



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:19 AM UTC

PDB ID : 9F5H / pdb_00009f5h
Title : Crystal structure of MGAT5 bump-and-hole mutant in complex with UDP and M592
Authors : Liu, Y.; Bineva-Todd, G.; Meek, R.; Mazo, L.; Piniello, B.; Moroz, O.V.; Begum, N.; Roustan, C.; Tomita, S.; Kjaer, S.; Rovira, C.; Davies, G.J.; Schumann, B.
Deposited on : 2024-04-28
Resolution : 1.97 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](#) ①) 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

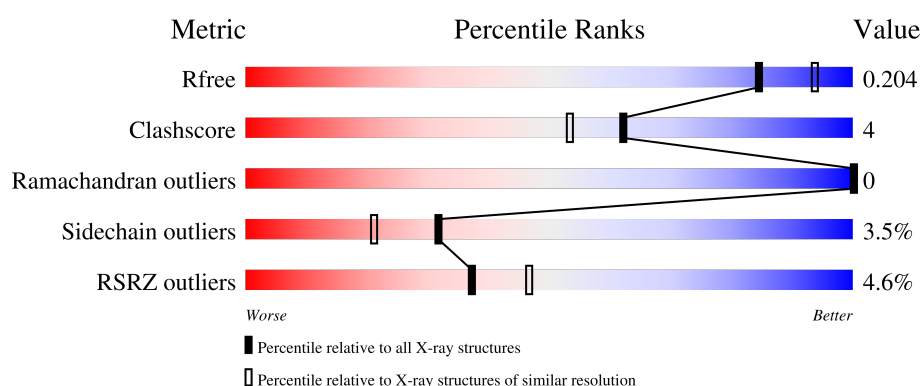
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	515	5% 85% 11% ..
1	B	515	4% 83% 12% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8396 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.

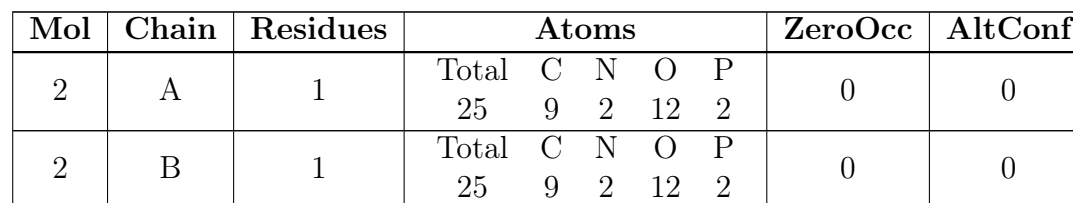
- Molecule 1 is a protein called Secreted alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4033	2595	687	726	25			
1	B	499	Total	C	N	O	S	0	0	0
			3985	2561	683	715	26			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	GLU	engineered mutation	UNP Q09328
A	329	GLY	-	linker	UNP Q09328
A	330	GLY	-	linker	UNP Q09328
A	331	GLY	-	linker	UNP Q09328
A	332	GLY	-	linker	UNP Q09328
A	445	VAL	PHE	engineered mutation	UNP Q09328
A	504	LEU	PHE	engineered mutation	UNP Q09328
B	297	ALA	GLU	engineered mutation	UNP Q09328
B	329	GLY	-	linker	UNP Q09328
B	330	GLY	-	linker	UNP Q09328
B	331	GLY	-	linker	UNP Q09328
B	332	GLY	-	linker	UNP Q09328
B	445	VAL	PHE	engineered mutation	UNP Q09328
B	504	LEU	PHE	engineered mutation	UNP Q09328

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



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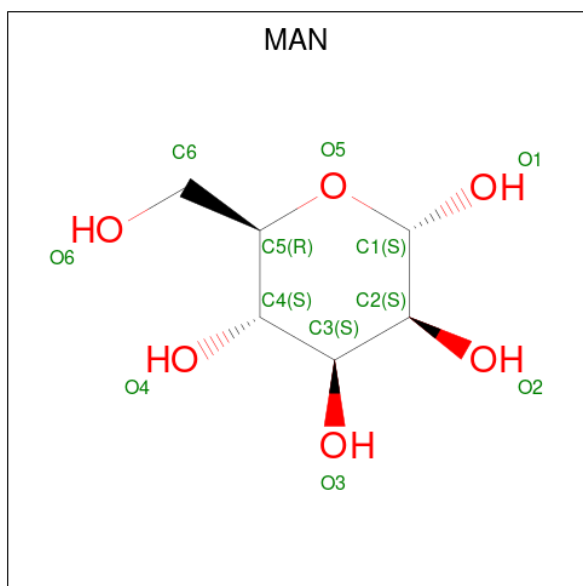
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

