



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 8P0Q / pdb_00008p0q
Title : Crystal structure of AaNGT complexed to UDP and a peptide
Authors : Piniello, B.; Macias-Leon, J.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2023-05-10
Resolution : 2.80 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

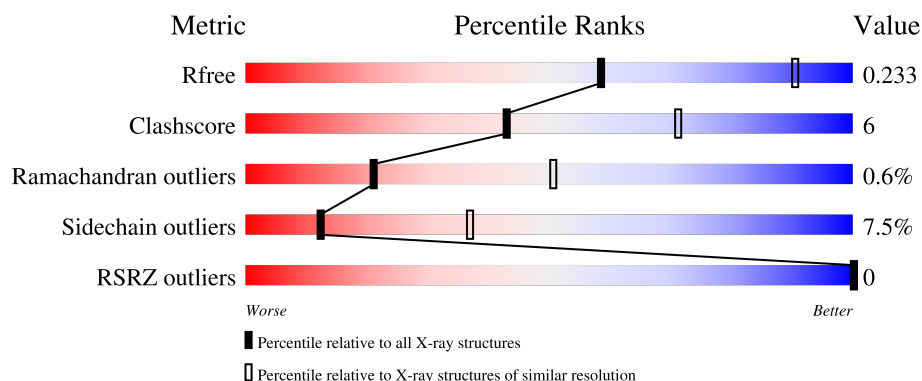
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	621	 81% 17% .
1	B	621	 77% 19% . .
2	C	6	 67% 33%
2	D	6	 33% 17% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10053 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 Adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4967	3171	846	921	29			
1	B	617	Total	C	N	O	S	0	0	0
			4952	3163	843	917	29			

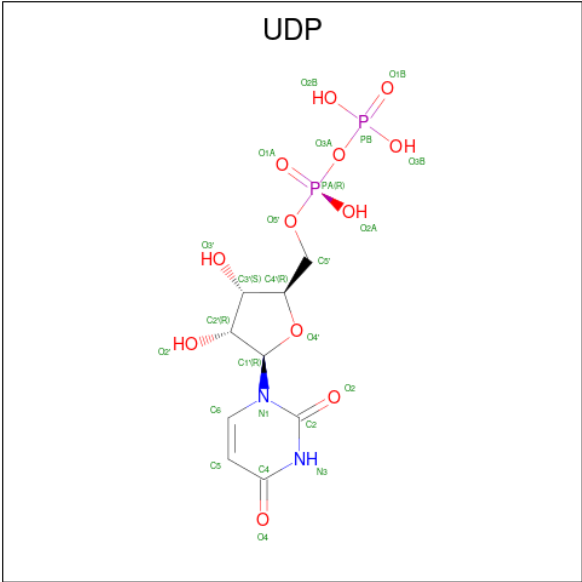
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ARG	GLU	conflict	UNP A0A3M6PNT1
B	3	ARG	GLU	conflict	UNP A0A3M6PNT1

- Molecule 2 is a protein called PHE-GLY-ASN-TRP-THR-THR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			51	34	8	9			
2	D	3	Total	C	N	O	0	0	0
			28	19	4	5			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



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

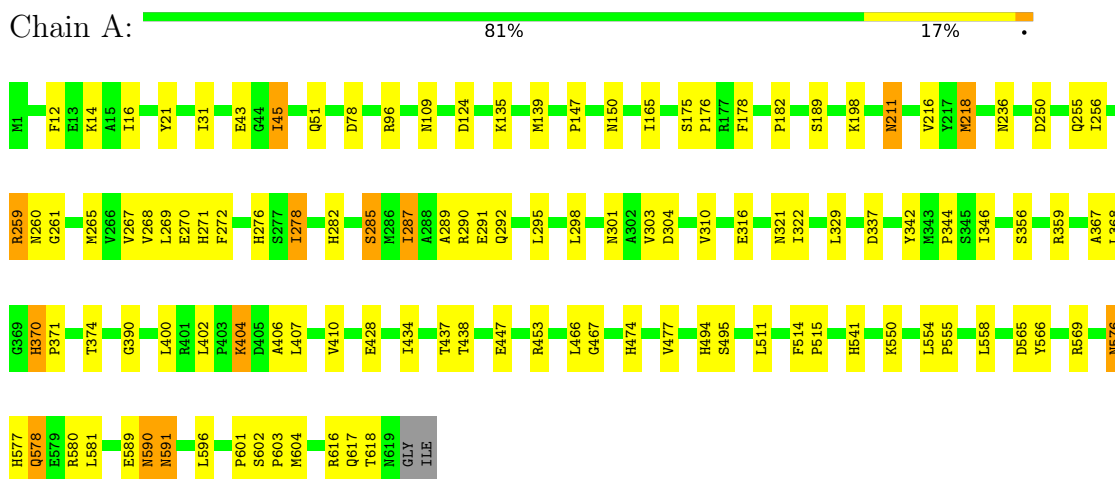
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		

