2
1	A	181	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	184	VAL	2.2
1	A	238	SER	2.2
1	B	162	PHE	2.2
1	B	177	ASN	2.2
1	B	179	GLU	2.2
1	D	162	PHE	2.1
1	D	0	HIS	2.1
1	A	199	LYS	2.1
1	B	159	SER	2.1
1	A	177	ASN	2.1
1	A	108	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

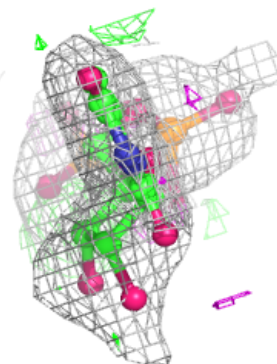
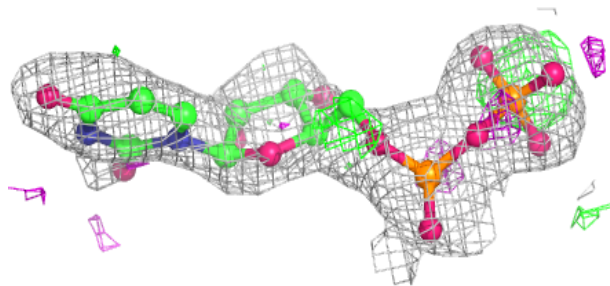
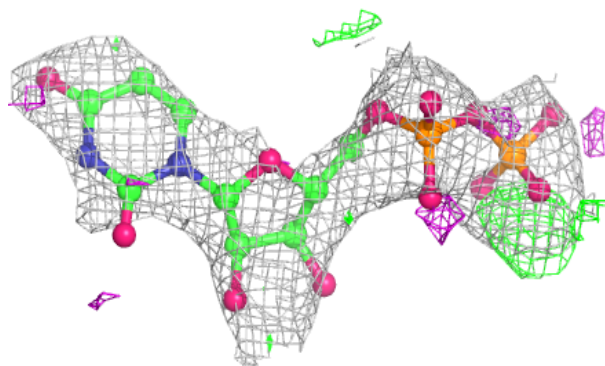
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EPE	B	402	15/15	0.58	0.20	52,65,102,111	0
3	CIT	A	402	13/13	0.65	0.15	53,58,65,66	0
6	EPE	C	403	15/15	0.65	0.20	65,68,98,111	0
4	GOL	A	403	6/6	0.74	0.24	56,60,61,64	0
4	GOL	C	402	6/6	0.74	0.17	64,67,70,70	0
2	UDP	A	401	25/25	0.79	0.17	53,63,66,68	25
5	UD1	C	401	39/39	0.87	0.14	43,51,60,61	39
5	UD1	B	401	39/39	0.91	0.12	42,47,53,55	39

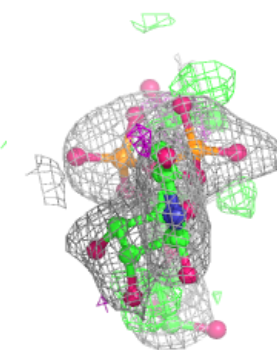
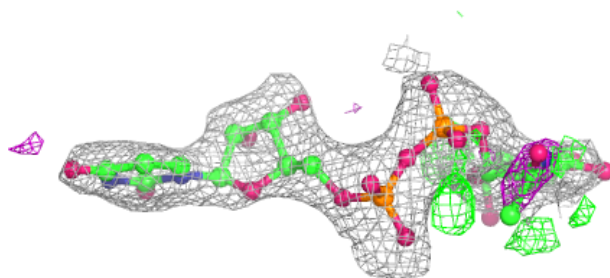
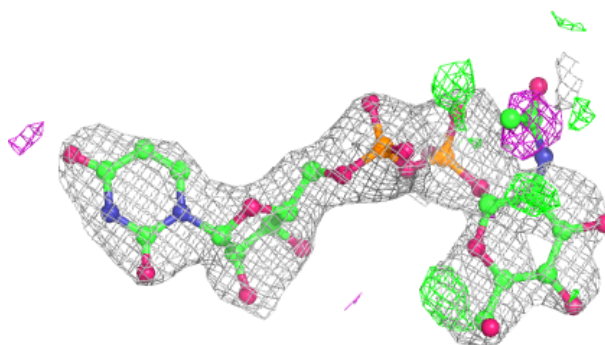
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

