Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2025 – 01:08 pm BST

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:

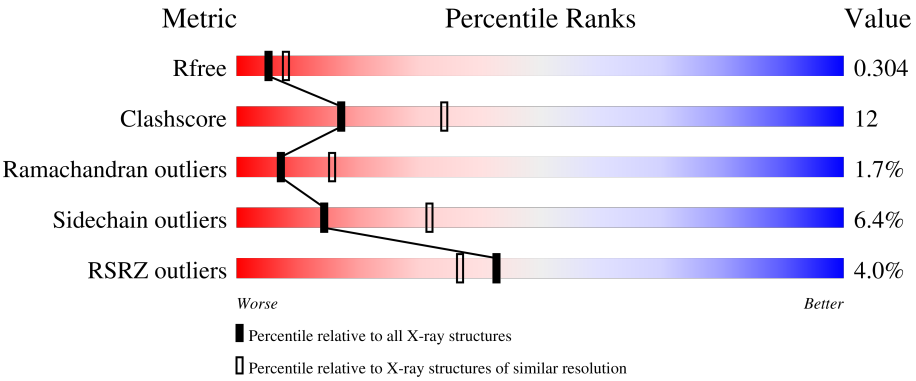
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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 <=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	67% 26% • 5%
1	B	354	4% 64% 25% • 9%
1	C	354	71% 22% • 5%
1	D	354	9% 51% 38% 5% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10767 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	335	Total	C	N	O	S	0	1	0
			2720	1756	452	505	7			
1	B	322	Total	C	N	O	S	0	0	0
			2576	1662	429	480	5			
1	C	335	Total	C	N	O	S	0	0	0
			2704	1744	449	504	7			
1	D	330	Total	C	N	O	S	0	0	0
			2638	1699	441	491	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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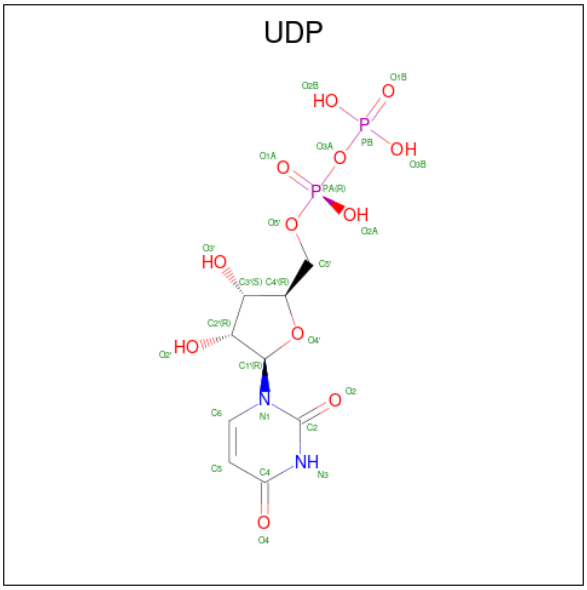
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP B3XPQ7
D	-18	GLY	-	expression tag	UNP B3XPQ7
D	-17	SER	-	expression tag	UNP B3XPQ7
D	-16	SER	-	expression tag	UNP B3XPQ7
D	-15	HIS	-	expression tag	UNP B3XPQ7
D	-14	HIS	-	expression tag	UNP B3XPQ7
D	-13	HIS	-	expression 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	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is water.

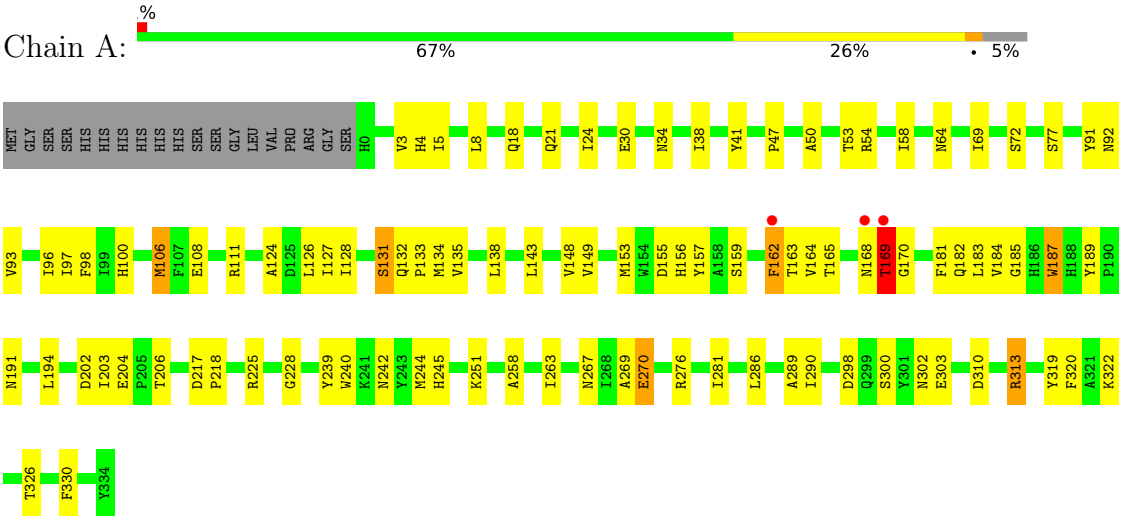
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	11	Total	O	0	0
			11	11		
3	C	28	Total	O	0	0
			28	28		
3	D	4	Total	O	0	0
			4	4		

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.

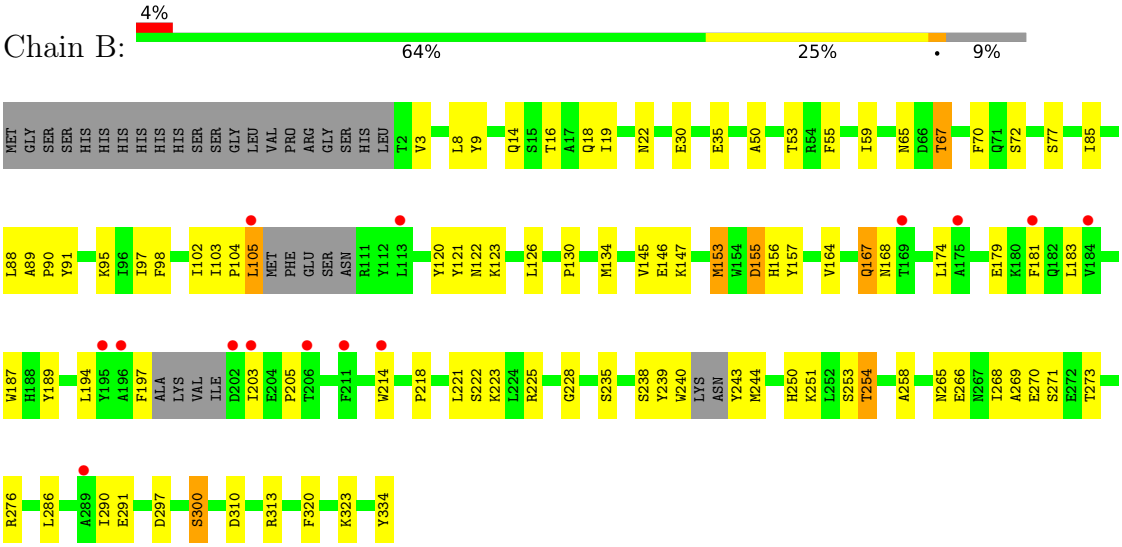
• Molecule 1: Glucosyltransferase 3

Chain A:



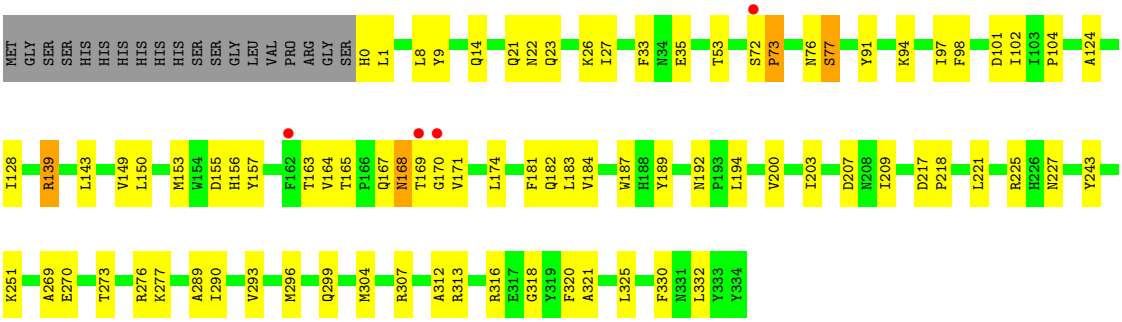
• Molecule 1: Glucosyltransferase 3

Chain B:

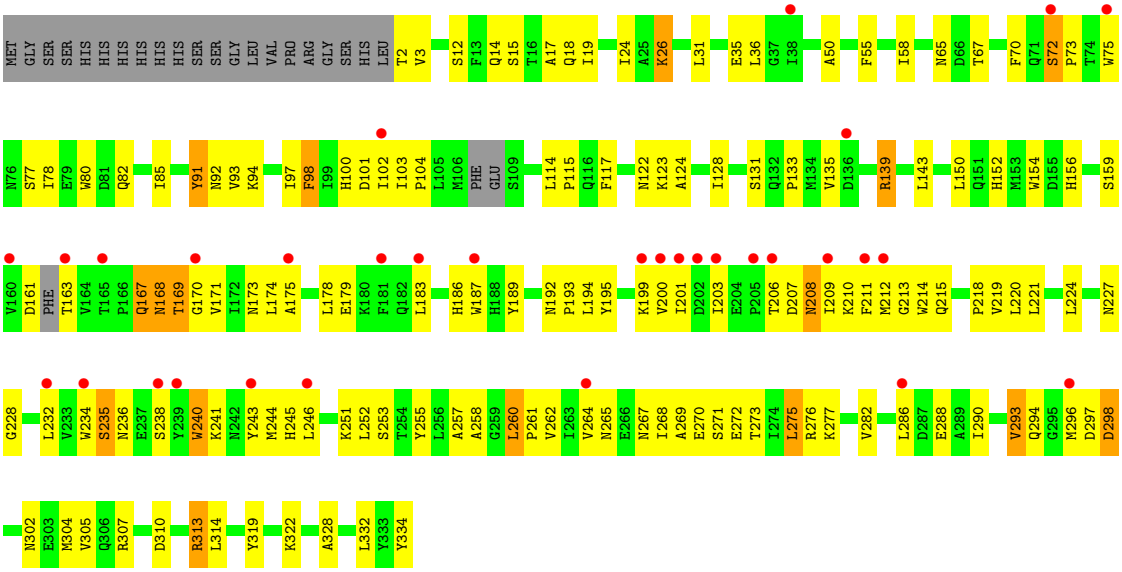


• Molecule 1: Glucosyltransferase 3

Chain C:



- Molecule 1: Glucosyltransferase 3



4 Data and refinement statistics (i)

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)	70.14 – 2.60 70.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.14-2.60) 87.0 (70.14-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.230 , 0.308 0.230 , 0.304	Depositor DCC
R_{free} test set	2170 reflections (4.89%)	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)	0.33 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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	0.93	EDS
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/2795	0.61	0/3809
1	B	0.44	0/2644	0.62	0/3604
1	C	0.46	0/2777	0.67	0/3785
1	D	0.40	0/2705	0.63	0/3684
All	All	0.43	0/10921	0.64	0/14882

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

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	2720	0	2627	59	0
1	B	2576	0	2453	56	0
1	C	2704	0	2614	61	0
1	D	2638	0	2547	98	0
2	A	25	0	11	1	0
2	B	25	0	11	3	0
2	C	25	0	11	1	0
3	A	11	0	0	3	0
3	B	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	0	8	0
3	D	4	0	0	1	0
All	All	10767	0	10274	261	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 12.