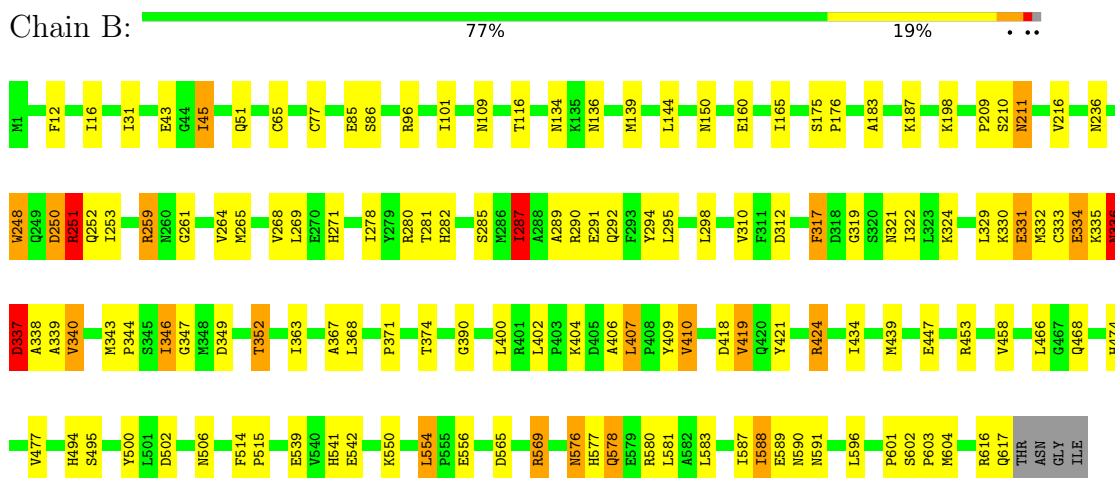
3 Residue-property plots

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.

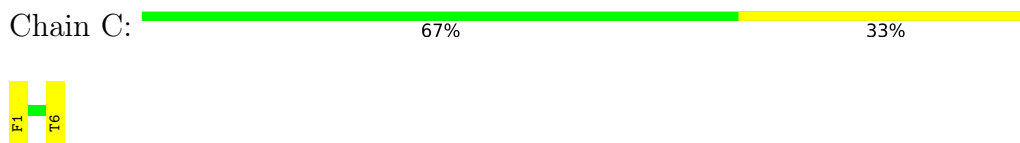
• Molecule 1: Adhesin



• Molecule 1: Adhesin



• Molecule 2: PHE-GLY-ASN-TRP-THR-THR



- Molecule 2: PHE-GLY-ASN-TRP-THR-THR

Chain D:  33% 17% 50%

PHE	GLY	ASN	TRP	THR	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.02Å 111.48Å 256.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.96-2.80) 99.4 (19.96-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.237 0.181 , 0.233	Depositor DCC
R_{free} test set	1351 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10053	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.09	1/5088 (0.0%)	1.49	14/6906 (0.2%)
1	B	1.07	0/5073	1.48	17/6885 (0.2%)
2	C	1.09	0/53	1.87	2/72 (2.8%)
2	D	1.04	0/29	1.32	0/40
All	All	1.08	1/10243 (0.0%)	1.49	33/13903 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	HIS	CE1-NE2	5.07	1.37	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ASP	CA-CB-CG	7.82	120.42	112.60
1	B	336	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	390	GLY	O-C-N	6.70	125.60	121.85
1	B	317	PHE	CA-CB-CG	6.26	120.06	113.80
2	C	6	THR	CA-C-O	-6.20	110.26	120.80
1	A	304	ASP	CA-CB-CG	5.92	118.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	GLU	CB-CG-CD	5.87	122.58	112.60
1	B	390	GLY	O-C-N	5.75	125.07	121.85
1	B	216	VAL	CA-C-N	5.70	128.19	120.44
1	B	216	VAL	C-N-CA	5.70	128.19	120.44
1	B	474	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	578	GLN	CB-CA-C	5.62	120.41	110.85
1	A	189	SER	CA-C-N	5.57	127.68	120.44
1	A	189	SER	C-N-CA	5.57	127.68	120.44
1	A	124	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	209	PRO	CA-C-N	5.43	127.56	120.28
1	B	209	PRO	C-N-CA	5.43	127.56	120.28
1	A	601	PRO	CA-C-N	5.36	126.79	120.09
1	A	601	PRO	C-N-CA	5.36	126.79	120.09
1	A	216	VAL	CA-C-N	5.35	127.71	120.44
1	A	216	VAL	C-N-CA	5.35	127.71	120.44
1	A	287	ILE	CA-C-N	5.32	127.41	120.28
1	A	287	ILE	C-N-CA	5.32	127.41	120.28
1	B	502	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	287	ILE	CA-C-N	5.17	127.20	120.28
1	B	287	ILE	C-N-CA	5.17	127.20	120.28
2	C	1	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	601	PRO	CA-C-N	5.15	126.53	120.09
1	B	601	PRO	C-N-CA	5.15	126.53	120.09
1	A	590	ASN	CB-CA-C	-5.11	103.14	111.06
1	B	578	GLN	CB-CA-C	5.10	119.53	110.85
1	A	474	HIS	CA-CB-CG	-5.10	108.70	113.80
1	B	418	ASP	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	368	LEU	Peptide
1	B	248	TRP	Peptide
1	B	261	GLY	Peptide
1	B	368	LEU	Peptide