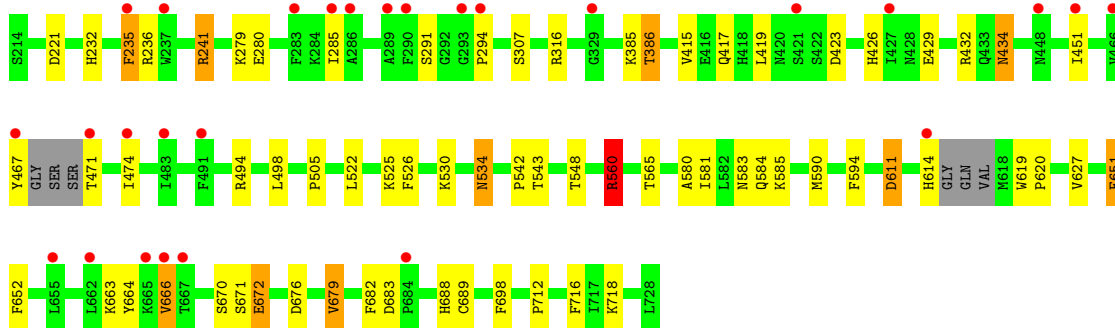
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	B	143	Total	O	0	0
			143	143		

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.

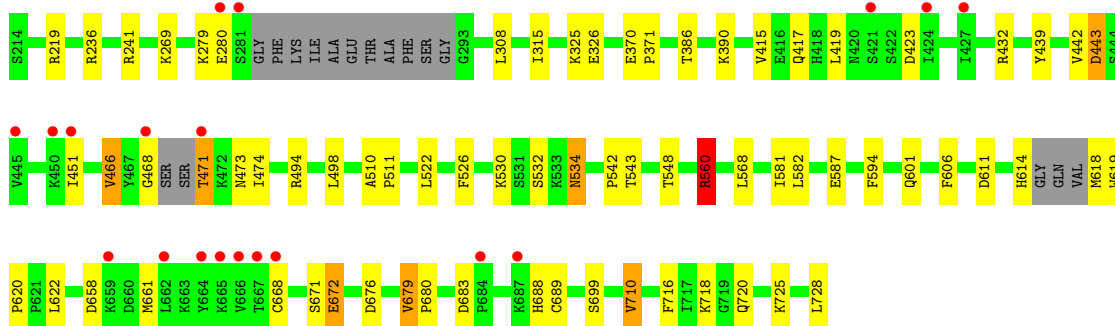
- Molecule 1: Secreted alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain A: 



- Molecule 1: Secreted alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.51Å 69.07Å 90.99Å 108.21° 92.09° 106.75°	Depositor
Resolution (Å)	44.10 – 1.97 44.10 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.6 (44.10-1.97) 94.6 (44.10-1.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.200 , 0.242 (Not available) , 0.204	Depositor DCC
R_{free} test set	3269 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, UDP, SO4

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	0.83	1/4136 (0.0%)	1.35	23/5605 (0.4%)
1	B	0.84	0/4086	1.37	27/5533 (0.5%)
All	All	0.83	1/8222 (0.0%)	1.36	50/11138 (0.4%)