All (261) 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	2.03	0.90
1:C:153:MET:O	3:C:501:HOH:O	1.90	0.88
1:C:23:GLN:HE22	1:C:157:TYR:H	1.20	0.86
1:B:103:ILE:HG13	1:B:104:PRO:HD3	1.59	0.85
1:D:173:ASN:ND2	1:D:228:GLY:O	2.12	0.83
1:B:155:ASP:OD1	3:B:501:HOH:O	1.99	0.81
1:C:168:ASN:O	1:C:170:GLY:N	2.15	0.79
1:D:215:GLN:HB3	1:D:219:VAL:HG23	1.62	0.79
1:A:153:MET:O	3:A:501:HOH:O	2.02	0.78
1:D:72:SER:HB3	1:D:100:HIS:H	1.54	0.73
1:B:14:GLN:HG2	1:B:214:TRP:CE2	2.24	0.72
1:D:199:LYS:HG2	1:D:214:TRP:H	1.52	0.72
1:D:232:LEU:HD21	1:D:234:TRP:HD1	1.55	0.72
1:C:168:ASN:HD22	1:C:171:VAL:HB	1.54	0.72
1:D:220:LEU:HD22	1:D:221:LEU:HD12	1.71	0.71
1:A:310:ASP:OD1	1:A:313:ARG:NH1	2.23	0.71
1:D:194:LEU:HD22	1:D:209:ILE:HD12	1.73	0.70
1:A:185:GLY:HA2	1:A:204:GLU:HG3	1.72	0.70
1:A:298:ASP:O	1:A:302:ASN:ND2	2.22	0.70
1:D:168:ASN:O	1:D:170:GLY:N	2.25	0.70
1:C:22:ASN:O	1:C:26:LYS:HG2	1.92	0.70
1:D:236:ASN:HB3	1:D:240:TRP:HB3	1.73	0.69
1:D:2:THR:N	3:D:401:HOH:O	2.25	0.69
1:D:168:ASN:ND2	1:D:227:ASN:O	2.25	0.69
1:C:0:HIS:NE2	3:C:505:HOH:O	2.26	0.68
1:A:69:ILE:HG22	1:A:96:ILE:HB	1.76	0.67
1:C:207:ASP:OD1	3:C:502:HOH:O	2.12	0.67
1:D:72:SER:CB	1:D:100:HIS:H	2.07	0.67
1:D:175:ALA:O	1:D:251:LYS:NZ	2.27	0.67
1:C:97:ILE:HD12	1:C:124:ALA:HB2	1.75	0.66
1:A:5:ILE:HD12	1:A:69:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	3:C:503:HOH:O	2.12	0.66
1:C:182:GLN:N	3:C:504:HOH:O	2.28	0.66
1:C:184:VAL:HG22	1:C:203:ILE:HG22	1.78	0.66
1:D:234:TRP:HE3	1:D:235:SER:H	1.44	0.65
1:A:239:TYR:O	3:A:502:HOH:O	2.15	0.65
1:D:212:MET:SD	1:D:213:GLY:N	2.70	0.65
1:C:168:ASN:ND2	1:C:227:ASN:O	2.30	0.64
1:B:197:PHE:HE2	1:B:223:LYS:HD2	1.61	0.64
1:B:130:PRO:HD2	1:B:134:MET:HG2	1.79	0.64
1:B:250:HIS:ND1	2:B:401:UDP:O3'	2.26	0.64
1:D:26:LYS:NZ	1:D:35:GLU:OE1	2.30	0.63
1:D:224:LEU:HD22	1:D:260:LEU:HD21	1.80	0.63
1:B:156:HIS:CE1	1:B:254:THR:HB	2.34	0.62
1:D:161:ASP:O	1:D:163:THR:N	2.32	0.62
1:D:310:ASP:O	1:D:313:ARG:HD3	1.99	0.62
1:B:9:TYR:OH	1:B:35:GLU:OE2	2.17	0.62
1:A:251:LYS:NZ	2:A:401:UDP:O1A	2.32	0.61
1:C:156:HIS:NE2	1:C:217:ASP:OD1	2.30	0.61
1:C:167:GLN:NE2	1:C:296:MET:HB3	2.15	0.61
1:D:183:LEU:HA	1:D:186:HIS:CD2	2.36	0.61
1:D:236:ASN:HB3	1:D:240:TRP:CB	2.31	0.60
1:A:106:MET:HB3	1:A:240:TRP:HZ3	1.66	0.60
1:D:183:LEU:HD21	1:D:187:TRP:CE3	2.37	0.59
1:C:23:GLN:HE22	1:C:157:TYR:N	1.97	0.59
1:A:276:ARG:NH1	1:D:334:TYR:OXT	2.35	0.58
1:B:55:PHE:O	1:B:59:ILE:HG12	2.04	0.58
1:A:50:ALA:HB1	1:B:53:THR:HG21	1.84	0.58
1:D:193:PRO:HG2	1:D:195:TYR:HE1	1.68	0.58
1:C:33:PHE:HE2	1:C:325:LEU:HD13	1.69	0.58
1:B:126:LEU:HD12	1:B:147:LYS:HB3	1.86	0.57
1:D:199:LYS:HB2	1:D:214:TRP:HB2	1.86	0.57
1:D:174:LEU:HD13	1:D:175:ALA:N	2.20	0.57
1:A:242:ASN:O	1:A:245:HIS:HB2	2.05	0.57
1:A:225:ARG:NH1	1:A:258:ALA:O	2.31	0.57
1:D:3:VAL:HG22	1:D:67:THR:HB	1.87	0.57
1:B:18:GLN:HE21	1:B:22:ASN:HD21	1.53	0.56
1:B:240:TRP:O	1:B:243:TYR:N	2.38	0.56
1:C:221:LEU:O	1:C:225:ARG:HG2	2.05	0.56
1:A:156:HIS:NE2	1:A:217:ASP:OD1	2.38	0.56
1:D:245:HIS:NE2	1:D:267:ASN:HB2	2.21	0.56
1:D:235:SER:HA	1:D:244:MET:SD	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:CZ3	1:A:286:LEU:HD22	2.40	0.55
1:A:322:LYS:O	1:A:326:THR:HG23	2.07	0.55
1:D:200:VAL:HG13	1:D:201:ILE:HG12	1.88	0.55
1:B:334:TYR:OXT	1:C:276:ARG:NH1	2.39	0.55
1:D:271:SER:O	1:D:275:LEU:HD23	2.07	0.54
1:A:91:TYR:O	1:A:93:VAL:N	2.41	0.54
1:B:181:PHE:HB3	1:B:235:SER:HA	1.88	0.54
1:B:313:ARG:NE	1:C:1:LEU:HB2	2.22	0.54
1:D:252:LEU:HD12	1:D:262:VAL:HG11	1.89	0.54
1:D:183:LEU:HA	1:D:186:HIS:HD2	1.72	0.54
1:D:78:ILE:HD12	1:D:117:PHE:CD1	2.44	0.53
1:D:277:LYS:O	1:D:307:ARG:HD2	2.08	0.53
1:A:245:HIS:CE1	1:A:267:ASN:HB3	2.44	0.53
1:C:312:ALA:O	1:C:316:ARG:HG3	2.09	0.53
1:D:194:LEU:HB3	1:D:209:ILE:HB	1.90	0.52
