Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 01:36 am GMT

PDB ID	:	6YJT
Title	:	Crystal structure of MGAT5 (alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase V) luminal domain with a Lys329-Ile345 loop truncation, in complex with UDP
Authors	:	Wu, L.; Darby, J.F.; Gilio, A.K.; Davies, G.J.
Deposited on	:	2020-04-04
Resolution	:	1.70 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:

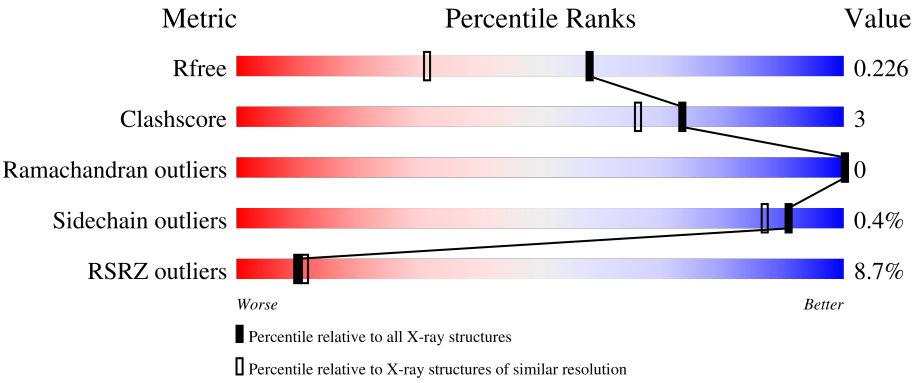
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	515	8% 90% 9%
1	BBB	515	10% 90% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17000 atoms, of which 8312 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 Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyl transferase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	513	Total	C	H	N	O	S	208	0	0
			8274	2662	4136	712	738	26			
1	BBB	506	Total	C	H	N	O	S	204	0	0
			8158	2625	4078	703	726	26			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	ASN	deletion	UNP Q09328
AAA	?	-	ARG	deletion	UNP Q09328
AAA	?	-	SER	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	CYS	deletion	UNP Q09328