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	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	SER	CA-CB	-5.33	1.45	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	679	VAL	N-CA-CB	-8.97	98.65	111.21
1	A	679	VAL	N-CA-CB	-8.29	99.60	111.21
1	A	548	THR	CA-CB-OG1	-8.15	97.38	109.60
1	A	280	GLU	CB-CG-CD	8.12	126.40	112.60
1	B	526	PHE	CA-CB-CG	7.71	121.51	113.80
1	B	606	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	542	PRO	N-CA-CB	-6.83	97.15	102.28
1	B	417	GLN	N-CA-CB	-6.78	98.92	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	683	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	542	PRO	N-CA-CB	-6.67	98.39	102.79
1	A	590	MET	CB-CA-C	-6.61	101.37	110.16
1	B	728	LEU	CA-C-O	-6.58	109.61	120.80
1	B	676	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	417	GLN	N-CA-CB	-6.08	100.74	111.39
1	A	716	PHE	CA-CB-CG	6.06	119.86	113.80
1	B	587	GLU	CB-CG-CD	6.05	122.88	112.60
1	B	443	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	560	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	B	725	LYS	CB-CA-C	5.98	120.38	110.81
1	A	683	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	543	THR	CA-CB-OG1	-5.95	100.68	109.60
1	B	386	THR	O-C-N	-5.89	116.55	121.38
1	A	279	LYS	CA-C-N	5.83	130.01	120.63
1	A	279	LYS	C-N-CA	5.83	130.01	120.63
1	A	494	ARG	CB-CA-C	5.82	120.46	110.79
1	B	560	ARG	CG-CD-NE	5.81	124.78	112.00
1	B	423	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	611	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	585	LYS	N-CA-CB	5.70	118.35	109.97
1	A	417	GLN	CB-CA-C	5.63	120.46	110.16
1	A	676	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	386	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	235	PHE	CA-CB-CG	5.52	119.32	113.80
1	B	548	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	543	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	370	GLU	CB-CA-C	5.43	116.68	108.86
1	A	526	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	611	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	423	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	658	ASP	CA-CB-CG	5.25	117.84	112.60
1	B	466	VAL	CA-C-N	5.22	127.27	120.28
1	B	466	VAL	C-N-CA	5.22	127.27	120.28
1	A	221	ASP	CB-CA-C	5.20	119.31	109.37
1	B	716	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	494	ARG	CB-CA-C	5.14	119.33	110.79
1	A	651	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	279	LYS	N-CA-CB	5.10	117.62	110.12
1	B	442	VAL	CA-C-N	5.09	127.36	120.38
1	B	442	VAL	C-N-CA	5.09	127.36	120.38
1	B	269	LYS	CB-CA-C	5.06	118.59	110.29

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Sidechain
1	A	316	ARG	Sidechain
1	A	432	ARG	Sidechain
1	A	560	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	432	ARG	Sidechain
1	B	560	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4033	0	3939	27	0
1	B	3985	0	3896	31	0
2	A	25	0	11	1	0
2	B	25	0	11	1	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
4	A	23	0	22	4	0
5	B	5	0	0	0	0
6	A	129	0	0	3	0
6	B	143	0	0	5	0
All	All	8396	0	7905	63	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 4.