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	4967	0	4886	50	0
1	B	4952	0	4873	76	0
2	C	51	0	44	0	0
2	D	28	0	23	2	0
3	A	25	0	11	0	0
3	B	25	0	11	1	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
All	All	10053	0	9848	123	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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LEU:HD11	1:B:587:ILE:HD11	1.40	1.02
1:B:85:GLU:HA	1:B:139:MET:HE1	1.46	0.97
1:B:583:LEU:O	1:B:587:ILE:HD13	1.81	0.79
1:B:85:GLU:HA	1:B:139:MET:CE	2.19	0.70
1:A:265:MET:HE2	1:A:295:LEU:HD11	1.75	0.69
1:B:280:ARG:HG3	1:B:410:VAL:O	1.93	0.67
1:B:265:MET:HE2	1:B:295:LEU:HD11	1.77	0.67
1:A:466:LEU:HD13	1:A:477:VAL:HG11	1.77	0.65
1:B:583:LEU:O	1:B:587:ILE:CD1	2.44	0.65
1:B:466:LEU:HD13	1:B:477:VAL:HG11	1.78	0.65
1:B:250:ASP:OD2	1:B:330:LYS:HG2	1.99	0.63
1:B:264:VAL:O	1:B:339:ALA:HB3	1.99	0.63
1:B:334:GLU:N	1:B:338:ALA:HB2	2.15	0.62
1:A:236:ASN:ND2	1:A:374:THR:O	2.37	0.58
1:B:406:ALA:O	1:B:407:LEU:HB2	2.02	0.57
1:B:468:GLN:H	1:B:494:HIS:HD2	1.52	0.57
1:A:576:ASN:HD22	1:A:576:ASN:N	2.03	0.56
1:B:282:HIS:CE1	1:B:407:LEU:HD21	2.40	0.56
1:B:85:GLU:CA	1:B:139:MET:HE1	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:CYS:O	1:B:336:ASN:N	2.32	0.56
1:B:554:LEU:HD11	1:B:587:ILE:CD1	2.26	0.54
1:A:150:ASN:HD21	1:B:51:GLN:HE21	1.55	0.54
1:B:331:GLU:O	1:B:336:ASN:ND2	2.41	0.53
1:B:236:ASN:ND2	1:B:374:THR:O	2.41	0.53
1:B:298:LEU:HD22	1:B:329:LEU:HD13	1.90	0.53
1:A:211:ASN:ND2	1:A:211:ASN:H	2.07	0.53
1:B:251:ARG:O	1:B:253:ILE:N	2.42	0.53
1:B:12:PHE:CE1	1:B:16:ILE:HD11	2.43	0.52
1:B:211:ASN:ND2	1:B:211:ASN:H	2.08	0.52
1:B:421:TYR:CD2	1:B:588:ILE:HD11	2.45	0.52
1:A:346:ILE:CD1	1:A:356:SER:HB3	2.40	0.52
1:B:211:ASN:H	1:B:211:ASN:HD22	1.57	0.52
1:B:278:ILE:HD11	1:B:344:PRO:HB2	1.92	0.51
1:B:419:VAL:HG23	1:B:419:VAL:O	2.09	0.51
1:A:12:PHE:CE1	1:A:16:ILE:HD11	2.45	0.51
1:B:554:LEU:CD1	1:B:587:ILE:HD11	2.26	0.51
1:B:576:ASN:HD22	1:B:576:ASN:N	2.08	0.51
1:A:282:HIS:CE1	1:A:367:ALA:HB1	2.46	0.50
1:A:175:SER:N	1:A:176:PRO:CD	2.74	0.50
1:A:255:GLN:O	1:A:337:ASP:HB3	2.12	0.50
1:B:514:PHE:HB2	1:B:515:PRO:HA	1.94	0.50
1:A:285:SER:OG	1:A:407:LEU:HG	2.11	0.50
1:A:150:ASN:ND2	1:B:51:GLN:HE21	2.10	0.50
1:B:349:ASP:HB3	1:B:352:THR:HG23	1.92	0.50
1:A:289:ALA:HB2	1:A:604:MET:HE2	1.93	0.49
1:B:280:ARG:HB2	1:B:280:ARG:NH1	2.27	0.49
1:A:51:GLN:HE21	1:B:150:ASN:HD21	1.59	0.49
1:B:287:ILE:O	1:B:290:ARG:HB3	2.12	0.49
1:B:289:ALA:HB2	1:B:604:MET:HE2	1.95	0.49
1:B:282:HIS:CE1	1:B:367:ALA:HB1	2.48	0.49
1:B:424:ARG:NH2	1:B:506:ASN:O	2.46	0.49
1:A:514:PHE:HB2	1:A:515:PRO:HA	1.94	0.49
1:A:31:ILE:HG23	1:A:45:ILE:HD12	1.95	0.48
1:A:565:ASP:O	1:A:569:ARG:HG2	2.13	0.48
1:B:500:TYR:CD2	3:B:701:UDP:C5	3.02	0.48
1:B:565:ASP:O	1:B:569:ARG:HG2	2.14	0.48
1:A:298:LEU:HD22	1:A:329:LEU:HD13	1.95	0.48
1:A:467:GLY:HA2	1:A:494:HIS:HD2	1.80	0.47
1:A:346:ILE:HD11	1:A:356:SER:HB3	1.95	0.47
1:B:346:ILE:HD13	1:B:347:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:O	1:B:402:LEU:HD13	2.14	0.47
1:A:271:HIS:HB3	1:A:276:HIS:CD2	2.50	0.46
1:A:400:LEU:O	1:A:402:LEU:HD13	2.15	0.46
1:B:134:ASN:ND2	1:B:136:ASN:HB3	2.30	0.46
1:B:321:ASN:HD22	1:B:324:LYS:H	1.62	0.46