1:A:135:VAL:HG21	1:A:148:VAL:HG11	1.91	0.52
1:A:108:GLU:HG3	1:A:239:TYR:CE1	2.43	0.52
1:B:14:GLN:HG2	1:B:214:TRP:CZ2	2.45	0.52
1:C:102:ILE:HG22	1:C:104:PRO:HD2	1.91	0.52
1:A:263:ILE:HG21	1:A:289:ALA:HB1	1.92	0.51
1:D:15:SER:HB3	1:D:18:GLN:HB3	1.91	0.51
1:A:181:PHE:O	1:A:183:LEU:N	2.43	0.51
1:B:251:LYS:NZ	2:B:401:UDP:O3B	2.43	0.51
1:B:273:THR:OG1	1:B:276:ARG:NH1	2.43	0.51
1:B:286:LEU:HD12	1:B:286:LEU:H	1.76	0.51
1:B:187:TRP:CE2	1:B:194:LEU:HB2	2.45	0.51
1:B:95:LYS:HE2	1:B:123:LYS:O	2.11	0.51
1:D:290:ILE:HA	1:D:293:VAL:HG13	1.93	0.51
1:C:8:LEU:HB2	1:C:21:GLN:OE1	2.11	0.50
1:C:189:TYR:CD1	1:C:290:ILE:HG21	2.46	0.50
1:A:218:PRO:HB2	1:C:218:PRO:HB2	1.93	0.50
1:C:139:ARG:HG2	1:C:143:LEU:HD23	1.92	0.50
1:A:240:TRP:O	1:A:244:MET:HG3	2.12	0.50
1:D:70:PHE:CZ	1:D:85:ILE:HG13	2.47	0.50
1:D:273:THR:HG22	1:D:276:ARG:HH21	1.77	0.50
1:A:38:ILE:HD12	1:A:58:ILE:HD13	1.93	0.50
1:A:153:MET:HB2	1:A:320:PHE:CE1	2.46	0.50
1:A:330:PHE:HA	1:D:314:LEU:HD21	1.93	0.50
1:B:244:MET:O	1:B:268:ILE:HG13	2.12	0.50
1:D:169:THR:HG22	1:D:169:THR:O	2.12	0.50
1:A:269:ALA:O	1:A:270:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ASP:HB3	1:C:209:ILE:HG13	1.93	0.49
1:B:122:ASN:HA	1:B:145:VAL:HG23	1.93	0.49
1:D:78:ILE:CD1	1:D:117:PHE:HA	2.43	0.49
1:C:76:ASN:O	1:C:77:SER:HB3	2.12	0.49
1:D:72:SER:HB2	1:D:73:PRO:HD3	1.94	0.49
1:B:97:ILE:HD13	1:B:120:TYR:CE2	2.47	0.49
1:A:128:ILE:HA	1:A:149:VAL:O	2.12	0.48
1:D:243:TYR:HA	1:D:246:LEU:HD13	1.95	0.48
1:B:253:SER:OG	3:B:502:HOH:O	2.20	0.48
1:A:189:TYR:CD1	1:A:290:ILE:HG21	2.49	0.48
1:B:269:ALA:O	1:B:270:GLU:HB2	2.14	0.48
1:B:65:ASN:O	1:C:313:ARG:NH1	2.37	0.48
1:A:131:SER:O	1:A:134:MET:HB3	2.14	0.48
1:B:189:TYR:CE1	1:B:290:ILE:HD12	2.49	0.48
1:A:187:TRP:HZ3	1:A:286:LEU:HD22	1.77	0.48
1:A:187:TRP:CD1	1:A:194:LEU:HB2	2.49	0.47
1:C:23:GLN:NE2	1:C:157:TYR:H	1.99	0.47
1:D:91:TYR:O	1:D:93:VAL:N	2.46	0.47
1:D:192:ASN:HD22	1:D:290:ILE:HG22	1.78	0.47
1:A:240:TRP:HE1	1:A:244:MET:HE2	1.79	0.47
1:C:304:MET:HB2	1:C:307:ARG:NH2	2.30	0.47
1:A:53:THR:HG21	1:B:50:ALA:HB1	1.96	0.47
1:B:59:ILE:HG21	1:B:88:LEU:HD21	1.95	0.47
1:C:164:VAL:HG12	1:C:165:THR:H	1.78	0.47
1:D:12:SER:O	1:D:14:GLN:N	2.47	0.47
1:B:297:ASP:OD1	1:B:300:SER:HB2	2.14	0.47
1:C:76:ASN:N	3:C:513:HOH:O	2.48	0.47
1:D:199:LYS:H	1:D:214:TRP:HE3	1.62	0.47
1:B:203:ILE:O	1:B:205:PRO:HD3	2.14	0.47
1:D:55:PHE:HE1	1:D:80:TRP:CZ2	2.33	0.47
1:C:187:TRP:O	1:C:207:ASP:HA	2.15	0.46
1:C:251:LYS:HG3	2:C:401:UDP:O2B	2.15	0.46
1:D:221:LEU:HG	1:D:258:ALA:HB2	1.97	0.46
1:D:179:GLU:HG2	1:D:203:ILE:HD11	1.97	0.46
1:C:8:LEU:HD23	1:C:9:TYR:N	2.31	0.46
1:D:102:ILE:HG22	1:D:104:PRO:HD2	1.98	0.46
1:C:164:VAL:HG12	1:C:165:THR:N	2.30	0.46
1:D:19:ILE:HD12	1:D:19:ILE:HA	1.88	0.46
1:D:224:LEU:HD23	1:D:224:LEU:HA	1.74	0.46
1:D:82:GLN:OE1	1:D:123:LYS:HE3	2.16	0.45
1:A:8:LEU:HB2	1:A:21:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:HB3	1:C:332:LEU:HD13	1.99	0.45
1:D:171:VAL:HG13	1:D:195:TYR:CD1	2.51	0.45
1:B:225:ARG:NH1	1:B:258:ALA:O	2.50	0.45
1:B:251:LYS:HZ3	2:B:401:UDP:PB	2.39	0.45
1:D:94:LYS:HB3	1:D:332:LEU:HD21	1.98	0.45
1:D:302:ASN:HA	1:D:305:VAL:HG22	1.99	0.45
1:A:5:ILE:CD1	1:A:69:ILE:HD11	2.47	0.45
1:A:96:ILE:HG23	1:A:126:LEU:HD23	1.98	0.45
1:C:156:HIS:O	1:C:316:ARG:HA	2.16	0.45
1:D:24:ILE:HG21	1:D:98:PHE:CE2	2.51	0.45
1:D:319:TYR:HA	1:D:322:LYS:HB2	1.99	0.45
1:D:131:SER:OG	1:D:133:PRO:HD2	2.17	0.45
1:D:156:HIS:HB3	1:D:257:ALA:HB2	1.99	0.45
1:D:270:GLU:O	1:D:273:THR:N	2.48	0.45
1:B:103:ILE:O	1:B:105:LEU:HG	2.17	0.45
1:C:53:THR:HG21	1:D:50:ALA:HB1	1.98	0.45
1:C:189:TYR:HB3	1:C:192:ASN:HB2	1.99	0.45
1:C:101:ASP:OD1	1:C:243:TYR:OH	2.27	0.44
1:D:78:ILE:HD11	1:D:117:PHE:HA	2.00	0.44
1:A:169:THR:O	1:A:170:GLY:C	2.56	0.44