All (63) 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)
4:A:803:MAN:C1	4:A:804:MAN:O6	1.81	1.26
3:A:802:NAG:C1	4:A:803:MAN:O2	1.84	1.24
1:A:611:ASP:OD2	1:A:614:HIS:ND1	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:802:NAG:C1	4:A:803:MAN:HO2	1.88	0.85
1:A:614:HIS:NE2	6:A:901:HOH:O	2.12	0.82
1:B:661:MET:HE1	1:B:710:VAL:HG21	1.62	0.82
1:B:601:GLN:HE21	1:B:720:GLN:HE21	1.28	0.81
1:B:718:LYS:HA	6:B:917:HOH:O	1.83	0.77
1:B:308:LEU:HB3	1:B:315:ILE:HD11	1.64	0.77
1:B:471:THR:HG21	1:B:474:ILE:HD12	1.71	0.72
1:A:671:SER:HA	1:A:689:CYS:O	1.91	0.71
1:B:671:SER:HA	1:B:689:CYS:O	1.91	0.70
1:A:426:HIS:CB	6:A:1020:HOH:O	2.40	0.69
1:A:672:GLU:OE2	1:A:688:HIS:NE2	2.26	0.67
1:A:611:ASP:OD2	1:A:614:HIS:CE1	2.50	0.65
1:B:672:GLU:OE2	1:B:688:HIS:NE2	2.25	0.64
1:B:468:GLY:HA3	1:B:471:THR:HG22	1.78	0.64
1:B:560:ARG:NH2	6:B:901:HOH:O	2.35	0.59
1:B:668:CYS:HG	1:B:689:CYS:HG	1.51	0.59
1:A:530:LYS:HA	1:A:534:ASN:HD21	1.68	0.57
1:A:434:ASN:C	1:A:434:ASN:HD22	2.13	0.57
1:A:666:VAL:HG23	1:A:682:PHE:CE1	2.40	0.56
1:A:241:ARG:HH21	1:A:241:ARG:HG3	1.71	0.56
1:A:291:SER:HB2	1:A:467:TYR:CE2	2.42	0.55
1:B:530:LYS:HA	1:B:534:ASN:HD21	1.72	0.55
1:B:618:MET:HE2	1:B:622:LEU:HB2	1.89	0.54
4:A:803:MAN:C1	4:A:804:MAN:C6	2.85	0.53
1:B:325:LYS:CG	6:B:1022:HOH:O	2.57	0.52
1:A:415:VAL:HG23	1:A:594:PHE:HB3	1.92	0.51
1:B:415:VAL:HG23	1:B:594:PHE:HB3	1.94	0.49
1:A:385:LYS:O	1:A:386:THR:C	2.55	0.49
1:A:611:ASP:CG	1:A:614:HIS:HD1	2.17	0.49
1:B:601:GLN:NE2	1:B:720:GLN:HE21	2.04	0.49
1:B:308:LEU:CB	1:B:315:ILE:HD11	2.37	0.48
1:B:468:GLY:CA	1:B:471:THR:HG22	2.43	0.47
1:B:534:ASN:C	1:B:534:ASN:HD22	2.22	0.47
1:A:525:LYS:HB2	1:A:565:THR:HG22	1.96	0.47
1:A:619:TRP:HA	1:A:620:PRO:C	2.40	0.46
1:A:534:ASN:C	1:A:534:ASN:HD22	2.22	0.46
1:B:498:LEU:HD13	1:B:581:ILE:HD13	1.97	0.46
1:A:652:PHE:HB3	1:A:698:PHE:CD1	2.51	0.46
1:A:498:LEU:HD11	1:A:522:LEU:HB2	1.97	0.45
1:A:580:ALA:O	1:A:584:GLN:HG3	2.16	0.45
1:A:627:VAL:HG21	1:A:664:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:TRP:HA	1:B:620:PRO:C	2.41	0.45
1:B:498:LEU:HD11	1:B:522:LEU:HB2	1.98	0.45
1:B:614:HIS:C	6:B:941:HOH:O	2.60	0.45
1:B:241:ARG:HH11	1:B:241:ARG:HG3	1.81	0.45
1:B:439:TYR:OH	2:B:801:UDP:O1A	2.25	0.44
1:B:560:ARG:HB2	1:B:560:ARG:HH21	1.81	0.44
1:B:443:ASP:O	1:B:473:ASN:OD1	2.36	0.44
1:A:232:HIS:HB2	1:A:235:PHE:CE2	2.53	0.44
1:B:680:PRO:HG2	1:B:710:VAL:HG13	1.98	0.44
1:B:510:ALA:N	1:B:511:PRO:CD	2.81	0.44
1:B:390:LYS:HE2	6:B:1036:HOH:O	2.18	0.43
1:B:618:MET:HE3	1:B:618:MET:HB3	1.95	0.43
1:A:285:ILE:HD13	1:A:294:PRO:HG2	2.00	0.42
1:A:498:LEU:HD13	1:A:581:ILE:HD13	2.01	0.42
1:A:651:PHE:HB2	1:A:712:PRO:HB2	2.01	0.41
1:A:434:ASN:C	1:A:434:ASN:ND2	2.77	0.41
1:A:670:SER:OG	1:A:688:HIS:ND1	2.40	0.41
2:A:801:UDP:H6	6:A:909:HOH:O	2.03	0.41
1:B:371:PRO:HG2	1:B:699:SER:HA	2.04	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	503/515 (98%)	489 (97%)	14 (3%)	0	100	100
1	B	491/515 (95%)	474 (96%)	17 (4%)	0	100	100
All	All	994/1030 (96%)	963 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	433/455 (95%)	417 (96%)	16 (4%)	30	20
1	B	430/455 (94%)	416 (97%)	14 (3%)	33	23
All	All	863/910 (95%)	833 (96%)	30 (4%)	32	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	419	LEU
1	A	429	GLU
1	A	434	ASN
1	A	451	ILE
1	A	471	THR
1	A	474	ILE
1	A	505	PRO
1	A	534	ASN
1	A	560	ARG
1	A	583	ASN
1	A	663	LYS
1	A	666	VAL
1	A	672	GLU
1	A	679	VAL
1	A	718	LYS
1	B	280	GLU
1	B	326	GLU
1	B	419	LEU
1	B	451	ILE
1	B	466	VAL
1	B	471	THR
1	B	532	SER
1	B	534	ASN
1	B	560	ARG
1	B	568	LEU
1	B	582	LEU