1:B:259:ARG:CZ	1:B:259:ARG:HB2	2.45	0.46
1:B:371:PRO:HG2	1:B:541:HIS:HB3	1.96	0.46
1:B:31:ILE:HG23	1:B:45:ILE:HD12	1.96	0.46
1:A:371:PRO:HG2	1:A:541:HIS:HB3	1.97	0.46
1:B:587:ILE:HD12	1:B:587:ILE:N	2.30	0.46
1:A:21:TYR:OH	1:A:78:ASP:OD2	2.31	0.45
1:A:602:SER:N	1:A:603:PRO:CD	2.80	0.45
1:A:511:LEU:HB3	1:A:566:TYR:OH	2.16	0.45
1:B:175:SER:N	1:B:176:PRO:CD	2.79	0.45
1:B:337:ASP:OD1	1:B:337:ASP:N	2.50	0.44
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.87	0.44
1:B:268:VAL:HB	1:B:343:MET:HG2	1.98	0.44
1:A:259:ARG:HB2	1:A:259:ARG:CZ	2.47	0.44
1:A:576:ASN:N	1:A:576:ASN:ND2	2.63	0.44
1:B:344:PRO:HA	1:B:367:ALA:HB3	1.99	0.44
1:B:576:ASN:N	1:B:576:ASN:ND2	2.65	0.44
1:B:439:MET:HE1	2:D:4:TRP:CB	2.48	0.44
1:B:578:GLN:H	1:B:578:GLN:CD	2.25	0.44
1:A:218:MET:HG2	1:A:370:HIS:CE1	2.53	0.43
1:A:287:ILE:O	1:A:290:ARG:HB3	2.17	0.43
1:A:577:HIS:CD2	1:A:580:ARG:HH22	2.36	0.43
1:A:578:GLN:H	1:A:578:GLN:CD	2.26	0.43
1:A:555:PRO:HD2	1:A:558:LEU:HD12	1.99	0.43
1:A:514:PHE:HA	1:A:515:PRO:C	2.44	0.43
1:A:576:ASN:HB3	1:A:578:GLN:NE2	2.33	0.43
1:B:439:MET:HE1	2:D:4:TRP:HB3	2.00	0.43
1:A:272:PHE:O	1:A:303:VAL:HA	2.19	0.43
1:B:602:SER:N	1:B:603:PRO:CD	2.80	0.43
1:A:590:ASN:O	1:A:591:ASN:C	2.62	0.43
1:B:539:GLU:HB2	1:B:542:GLU:HG3	2.01	0.43
1:A:267:VAL:HA	1:A:342:TYR:O	2.19	0.42
1:A:301:ASN:HB3	1:A:316:GLU:OE2	2.19	0.42
1:B:65:CYS:HB3	1:B:101:ILE:O	2.20	0.42
1:B:340:VAL:HG22	1:B:363:ILE:HB	2.01	0.42
1:B:248:TRP:CZ3	1:B:330:LYS:HD3	2.54	0.42
1:B:77:CYS:SG	1:B:116:THR:HG21	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PHE:HD1	1:A:278:ILE:HG22	1.84	0.42
1:B:332:MET:O	1:B:332:MET:CG	2.68	0.41
1:A:178:PHE:HB2	1:A:438:THR:HB	2.01	0.41
1:B:577:HIS:CD2	1:B:580:ARG:HH22	2.38	0.41
1:B:183:ALA:O	1:B:187:LYS:HG3	2.21	0.41
1:B:281:THR:HG22	1:B:409:TYR:CZ	2.55	0.41
1:B:514:PHE:HA	1:B:515:PRO:C	2.45	0.41
1:A:175:SER:N	1:A:176:PRO:HD3	2.36	0.41
1:B:109:ASN:OD1	1:B:109:ASN:C	2.63	0.41
1:B:281:THR:HG22	1:B:409:TYR:CE1	2.55	0.41
1:A:109:ASN:OD1	1:A:109:ASN:C	2.64	0.41
1:A:250:ASP:HB3	1:A:359:ARG:HB3	2.02	0.41
1:B:590:ASN:O	1:B:591:ASN:C	2.63	0.41
1:A:139:MET:HE3	1:A:165:ILE:HD11	2.03	0.41
1:B:271:HIS:O	1:B:278:ILE:HG21	2.21	0.41
1:A:402:LEU:HB3	1:A:406:ALA:CB	2.51	0.40
1:A:577:HIS:HD2	1:A:580:ARG:HH22	1.69	0.40
1:B:139:MET:HE3	1:B:165:ILE:HD11	2.02	0.40
1:B:294:TYR:CE1	1:B:312:ASP:HB3	2.57	0.40
1:B:334:GLU:CA	1:B:338:ALA:HB2	2.52	0.40
1:A:256:ILE:HD12	1:A:256:ILE:N	2.36	0.40
1:A:344:PRO:HA	1:A:367:ALA:HB3	2.03	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	617/621 (99%)	593 (96%)	22 (4%)	2 (0%)	36 66
1	B	615/621 (99%)	581 (94%)	28 (5%)	6 (1%)	12 38
2	C	4/6 (67%)	4 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1237/1254 (99%)	1179 (95%)	50 (4%)	8 (1%)	21	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	GLN
1	B	251	ARG
1	B	419	VAL
1	A	404	LYS
1	B	404	LYS
1	B	319	GLY
1	A	591	ASN
1	B	588	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	550/551 (100%)	511 (93%)	39 (7%)	13	39
1	B	548/551 (100%)	504 (92%)	44 (8%)	11	34
2	C	5/5 (100%)	5 (100%)	0	100	100
2	D	3/5 (60%)	3 (100%)	0	100	100
All	All	1106/1112 (100%)	1023 (92%)	83 (8%)	12	37