1:D:17:ALA:HB2	1:D:75:TRP:CZ2	2.53	0.44
1:D:272:GLU:H	1:D:272:GLU:CD	2.21	0.44
1:A:5:ILE:HD11	1:A:24:ILE:HG22	1.99	0.44
1:C:73:PRO:HD3	1:C:101:ASP:H	1.83	0.44
1:C:170:GLY:HA2	1:C:192:ASN:OD1	2.18	0.44
1:D:187:TRP:HA	1:D:189:TYR:CE2	2.53	0.44
1:A:155:ASP:OD1	1:A:320:PHE:HB2	2.18	0.44
1:D:286:LEU:H	1:D:286:LEU:HD23	1.82	0.44
1:D:73:PRO:HB2	1:D:75:TRP:HD1	1.83	0.44
1:D:91:TYR:H	1:D:91:TYR:HD1	1.62	0.44
1:D:268:ILE:HG22	1:D:269:ALA:O	2.18	0.44
1:B:221:LEU:HD23	1:B:258:ALA:HB2	2.00	0.44
1:C:128:ILE:HA	1:C:149:VAL:O	2.18	0.44
1:D:78:ILE:HD12	1:D:117:PHE:CG	2.52	0.44
1:A:30:GLU:OE1	1:A:157:TYR:OH	2.36	0.43
1:A:41:TYR:OH	1:A:54:ARG:NE	2.50	0.43
1:B:85:ILE:HD11	1:B:95:LYS:HD2	2.00	0.43
1:B:265:ASN:OD1	1:B:266:GLU:N	2.52	0.43
1:C:128:ILE:HG12	1:C:149:VAL:HB	2.00	0.43
1:C:183:LEU:N	3:C:508:HOH:O	2.36	0.43
1:D:97:ILE:HD12	1:D:124:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LYS:CG	1:D:214:TRP:H	2.24	0.43
1:D:91:TYR:O	1:D:93:VAL:HG13	2.18	0.43
1:D:261:PRO:HD3	1:D:305:VAL:HG12	2.00	0.43
1:C:27:ILE:HD13	1:C:321:ALA:HB3	2.01	0.43
1:A:138:LEU:HB3	1:A:143:LEU:HB2	2.01	0.43
1:A:168:ASN:O	1:A:170:GLY:N	2.52	0.43
1:B:218:PRO:HB2	1:D:218:PRO:HB3	2.00	0.43
1:B:286:LEU:O	1:B:290:ILE:HG13	2.18	0.43
1:C:168:ASN:O	1:C:171:VAL:N	2.49	0.43
1:C:187:TRP:NE1	1:C:194:LEU:HB2	2.34	0.43
1:D:31:LEU:HD13	1:D:31:LEU:HA	1.85	0.43
1:D:36:LEU:HD22	1:D:58:ILE:O	2.19	0.43
1:D:167:GLN:O	1:D:169:THR:N	2.51	0.43
1:B:189:TYR:CZ	1:B:290:ILE:HD12	2.54	0.43
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.79	0.43
1:B:181:PHE:CG	1:B:235:SER:HB2	2.54	0.43
1:C:174:LEU:HB2	1:C:194:LEU:HD11	2.01	0.43
1:D:150:LEU:HD12	1:D:150:LEU:H	1.84	0.43
1:C:155:ASP:OD2	1:C:320:PHE:HB2	2.18	0.43
1:C:8:LEU:HD12	1:C:21:GLN:NE2	2.34	0.42
1:A:4:HIS:ND1	1:A:34:ASN:HB3	2.34	0.42
1:A:18:GLN:HB3	3:A:506:HOH:O	2.18	0.42
1:B:174:LEU:HB2	1:B:194:LEU:HD21	1.99	0.42
1:C:269:ALA:O	1:C:270:GLU:HB2	2.18	0.42
1:A:97:ILE:HD12	1:A:124:ALA:HB2	2.01	0.42
1:D:261:PRO:HB3	1:D:304:MET:HG2	2.01	0.42
1:B:70:PHE:CZ	1:B:85:ILE:HG13	2.54	0.42
1:B:102:ILE:HD13	1:B:121:TYR:HE2	1.84	0.42
1:C:277:LYS:NZ	3:C:512:HOH:O	2.48	0.42
1:D:187:TRP:CE2	1:D:194:LEU:HB2	2.55	0.42
1:D:207:ASP:HB3	1:D:208:ASN:H	1.71	0.41
1:D:232:LEU:HD21	1:D:234:TRP:CD1	2.45	0.41
1:B:8:LEU:HD12	1:B:9:TYR:H	1.85	0.41
1:B:323:LYS:HE3	1:C:330:PHE:CE2	2.56	0.41
1:C:164:VAL:CG1	1:C:165:THR:H	2.33	0.41
1:A:165:THR:O	1:A:165:THR:OG1	2.32	0.41
1:A:184:VAL:HG22	1:A:203:ILE:HG22	2.03	0.41
1:A:187:TRP:NE1	1:A:194:LEU:HB2	2.34	0.41
1:B:155:ASP:OD2	1:B:320:PHE:HB2	2.20	0.41
1:D:174:LEU:HD22	1:D:255:TYR:OH	2.19	0.41
1:B:167:GLN:H	1:B:167:GLN:HG2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TRP:NE1	1:B:194:LEU:HB2	2.35	0.41
1:C:155:ASP:HB3	1:C:318:GLY:HA2	2.03	0.41
1:D:65:ASN:HA	1:D:92:ASN:O	2.20	0.41
1:D:114:LEU:HB3	1:D:115:PRO:HD3	2.02	0.41
1:D:135:VAL:O	1:D:139:ARG:HG3	2.21	0.41
1:B:89:ALA:O	1:B:91:TYR:N	2.54	0.41
1:D:154:TRP:HB2	1:D:253:SER:OG	2.21	0.41
1:A:97:ILE:HB	1:A:127:ILE:HD13	2.02	0.41
1:B:323:LYS:HE3	1:C:330:PHE:CD2	2.56	0.41
1:D:264:VAL:HG23	1:D:268:ILE:HD12	2.03	0.41
1:D:273:THR:CG2	1:D:276:ARG:HH21	2.33	0.41
1:B:3:VAL:HG13	1:B:67:THR:HB	2.02	0.40
1:A:263:ILE:HG23	1:A:281:ILE:HB	2.02	0.40
1:A:319:TYR:HA	1:A:322:LYS:HB2	2.03	0.40
1:D:128:ILE:HD11	1:D:328:ALA:CB	2.51	0.40
1:A:300:SER:HA	1:A:303:GLU:HB2	2.03	0.40
1:B:153:MET:HG3	1:B:320:PHE:CE1	2.56	0.40
1:C:289:ALA:O	1:C:293:VAL:HG23	2.21	0.40
1:D:103:ILE:HB	1:D:117:PHE:CZ	2.56	0.40
1:B:30:GLU:OE2	1:B:157:TYR:OH	2.39	0.40
1:D:122:ASN:OD1	1:D:143:LEU:HD12	2.21	0.40
1:A:21:GLN:HG2	1:A:100:HIS:NE2	2.36	0.40
1:A:132:GLN:N	1:A:133:PRO:HD2	2.37	0.40
1:A:162:PHE:CD2	1:A:163:THR:N	2.89	0.40
1:C:9:TYR:OH	1:C:35:GLU:OE2	2.26	0.40