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Mol	Chain	Res	Type
1	B	672	GLU
1	B	679	VAL
1	B	710	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	A	517	ASN
1	A	534	ASN
1	A	571	GLN
1	A	601	GLN
1	A	720	GLN
1	B	435	GLN
1	B	473	ASN
1	B	534	ASN
1	B	571	GLN
1	B	601	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	MAN	A	803	-	11,11,12	1.42	2 (18%)	15,15,17	2.05	3 (20%)
3	NAG	B	802	-	14,14,15	1.14	1 (7%)	17,19,21	2.82	4 (23%)
4	MAN	A	804	-	12,12,12	1.21	1 (8%)	17,17,17	1.55	3 (17%)
2	UDP	A	801	-	25,26,26	0.57	0	38,40,40	0.84	2 (5%)
5	SO4	B	803	-	4,4,4	0.22	0	6,6,6	0.26	0
2	UDP	B	801	-	25,26,26	0.97	2 (8%)	38,40,40	0.86	1 (2%)
3	NAG	A	802	-	14,14,15	0.71	0	17,19,21	1.78	2 (11%)

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	MAN	A	803	-	-	2/2/19/22	0/1/1/1
3	NAG	B	802	-	-	3/6/23/26	0/1/1/1
4	MAN	A	804	-	-	0/2/22/22	0/1/1/1
2	UDP	A	801	-	-	5/16/32/32	0/2/2/2
2	UDP	B	801	-	-	3/16/32/32	0/2/2/2
3	NAG	A	802	-	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	MAN	C2-C3	-3.67	1.46	1.52
4	A	804	MAN	C1-C2	2.90	1.59	1.52
2	B	801	UDP	PA-O3A	2.76	1.62	1.59
4	A	803	MAN	C1-C2	-2.30	1.46	1.52
3	B	802	NAG	C1-C2	2.28	1.55	1.52
2	B	801	UDP	PB-O1B	-2.03	1.44	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	NAG	C2-N2-C7	8.12	133.78	122.90
3	B	802	NAG	C1-C2-N2	6.86	121.24	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	MAN	O3-C3-C2	-5.32	99.20	110.05
3	A	802	NAG	C2-N2-C7	4.70	129.20	122.90
4	A	803	MAN	O2-C2-C3	-4.21	101.44	110.15
3	A	802	NAG	C1-C2-N2	4.07	116.85	110.43
4	A	804	MAN	O1-C1-O5	-3.36	100.42	110.41
4	A	804	MAN	O5-C1-C2	2.91	115.41	110.30
3	B	802	NAG	C1-O5-C5	2.86	116.01	112.19
2	B	801	UDP	O3'-C3'-C4'	-2.62	103.56	111.08
3	B	802	NAG	O6-C6-C5	2.58	120.12	111.33
2	A	801	UDP	O2A-PA-O1A	2.09	122.15	112.44
4	A	804	MAN	C3-C4-C5	-2.06	106.49	110.23
4	A	803	MAN	O5-C1-C2	-2.04	105.92	110.79
2	A	801	UDP	O3B-PB-O3A	-2.00	97.91	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	UDP	C5'-O5'-PA-O1A
2	A	801	UDP	C5'-O5'-PA-O3A
2	B	801	UDP	O4'-C4'-C5'-O5'
3	A	802	NAG	C1-C2-N2-C7
3	B	802	NAG	C1-C2-N2-C7
3	B	802	NAG	C8-C7-N2-C2
3	B	802	NAG	O7-C7-N2-C2
4	A	803	MAN	C4-C5-C6-O6
3	A	802	NAG	C8-C7-N2-C2
4	A	803	MAN	O5-C5-C6-O6
3	A	802	NAG	O7-C7-N2-C2
2	B	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	C5'-O5'-PA-O2A
2	B	801	UDP	PB-O3A-PA-O1A

There are no ring outliers.

5 monomers are involved in 6 short contacts:

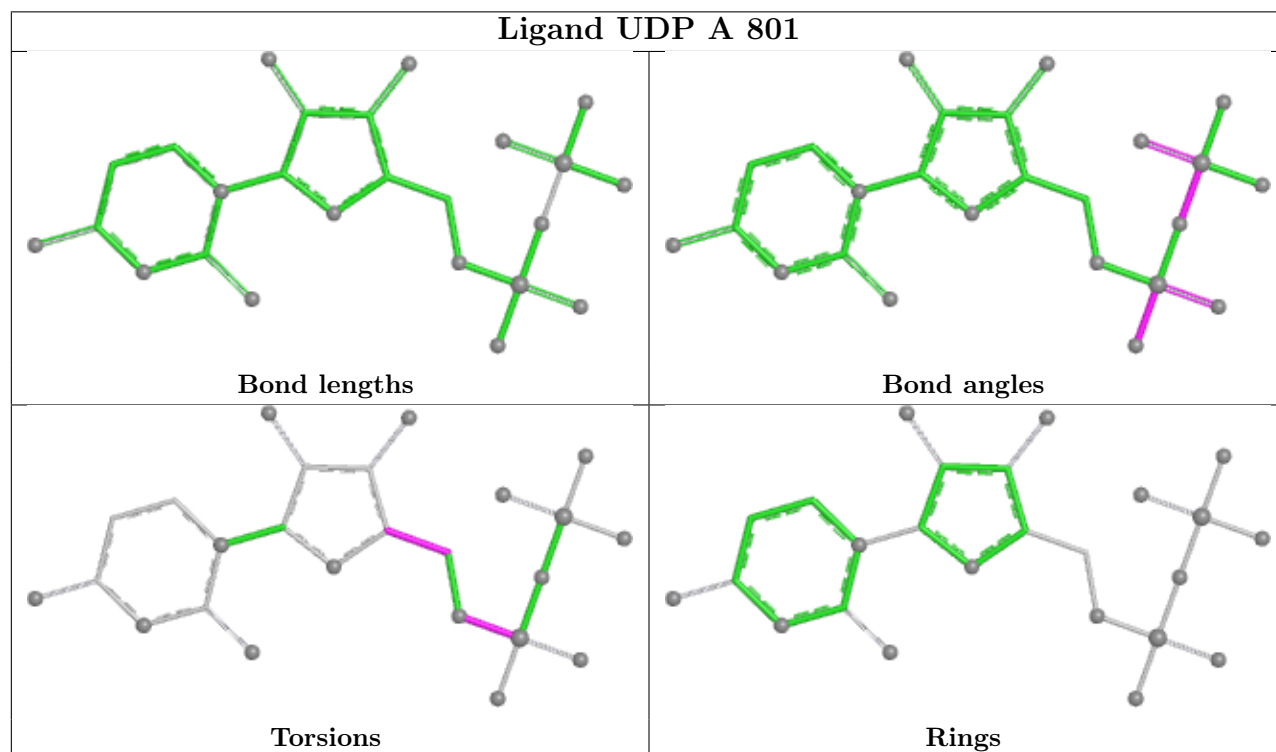
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	MAN	4	0
4	A	804	MAN	2	0