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	43	GLU
1	A	45	ILE
1	A	96	ARG
1	A	135	LYS
1	A	147	PRO

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Mol	Chain	Res	Type
1	A	182	PRO
1	A	198	LYS
1	A	211	ASN
1	A	218	MET
1	A	259	ARG
1	A	260	ASN
1	A	268	VAL
1	A	269	LEU
1	A	270	GLU
1	A	278	ILE
1	A	285	SER
1	A	291	GLU
1	A	292	GLN
1	A	310	VAL
1	A	321	ASN
1	A	322	ILE
1	A	404	LYS
1	A	410	VAL
1	A	428	GLU
1	A	434	ILE
1	A	437	THR
1	A	447	GLU
1	A	453	ARG
1	A	495	SER
1	A	550	LYS
1	A	554	LEU
1	A	576	ASN
1	A	581	LEU
1	A	589	GLU
1	A	596	LEU
1	A	616	ARG
1	A	617	GLN
1	A	618	THR
1	B	43	GLU
1	B	45	ILE
1	B	86	SER
1	B	96	ARG
1	B	198	LYS
1	B	210	SER
1	B	211	ASN
1	B	250	ASP
1	B	251	ARG

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Mol	Chain	Res	Type
1	B	259	ARG
1	B	269	LEU
1	B	285	SER
1	B	287	ILE
1	B	291	GLU
1	B	292	GLN
1	B	310	VAL
1	B	317	PHE
1	B	322	ILE
1	B	331	GLU
1	B	334	GLU
1	B	335	LYS
1	B	336	ASN
1	B	337	ASP
1	B	340	VAL
1	B	346	ILE
1	B	352	THR
1	B	407	LEU
1	B	410	VAL
1	B	424	ARG
1	B	434	ILE
1	B	447	GLU
1	B	453	ARG
1	B	458	VAL
1	B	495	SER
1	B	550	LYS
1	B	554	LEU
1	B	556	GLU
1	B	569	ARG
1	B	576	ASN
1	B	581	LEU
1	B	589	GLU
1	B	596	LEU
1	B	616	ARG
1	B	617	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	150	ASN