There are no symmetry-related clashes.

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	334/354 (94%)	317 (95%)	10 (3%)	7 (2%)	5 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	314/354 (89%)	289 (92%)	21 (7%)	4 (1%)	10 21
1	C	333/354 (94%)	304 (91%)	26 (8%)	3 (1%)	14 31
1	D	324/354 (92%)	287 (89%)	29 (9%)	8 (2%)	4 8
All	All	1305/1416 (92%)	1197 (92%)	86 (7%)	22 (2%)	7 16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PHE
1	A	228	GLY
1	A	270	GLU
1	B	77	SER
1	C	77	SER
1	C	169	THR
1	D	152	HIS
1	D	169	THR
1	D	298	ASP
1	A	77	SER
1	A	92	ASN
1	A	182	GLN
1	D	72	SER
1	B	168	ASN
1	A	169	THR
1	D	168	ASN
1	D	77	SER
1	D	167	GLN
1	D	238	SER
1	B	90	PRO
1	C	200	VAL
1	B	228	GLY

5.3.2 Protein sidechains (i)

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	293/309 (95%)	277 (94%)	16 (6%)	18 38
1	B	271/309 (88%)	250 (92%)	21 (8%)	10 22
1	C	291/309 (94%)	280 (96%)	11 (4%)	28 54
1	D	281/309 (91%)	256 (91%)	25 (9%)	8 17
All	All	1136/1236 (92%)	1063 (94%)	73 (6%)	14 32

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	47	PRO
1	A	64	ASN
1	A	72	SER
1	A	98	PHE
1	A	106	MET
1	A	111	ARG
1	A	131	SER
1	A	159	SER
1	A	164	VAL
1	A	169	THR
1	A	187	TRP
1	A	191	ASN
1	A	202	ASP
1	A	206	THR
1	A	313	ARG
1	B	16	THR
1	B	19	ILE
1	B	67	THR
1	B	72	SER
1	B	98	PHE
1	B	105	LEU
1	B	146	GLU
1	B	153	MET
1	B	155	ASP
1	B	164	VAL
1	B	167	GLN
1	B	179	GLU
1	B	183	LEU
1	B	222	SER
1	B	238	SER
1	B	239	TYR
1	B	254	THR

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Mol	Chain	Res	Type
1	B	271	SER
1	B	291	GLU
1	B	300	SER
1	B	310	ASP
1	C	14	GLN
1	C	72	SER
1	C	73	PRO
1	C	91	TYR
1	C	98	PHE
1	C	139	ARG
1	C	163	THR
1	C	168	ASN
1	C	181	PHE
1	C	273	THR
1	C	299	GLN
1	D	26	LYS
1	D	91	TYR
1	D	98	PHE
1	D	101	ASP
1	D	139	ARG
1	D	159	SER
1	D	178	LEU
1	D	206	THR
1	D	208	ASN
1	D	210	LYS
1	D	211	PHE
1	D	235	SER
1	D	240	TRP
1	D	241	LYS
1	D	260	LEU
1	D	265	ASN
1	D	275	LEU
1	D	282	VAL
1	D	288	GLU
1	D	293	VAL
1	D	294	GLN
1	D	296	MET
1	D	297	ASP
1	D	298	ASP
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	B	23	GLN
1	B	182	GLN
1	C	23	GLN
1	C	168	ASN
1	D	132	GLN
1	D	186	HIS
1	D	285	ASN
1	D	294	GLN

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)

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	C	401	-	24,26,26	0.31	0	37,40,40	0.53	0
2	UDP	B	401	-	24,26,26	0.25	0	37,40,40	0.59	1 (2%)
2	UDP	A	401	-	24,26,26	0.23	0	37,40,40	0.60	1 (2%)

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	C	401	-	-	2/16/32/32	0/2/2/2
2	UDP	B	401	-	-	4/16/32/32	0/2/2/2
2	UDP	A	401	-	-	4/16/32/32	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	UDP	PA-O3A-PB	-2.72	123.50	132.83
2	B	401	UDP	PA-O3A-PB	-2.58	123.98	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	UDP	C5'-O5'-PA-O1A
2	A	401	UDP	PA-O3A-PB-O2B
2	B	401	UDP	C3'-C4'-C5'-O5'
2	B	401	UDP	PA-O3A-PB-O3B
2	B	401	UDP	O4'-C4'-C5'-O5'
2	A	401	UDP	PA-O3A-PB-O3B
2	C	401	UDP	C3'-C4'-C5'-O5'
2	C	401	UDP	PA-O3A-PB-O1B
2	B	401	UDP	PA-O3A-PB-O1B
2	A	401	UDP	PA-O3A-PB-O1B

There are no ring outliers.

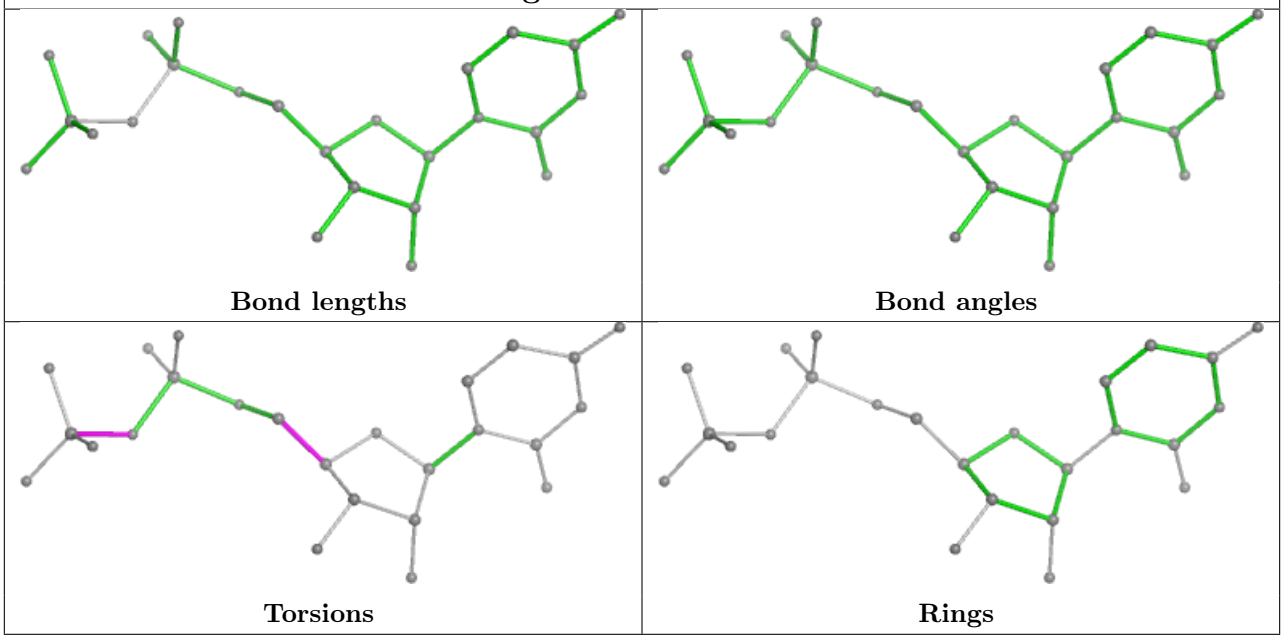
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	UDP	1	0
2	B	401	UDP	3	0
2	A	401	UDP	1	0