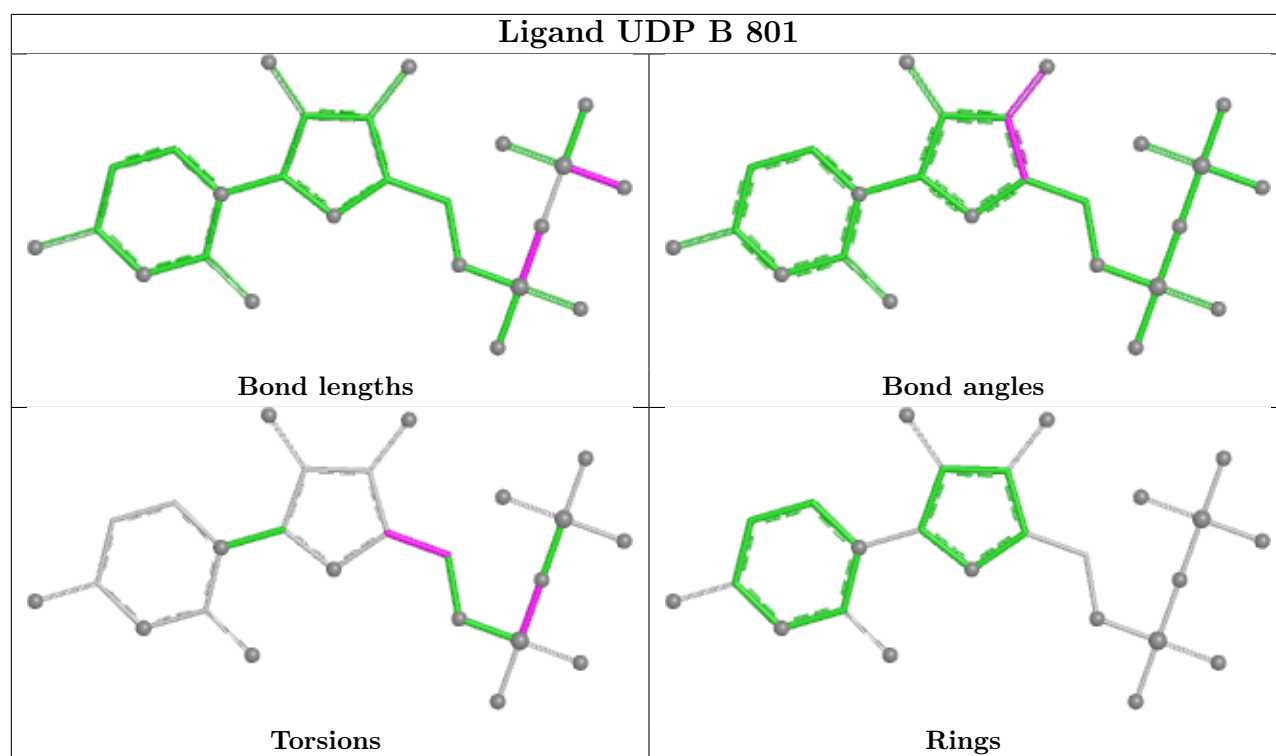
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	UDP	1	0
2	B	801	UDP	1	0
3	A	802	NAG	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/515 (98%)	0.23	27 (5%) 32 41	21, 36, 74, 94	0
1	B	499/515 (96%)	0.15	19 (3%) 44 54	19, 34, 72, 97	0
All	All	1008/1030 (97%)	0.19	46 (4%) 37 47	19, 35, 73, 97	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	PHE	3.8
1	A	662	LEU	3.7
1	A	474	ILE	3.7
1	A	289	ALA	3.7
1	A	471	THR	3.7
1	A	427	ILE	3.5
1	B	687	LYS	3.5
1	A	235	PHE	3.3
1	A	467	TYR	3.3
1	A	655	LEU	3.2
1	B	421	SER	3.2
1	B	666	VAL	3.2
1	B	662	LEU	3.1
1	A	491	PHE	3.0
1	A	294	PRO	2.9
1	A	421	SER	2.9
1	B	468	GLY	2.9
1	A	448	ASN	2.8
1	A	451	ILE	2.8
1	B	668	CYS	2.8
1	A	293	GLY	2.6
1	A	466	VAL	2.6
1	B	450	LYS	2.4
1	B	471	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	684	PRO	2.4
1	A	237	TRP	2.4
1	B	659	LYS	2.4
1	A	290	PHE	2.3
1	A	684	PRO	2.3
1	A	666	VAL	2.3
1	A	483	ILE	2.3
1	A	285	ILE	2.3
1	B	445	VAL	2.3
1	A	667	THR	2.3
1	B	427	ILE	2.2
1	A	665	LYS	2.2
1	B	451	ILE	2.2
1	A	329	GLY	2.1
1	A	286	ALA	2.1
1	B	664	TYR	2.1
1	B	667	THR	2.1
1	B	280	GLU	2.1
1	B	665	LYS	2.1
1	B	424	ILE	2.0
1	B	281	SER	2.0
1	A	614	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	A	804	12/12	0.63	0.18	73,90,104,108	0