1	A	211	ASN

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Mol	Chain	Res	Type
1	A	229	HIS
1	A	273	HIS
1	A	321	ASN
1	A	357	ASN
1	A	375	HIS
1	A	431	ASN
1	A	494	HIS
1	A	512	ASN
1	A	541	HIS
1	A	576	ASN
1	A	577	HIS
1	A	578	GLN
1	A	586	HIS
1	B	33	ASN
1	B	134	ASN
1	B	150	ASN
1	B	211	ASN
1	B	229	HIS
1	B	273	HIS
1	B	282	HIS
1	B	321	ASN
1	B	336	ASN
1	B	357	ASN
1	B	420	GLN
1	B	431	ASN
1	B	468	GLN
1	B	494	HIS
1	B	512	ASN
1	B	518	ASN
1	B	541	HIS
1	B	576	ASN
1	B	577	HIS
1	B	578	GLN
1	B	590	ASN
1	B	591	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UDP	A	701	-	25,26,26	0.60	0	38,40,40	1.02	1 (2%)
3	UDP	B	701	-	25,26,26	0.62	0	38,40,40	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	A	701	-	-	6/16/32/32	0/2/2/2
3	UDP	B	701	-	-	2/16/32/32	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	UDP	O2B-PB-O1B	3.38	124.00	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

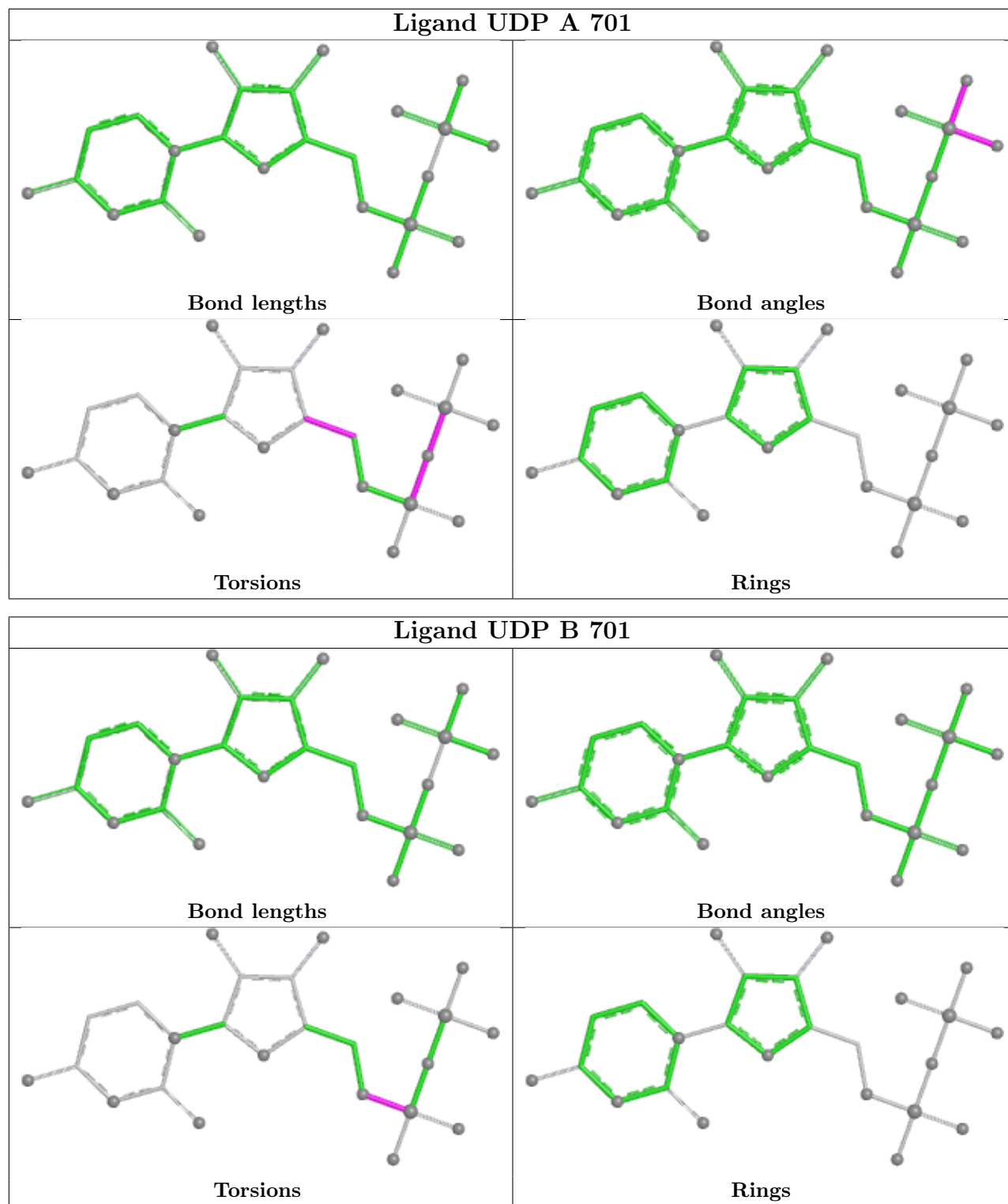
Mol	Chain	Res	Type	Atoms
3	A	701	UDP	O4'-C4'-C5'-O5'
3	A	701	UDP	PA-O3A-PB-O2B
3	B	701	UDP	C5'-O5'-PA-O1A
3	A	701	UDP	C3'-C4'-C5'-O5'
3	B	701	UDP	C5'-O5'-PA-O3A
3	A	701	UDP	PB-O3A-PA-O2A
3	A	701	UDP	PB-O3A-PA-O1A
3	A	701	UDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	UDP	1	0