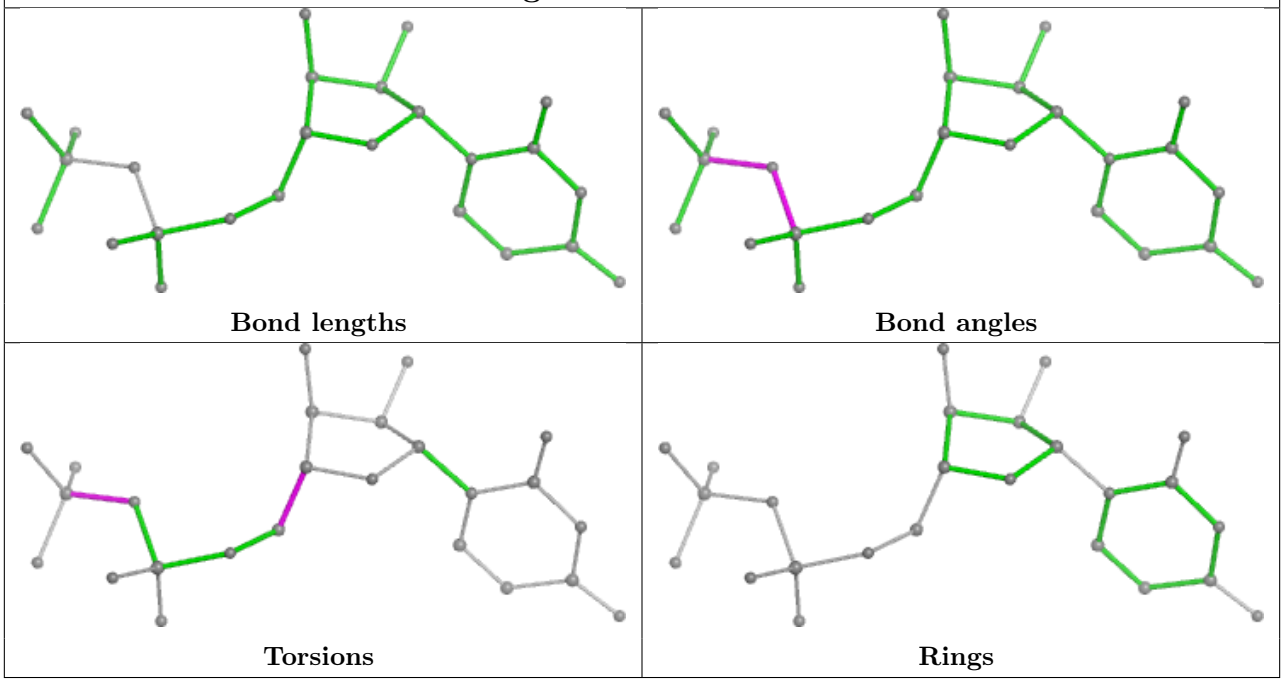
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

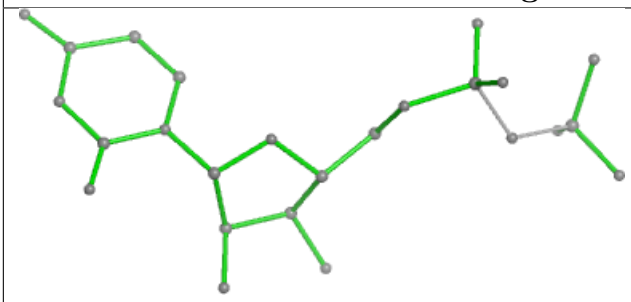
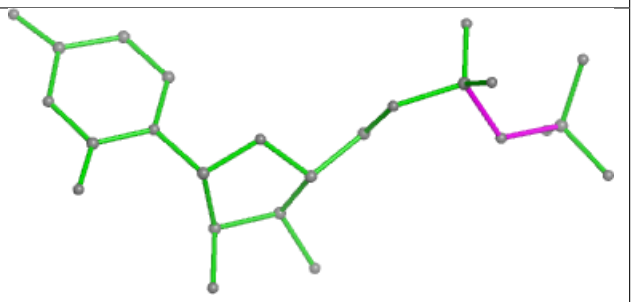
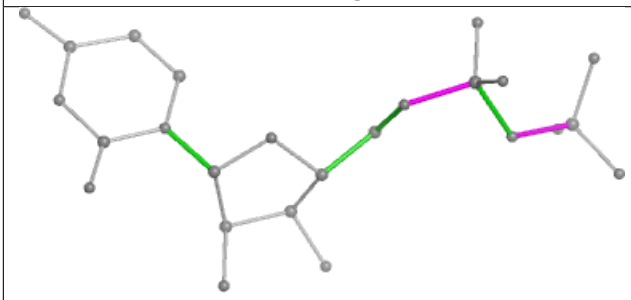
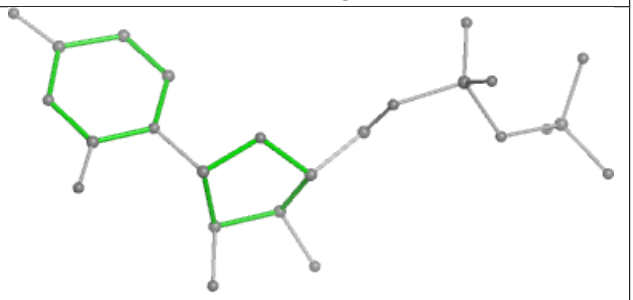
also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 UDP C 401



Ligand UDP B 401



Ligand UDP A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	0.24	3 (0%)	81	77	26, 62, 91, 154	1 (0%)
1	B	322/354 (90%)	0.34	14 (4%)	40	34	40, 62, 108, 148	0
1	C	335/354 (94%)	0.04	4 (1%)	76	72	37, 55, 76, 158	0
1	D	330/354 (93%)	0.84	32 (9%)	15	12	51, 88, 145, 183	0
All	All	1322/1416 (93%)	0.36	53 (4%)	43	37	26, 64, 123, 183	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	GLY	4.6
1	C	169	THR	4.6
1	D	200	VAL	4.1
1	B	203	ILE	4.1
1	B	175	ALA	3.4
1	D	183	LEU	3.2
1	D	160	VAL	3.1
1	D	170	GLY	3.0
1	D	209	ILE	2.9
1	D	234	TRP	2.9
1	D	243	TYR	2.9
1	D	201	ILE	2.9
1	D	264	VAL	2.8
1	B	181	PHE	2.8
1	D	102	ILE	2.7
1	D	203	ILE	2.7
1	D	286	LEU	2.6
1	D	212	MET	2.6
1	B	211	PHE	2.6
1	D	202	ASP	2.6
1	D	246	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	169	THR	2.6
1	D	163	THR	2.6
1	D	75	TRP	2.5
1	B	195	TYR	2.5
1	B	113	LEU	2.4
1	D	175	ALA	2.4
1	D	296	MET	2.4
1	A	168	ASN	2.4
1	B	206	THR	2.4
1	D	165	THR	2.4
1	D	181	PHE	2.4
1	D	206	THR	2.3
1	D	38	ILE	2.3
1	B	196	ALA	2.3
1	D	72	SER	2.3
1	B	105	LEU	2.3
1	D	199	LYS	2.3
1	D	136	ASP	2.3
1	D	205	PRO	2.2
1	B	214	TRP	2.2
1	D	187	TRP	2.2
1	D	238	SER	2.2
1	B	289	ALA	2.2
1	D	239	TYR	2.1
1	A	162	PHE	2.1
1	D	211	PHE	2.1
1	C	162	PHE	2.1
1	B	169	THR	2.1
1	D	232	LEU	2.1
1	B	184	VAL	2.0
1	B	202	ASP	2.0
1	C	72	SER	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