AAA	?	-	PRO	deletion	UNP Q09328
AAA	?	-	THR	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	330	GLY	ASP	conflict	UNP Q09328
AAA	331	GLY	ARG	conflict	UNP Q09328
AAA	332	GLY	ILE	conflict	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	ASN	deletion	UNP Q09328
BBB	?	-	ARG	deletion	UNP Q09328
BBB	?	-	SER	deletion	UNP Q09328

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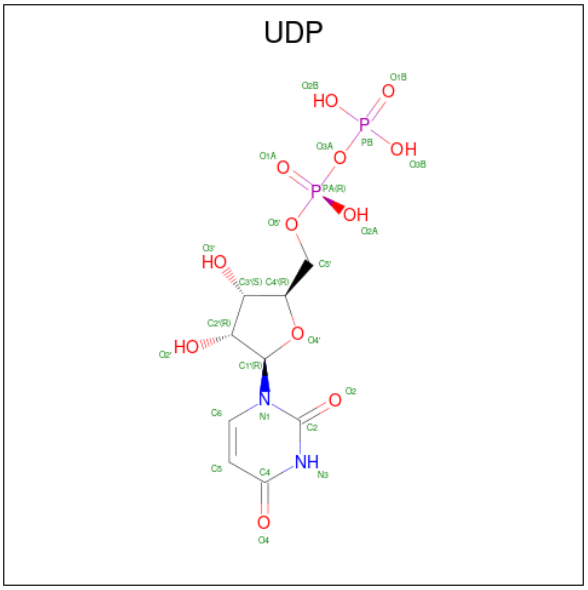
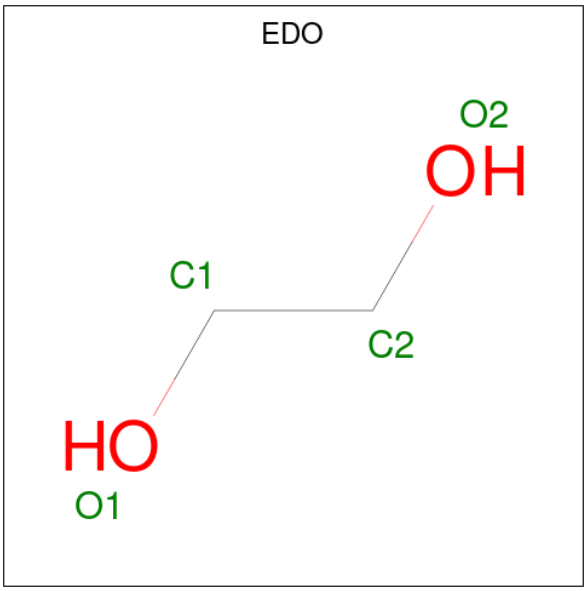
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	CYS	deletion	UNP Q09328
BBB	?	-	PRO	deletion	UNP Q09328
BBB	?	-	THR	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	330	GLY	ASP	conflict	UNP Q09328
BBB	331	GLY	ARG	conflict	UNP Q09328
BBB	332	GLY	ILE	conflict	UNP Q09328

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



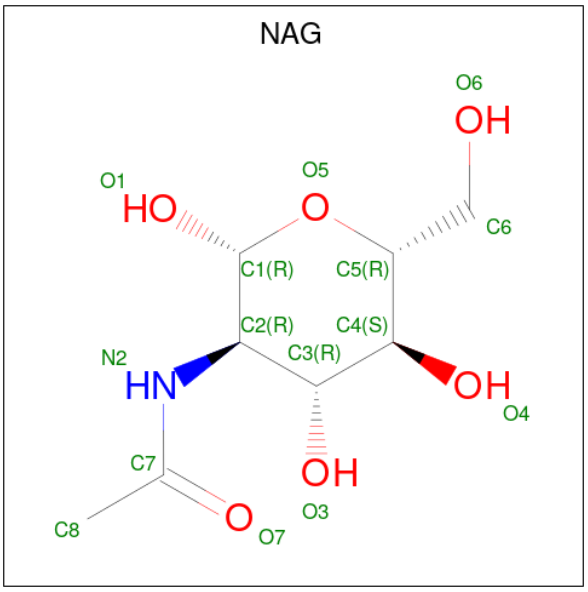
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	P	2	0
			36	9	11	2	12	2		
2	BBB	1	Total	C	H	N	O	P	2	0
			36	9	11	2	12	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



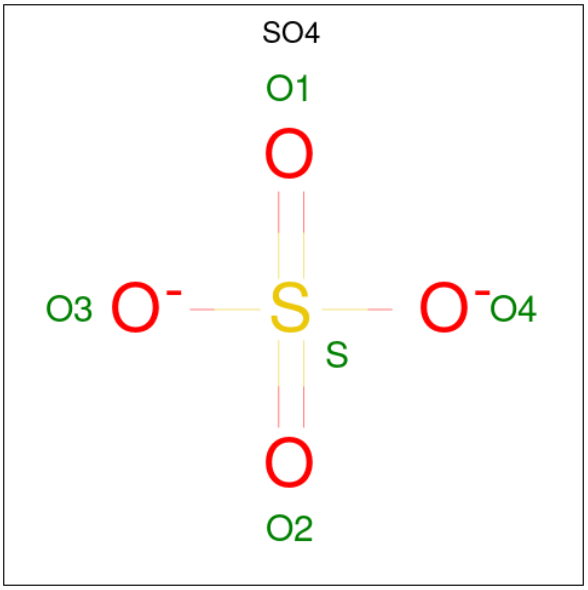
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 6 is water.