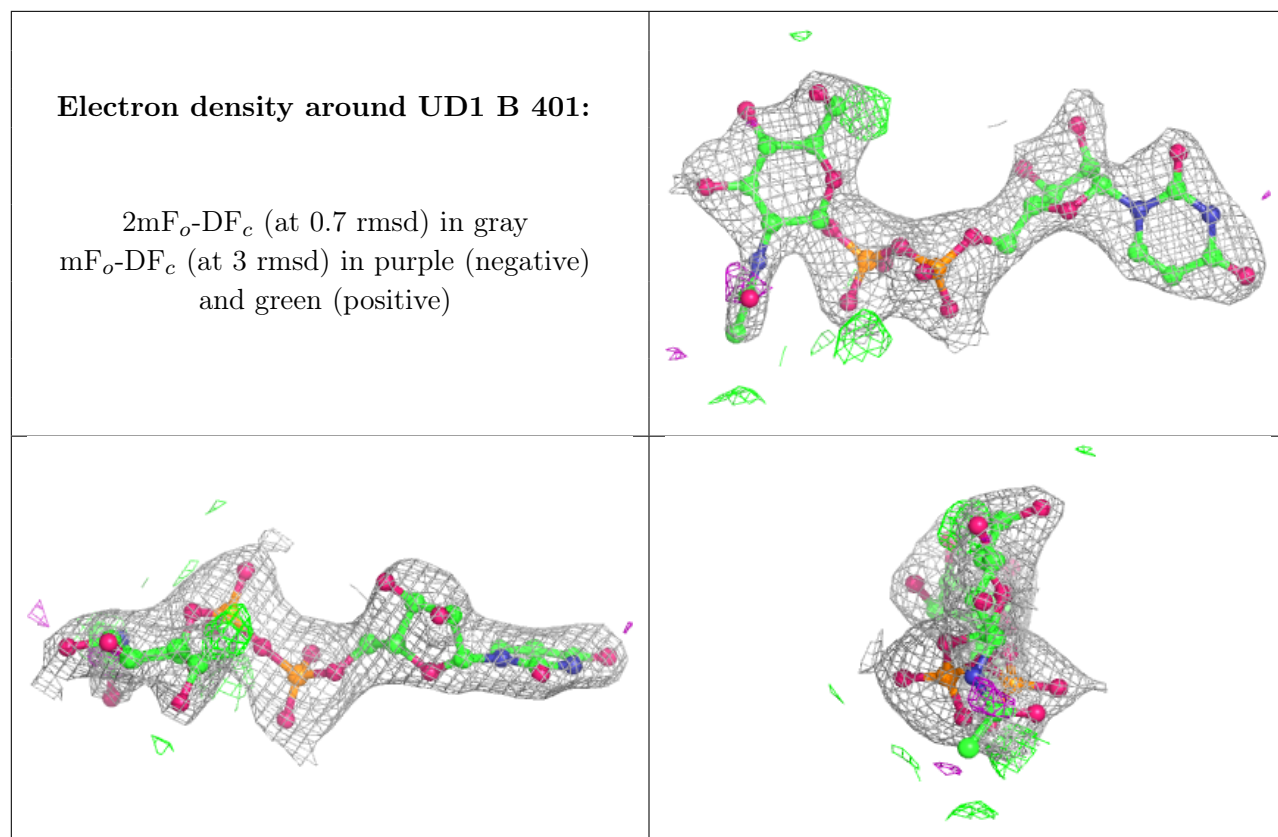
**Electron density around UDP A 401:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.