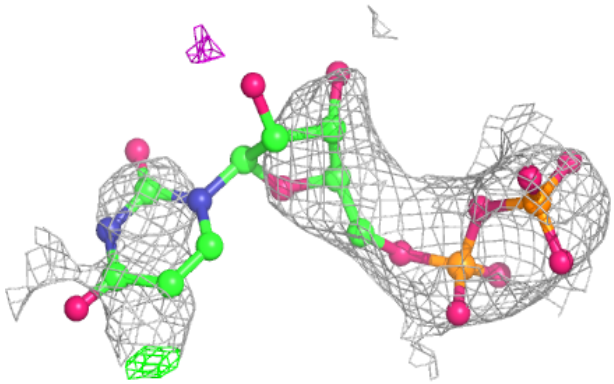
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

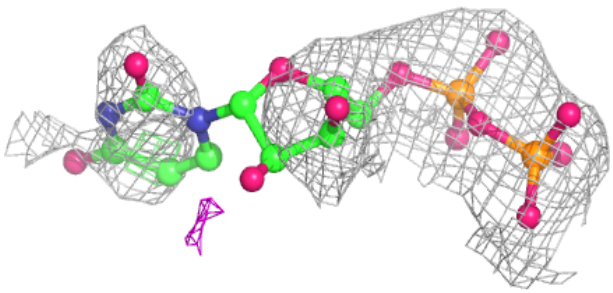
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDP	B	401	25/25	0.76	0.15	85,90,98,99	25
2	UDP	A	401	25/25	0.94	0.07	48,51,57,59	0
2	UDP	C	401	25/25	0.94	0.09	50,55,60,60	0

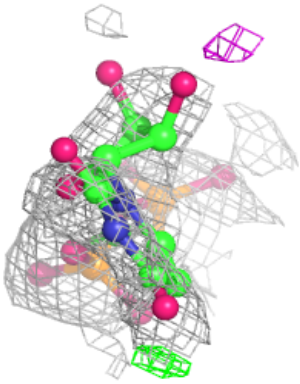
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP 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)

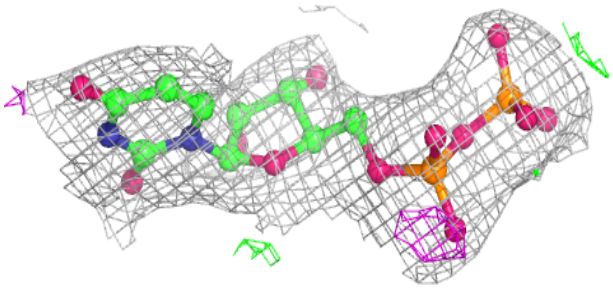


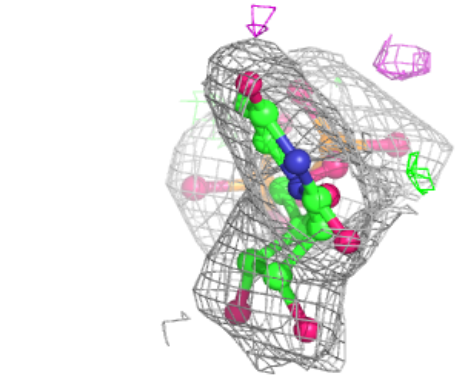


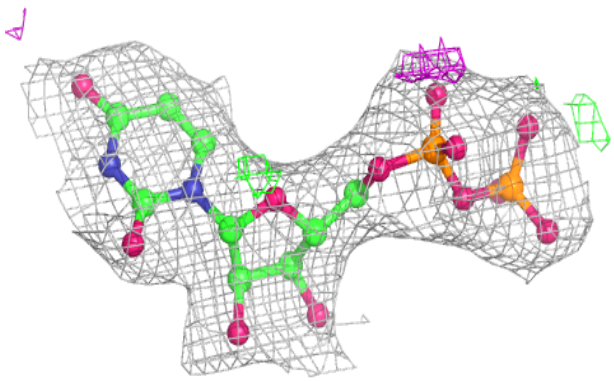


Electron density around UDP A 401:

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

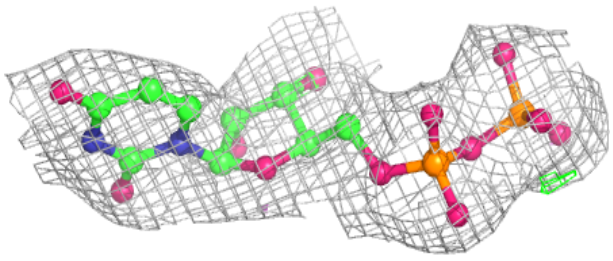


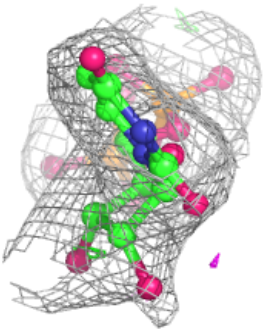


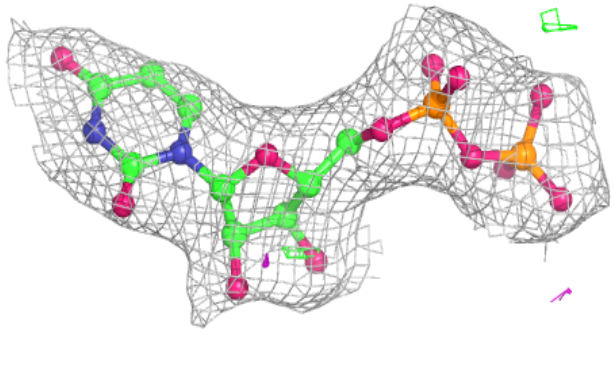


Electron density around UDP C 401:

$2mF_o$-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.