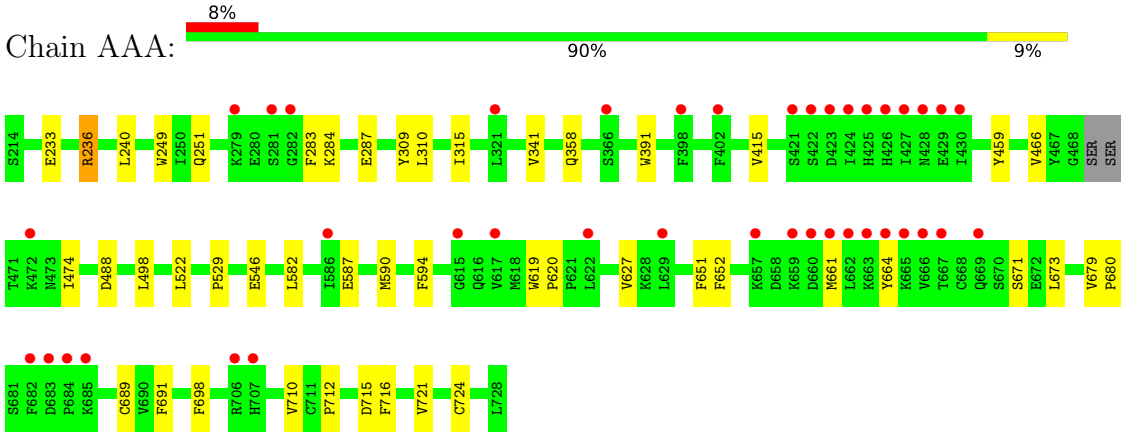
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	163	Total O 163 163	0	0
6	BBB	167	Total O 167 167	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

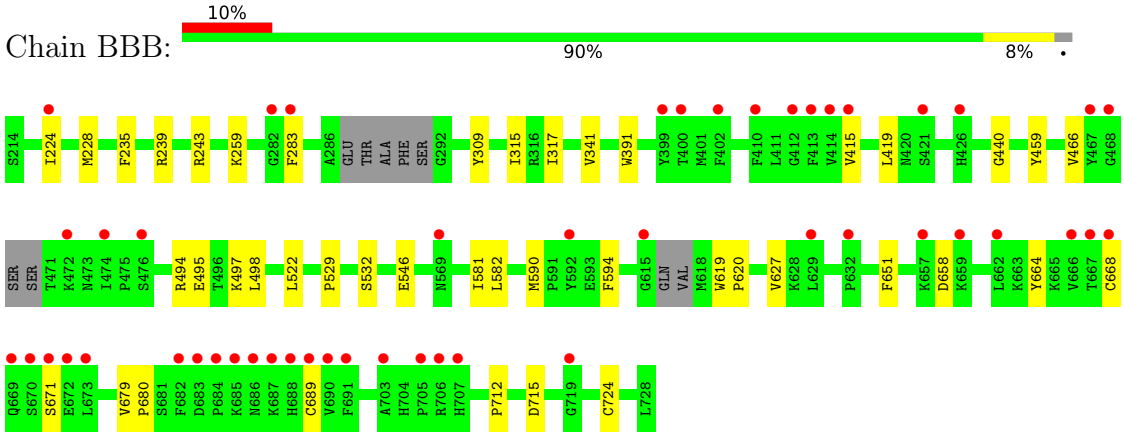
• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain AAA:



• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.03Å 69.59Å 90.00Å 107.77° 91.81° 106.94°	Depositor
Resolution (Å)	43.43 – 1.70 43.43 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (43.43-1.70) 95.6 (43.43-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.184 , 0.223 0.192 , 0.226	Depositor DCC
R_{free} test set	3727 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	17000	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% 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: NAG, UDP, EDO, 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	AAA	0.67	0/4246	0.78	0/5735
1	BBB	0.66	0/4185	0.82	0/5650
All	All	0.67	0/8431	0.80	0/11385

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	AAA	4138	4136	4112	27	0
1	BBB	4080	4078	4050	29	0
2	AAA	25	11	11	0	0
2	BBB	25	11	11	0	0
3	AAA	16	24	24	1	0
3	BBB	16	24	24	2	0
4	AAA	14	14	13	0	0
4	BBB	14	14	13	0	0
5	AAA	5	0	0	0	0
5	BBB	25	0	0	0	0
6	AAA	163	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	167	0	0	2	0
All	All	8688	8312	8258	54	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 3.