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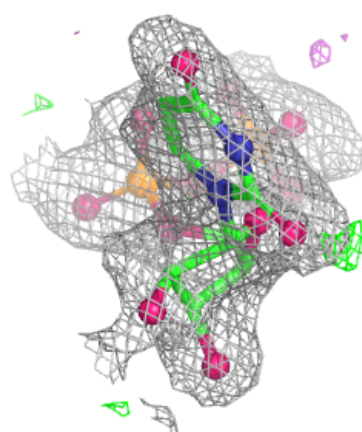
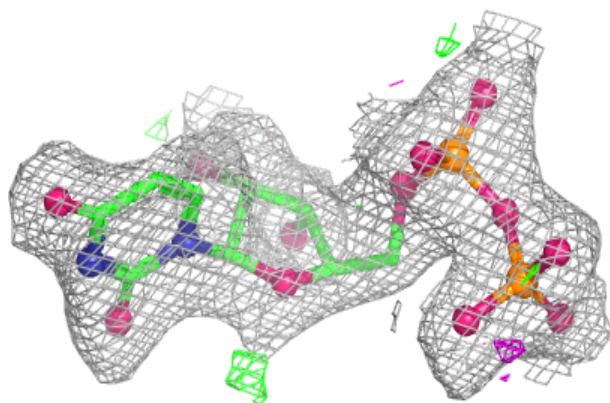
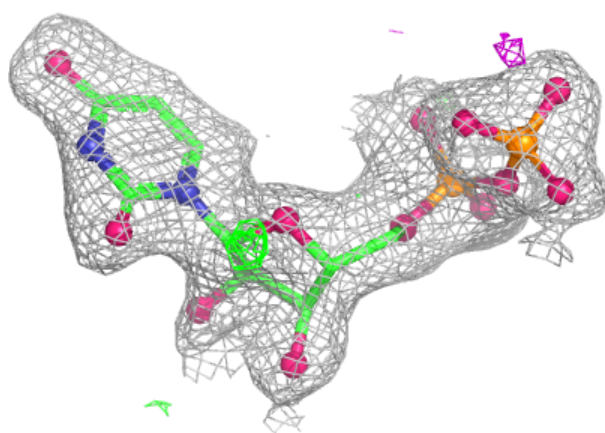
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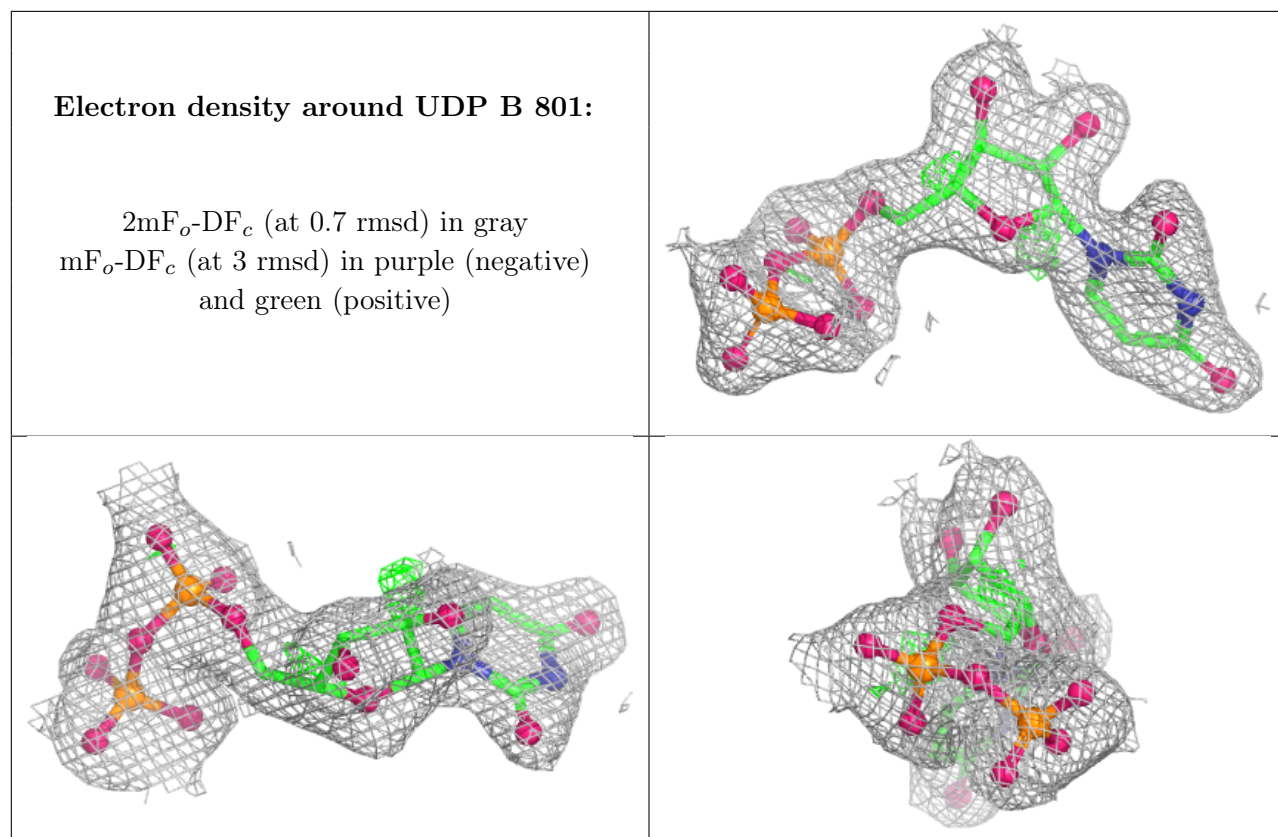
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	802	14/15	0.83	0.13	32,52,59,60	0
4	MAN	A	803	11/12	0.85	0.13	24,28,30,31	11
3	NAG	A	802	14/15	0.90	0.10	31,39,65,70	0
2	UDP	A	801	25/25	0.94	0.09	25,38,42,43	25
5	SO4	B	803	5/5	0.94	0.07	50,61,66,75	0
2	UDP	B	801	25/25	0.96	0.07	18,22,25,27	25

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 801:

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.