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



5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	619/621 (99%)	-0.88	0 100 100	51, 75, 101, 129	0
1	B	617/621 (99%)	-0.72	0 100 100	54, 97, 144, 173	0
2	C	6/6 (100%)	-0.49	0 100 100	74, 80, 91, 118	0
2	D	3/6 (50%)	0.14	0 100 100	130, 130, 137, 159	0
All	All	1245/1254 (99%)	-0.80	0 100 100	51, 83, 136, 173	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

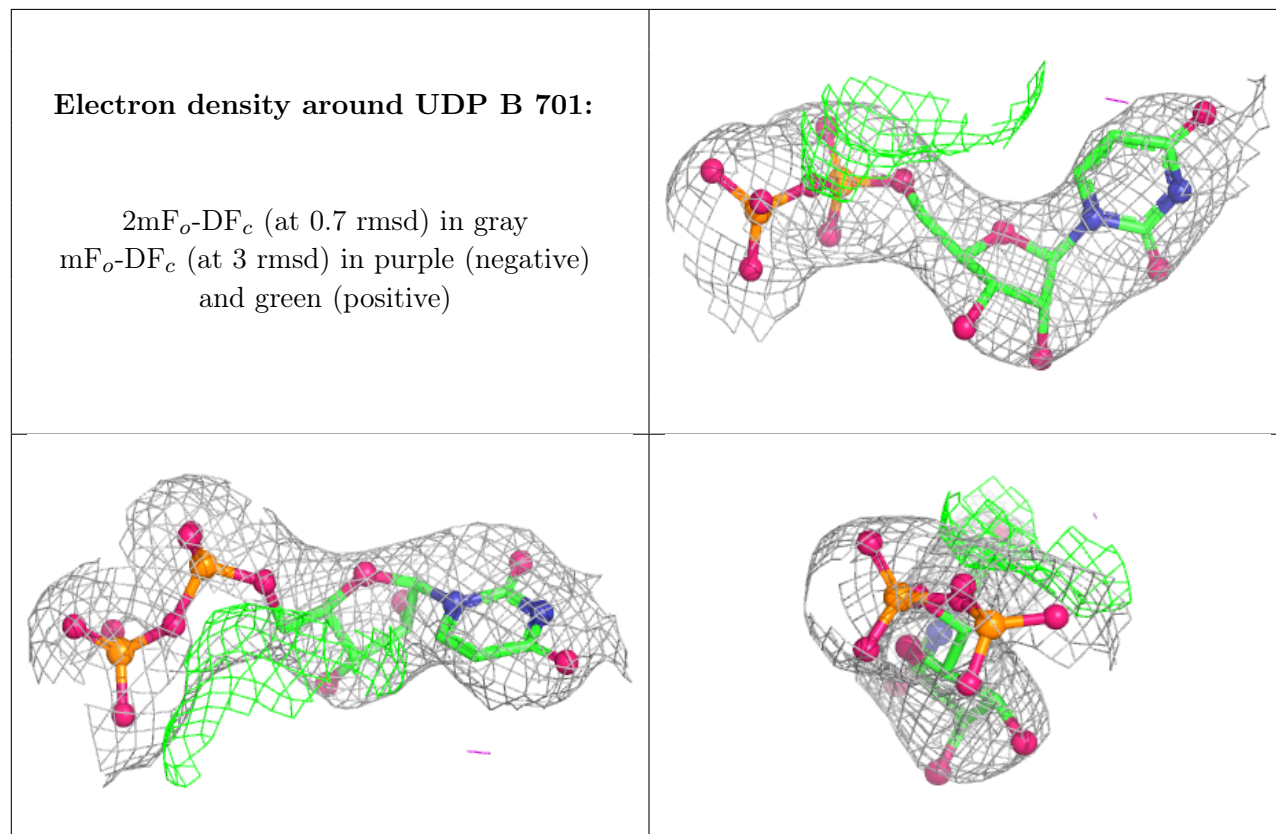
6.4 Ligands [i](#)