All (54) 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:AAA:236:ARG:NH2	1:BBB:495:GLU:OE2	2.22	0.72
1:AAA:671:SER:HA	1:AAA:689:CYS:O	1.97	0.64
1:BBB:671:SER:HA	1:BBB:689:CYS:O	1.97	0.64
1:AAA:283:PHE:HE2	1:AAA:341:VAL:HG21	1.64	0.63
1:AAA:529:PRO:HB2	1:AAA:546:GLU:HB3	1.82	0.60
1:BBB:419:LEU:HD21	1:BBB:494:ARG:HG3	1.84	0.60
1:AAA:661:MET:CE	1:AAA:710:VAL:HG21	2.32	0.59
1:BBB:224:ILE:O	1:BBB:228:MET:HG3	2.01	0.59
1:BBB:651:PHE:HB2	1:BBB:712:PRO:HB2	1.84	0.58
1:AAA:661:MET:HE3	1:AAA:710:VAL:HG21	1.85	0.57
1:BBB:459:TYR:HB3	1:BBB:582:LEU:HD11	1.88	0.55
1:BBB:497:LYS:HE3	6:BBB:1029:HOH:O	2.07	0.54
1:BBB:419:LEU:CD2	1:BBB:494:ARG:HG3	2.36	0.54
1:AAA:651:PHE:HB2	1:AAA:712:PRO:HB2	1.89	0.54
1:AAA:415:VAL:HG23	1:AAA:594:PHE:HB3	1.89	0.53
1:BBB:415:VAL:HG23	1:BBB:594:PHE:HB3	1.92	0.51
1:AAA:619:TRP:HA	1:AAA:620:PRO:C	2.31	0.51
1:AAA:466:VAL:HG11	1:AAA:474:ILE:CD1	2.41	0.51
1:BBB:619:TRP:HA	1:BBB:620:PRO:C	2.31	0.51
1:AAA:673:LEU:HD23	1:AAA:691:PHE:HB2	1.93	0.50
1:AAA:284:LYS:HA	1:AAA:287:GLU:HG3	1.94	0.49
1:AAA:415:VAL:HB	1:AAA:590:MET:HE3	1.95	0.49
1:BBB:283:PHE:CE2	1:BBB:341:VAL:HG21	2.47	0.49
1:BBB:415:VAL:HB	1:BBB:590:MET:HE3	1.97	0.47
1:AAA:459:TYR:HB3	1:AAA:582:LEU:HD11	1.96	0.47
1:BBB:235:PHE:O	1:BBB:239:ARG:HG3	2.14	0.47
1:BBB:529:PRO:HB2	1:BBB:546:GLU:HB3	1.96	0.46
1:BBB:627:VAL:HG21	1:BBB:664:TYR:CG	2.50	0.46
1:AAA:673:LEU:CD2	1:AAA:691:PHE:HB2	2.45	0.46
1:BBB:498:LEU:HD11	1:BBB:522:LEU:HB2	1.97	0.45
1:AAA:309:TYR:N	1:AAA:315:ILE:HD11	2.32	0.45
1:BBB:498:LEU:HD13	1:BBB:581:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:283:PHE:CZ	1:BBB:341:VAL:HG21	2.53	0.44
1:AAA:488:ASP:OD1	1:BBB:243:ARG:NH1	2.50	0.43
1:AAA:716:PHE:HB2	1:AAA:721:VAL:HA	2.00	0.43
1:AAA:498:LEU:HD11	1:AAA:522:LEU:HB2	2.00	0.43
1:BBB:309:TYR:N	1:BBB:315:ILE:HD11	2.33	0.43
1:BBB:658:ASP:OD1	1:BBB:668:CYS:HB2	2.17	0.43
1:AAA:679:VAL:HA	1:AAA:680:PRO:C	2.39	0.43
1:BBB:532:SER:CB	3:BBB:804:EDO:C2	2.97	0.43
1:AAA:249:TRP:HB3	1:AAA:310:LEU:HD11	2.00	0.43
1:BBB:679:VAL:HA	1:BBB:680:PRO:C	2.39	0.43
1:AAA:391:TRP:CE2	3:AAA:804:EDO:H12	2.54	0.42
1:BBB:497:LYS:HE2	1:BBB:581:ILE:O	2.19	0.42
1:AAA:652:PHE:HB3	1:AAA:698:PHE:CD1	2.54	0.42
1:AAA:251:GLN:HG3	6:AAA:941:HOH:O	2.19	0.42
1:AAA:233:GLU:OE1	1:AAA:236:ARG:NH1	2.53	0.41
1:BBB:440:GLY:O	1:BBB:466:VAL:HG22	2.20	0.41
1:AAA:715:ASP:OD1	1:AAA:724:CYS:HB2	2.19	0.41
1:BBB:715:ASP:OD1	1:BBB:724:CYS:HB2	2.19	0.41
1:AAA:627:VAL:HG21	1:AAA:664:TYR:CG	2.56	0.41
1:BBB:259:LYS:O	6:BBB:901:HOH:O	2.21	0.41
1:BBB:315:ILE:HG22	1:BBB:317:ILE:HG13	2.02	0.41
1:BBB:391:TRP:CZ2	3:BBB:805:EDO:H12	2.56	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	AAA	509/515 (99%)	499 (98%)	10 (2%)	0	100	100
1	BBB	498/515 (97%)	487 (98%)	11 (2%)	0	100	100
All	All	1007/1030 (98%)	986 (98%)	21 (2%)	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	AAA	454/456 (100%)	450 (99%)	4 (1%)	78 70