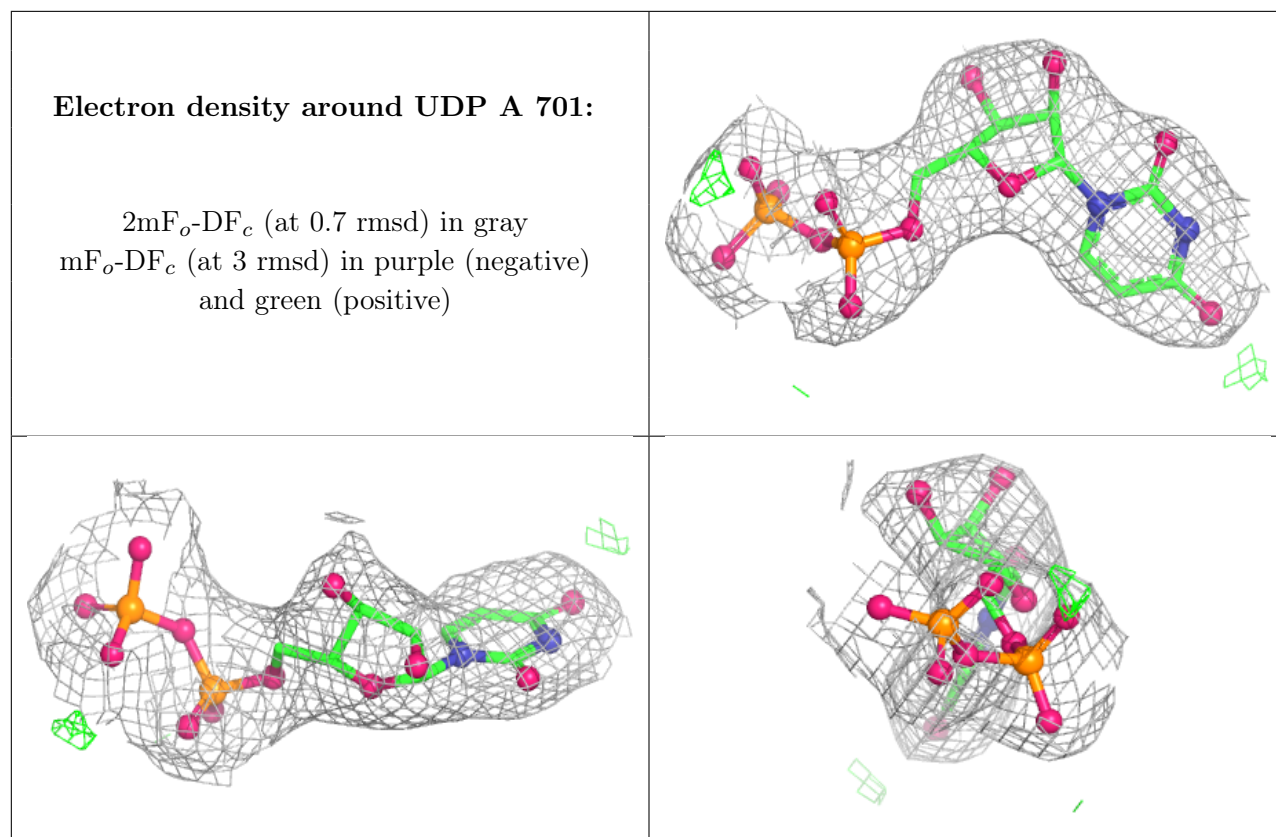
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UDP	B	701	25/25	0.93	0.06	88,105,114,117	0
3	UDP	A	701	25/25	0.97	0.04	60,64,72,81	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.