1	BBB	447/456 (98%)	447 (100%)	0	100 100
All	All	901/912 (99%)	897 (100%)	4 (0%)	91 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	236	ARG
1	AAA	240	LEU
1	AAA	358	GLN
1	AAA	587	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	SO4	BBB	809	-	4,4,4	0.39	0	6,6,6	0.13	0
3	EDO	BBB	803	-	3,3,3	0.15	0	2,2,2	0.05	0
5	SO4	AAA	807	-	4,4,4	0.32	0	6,6,6	0.07	0
3	EDO	AAA	805	-	3,3,3	0.08	0	2,2,2	0.08	0
4	NAG	AAA	806	1	14,14,15	0.83	0	17,19,21	1.50	4 (23%)
2	UDP	BBB	802	-	24,26,26	0.99	1 (4%)	37,40,40	1.70	9 (24%)
3	EDO	BBB	805	-	3,3,3	0.30	0	2,2,2	0.35	0
5	SO4	BBB	808	-	4,4,4	0.34	0	6,6,6	0.09	0
3	EDO	BBB	801	-	3,3,3	0.11	0	2,2,2	0.17	0
5	SO4	BBB	807	-	4,4,4	0.40	0	6,6,6	0.12	0
3	EDO	AAA	803	-	3,3,3	0.08	0	2,2,2	0.14	0
3	EDO	AAA	802	-	3,3,3	0.12	0	2,2,2	0.42	0
5	SO4	BBB	810	-	4,4,4	0.36	0	6,6,6	0.17	0
4	NAG	BBB	806	1	14,14,15	0.60	0	17,19,21	1.18	1 (5%)
3	EDO	AAA	804	-	3,3,3	0.24	0	2,2,2	0.06	0
2	UDP	AAA	801	-	24,26,26	1.19	3 (12%)	37,40,40	1.47	6 (16%)
3	EDO	BBB	804	-	3,3,3	0.39	0	2,2,2	0.20	0
5	SO4	BBB	811	-	4,4,4	0.28	0	6,6,6	0.12	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	EDO	BBB	803	-	-	1/1/1/1	-
3	EDO	AAA	805	-	-	0/1/1/1	-
4	NAG	AAA	806	1	-	1/6/23/26	0/1/1/1
2	UDP	BBB	802	-	-	3/16/32/32	0/2/2/2
3	EDO	BBB	805	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	BBB	801	-	-	0/1/1/1	-
3	EDO	AAA	803	-	-	0/1/1/1	-
3	EDO	AAA	802	-	-	1/1/1/1	-
4	NAG	BBB	806	1	-	2/6/23/26	0/1/1/1
3	EDO	AAA	804	-	-	0/1/1/1	-
2	UDP	AAA	801	-	-	3/16/32/32	0/2/2/2
3	EDO	BBB	804	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	802	UDP	C6-C5	2.69	1.41	1.35
2	AAA	801	UDP	C4-N3	-2.67	1.33	1.38
2	AAA	801	UDP	C2-N1	2.51	1.42	1.38
2	AAA	801	UDP	C2-N3	-2.50	1.33	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	802	UDP	N3-C2-N1	4.03	120.24	114.89
2	BBB	802	UDP	O2-C2-N1	-3.76	117.78	122.79
2	BBB	802	UDP	C4-N3-C2	-3.63	121.79	126.58
2	AAA	801	UDP	C4-N3-C2	-3.48	121.98	126.58
2	AAA	801	UDP	C5-C4-N3	3.29	119.76	114.84
2	BBB	802	UDP	O4-C4-C5	-3.26	119.42	125.16
2	AAA	801	UDP	O4-C4-C5	-3.13	119.66	125.16
2	BBB	802	UDP	C5-C4-N3	3.10	119.48	114.84
2	BBB	802	UDP	O4'-C1'-C2'	-3.06	99.96	106.64
2	AAA	801	UDP	N3-C2-N1	3.00	118.87	114.89
4	BBB	806	NAG	C1-O5-C5	2.92	116.14	112.19
4	AAA	806	NAG	C1-O5-C5	2.71	115.86	112.19
4	AAA	806	NAG	O5-C5-C6	2.69	111.42	107.20
2	AAA	801	UDP	O4'-C1'-N1	2.62	114.36	108.36
2	AAA	801	UDP	C4'-O4'-C1'	-2.34	104.31	109.47
4	AAA	806	NAG	O5-C1-C2	2.31	114.93	111.29
2	BBB	802	UDP	O3B-PB-O2B	2.23	116.16	107.64
2	BBB	802	UDP	O5'-PA-O1A	-2.18	100.55	109.07
2	BBB	802	UDP	O2B-PB-O3A	2.13	111.78	104.64
4	AAA	806	NAG	C1-C2-N2	2.12	114.10	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

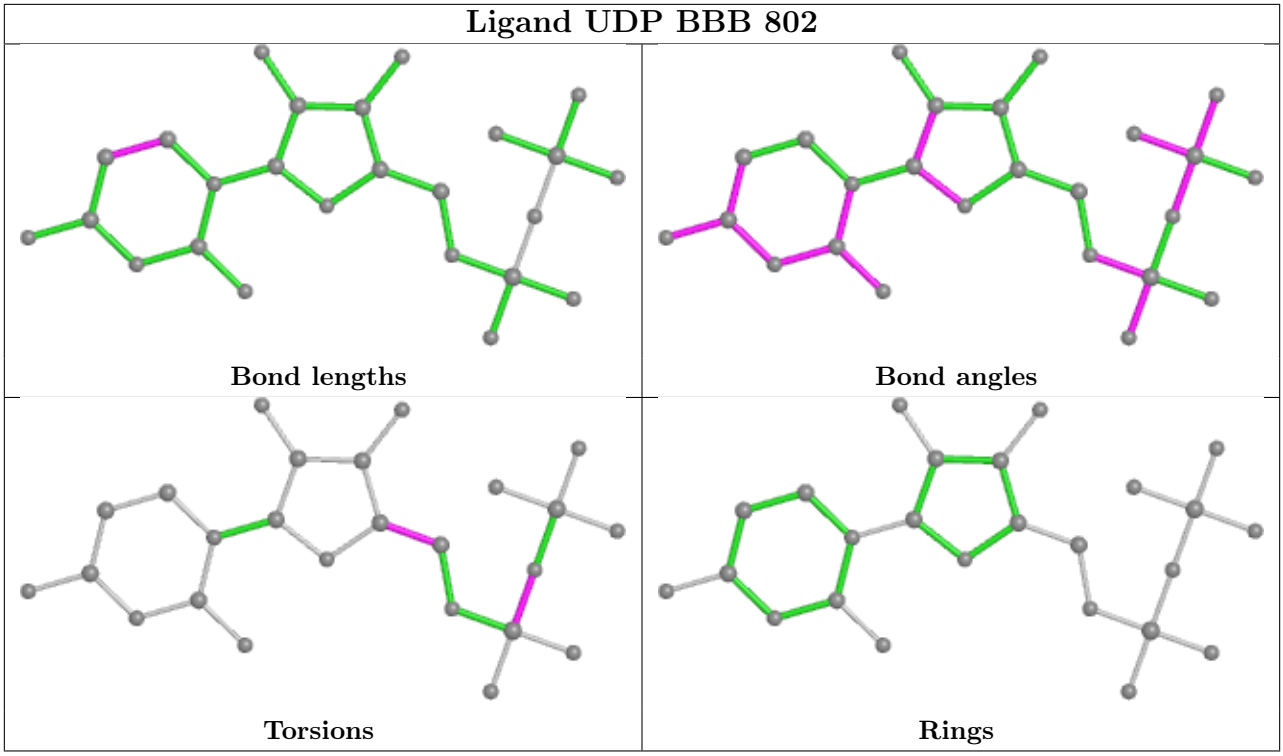
Mol	Chain	Res	Type	Atoms
2	AAA	801	UDP	C5'-O5'-PA-O1A
3	BBB	803	EDO	O1-C1-C2-O2
2	BBB	802	UDP	C3'-C4'-C5'-O5'
2	BBB	802	UDP	O4'-C4'-C5'-O5'
3	BBB	804	EDO	O1-C1-C2-O2
2	AAA	801	UDP	C5'-O5'-PA-O3A
2	AAA	801	UDP	C5'-O5'-PA-O2A
4	BBB	806	NAG	C4-C5-C6-O6
3	AAA	802	EDO	O1-C1-C2-O2
4	AAA	806	NAG	C4-C5-C6-O6
2	BBB	802	UDP	PB-O3A-PA-O2A
4	BBB	806	NAG	O5-C5-C6-O6

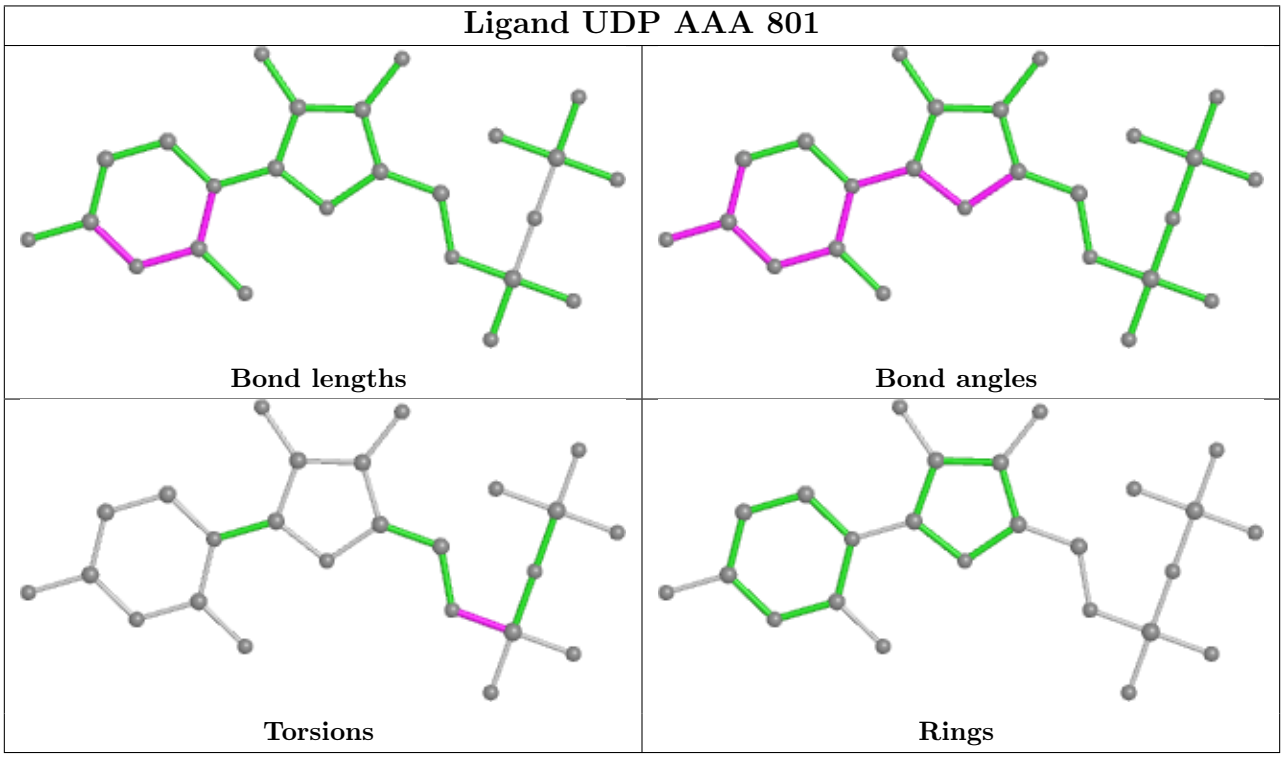
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	805	EDO	1	0
3	AAA	804	EDO	1	0
3	BBB	804	EDO	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.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	AAA	513/515 (99%)	0.42	40 (7%)	13	15	39, 54, 93, 137	0
1	BBB	506/515 (98%)	0.45	49 (9%)	7	8	39, 53, 92, 116	0
All	All	1019/1030 (98%)	0.44	89 (8%)	10	11	39, 54, 93, 137	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	662	LEU	6.9
1	AAA	424	ILE	6.7
1	AAA	425	HIS	6.7
1	AAA	666	VAL	6.0
1	BBB	667	THR	5.6
1	AAA	427	ILE	5.6
1	BBB	685	LYS	5.5
1	BBB	682	PHE	5.3
1	BBB	691	PHE	5.3
1	AAA	665	LYS	5.2
1	AAA	586	ILE	5.2
1	BBB	282	GLY	5.0
1	BBB	668	CYS	4.7
1	BBB	686	ASN	4.5
1	AAA	426	HIS	4.5
1	BBB	706	ARG	4.4
1	AAA	430	ILE	4.3
1	BBB	669	GLN	4.3
1	AAA	429	GLU	4.3
1	BBB	283	PHE	4.1
1	AAA	617	VAL	3.9
1	BBB	688	HIS	3.9
1	BBB	687	LYS	3.9
1	AAA	685	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	BBB	670	SER	3.8
1	AAA	615	GLY	3.8
1	BBB	684	PRO	3.7
1	AAA	664	TYR	3.6
1	BBB	671	SER	3.6
1	BBB	666	VAL	3.5
1	BBB	632	PRO	3.4
1	BBB	690	VAL	3.4
1	BBB	467	TYR	3.3
1	AAA	421	SER	3.3
1	BBB	707	HIS	3.2
1	AAA	669	GLN	3.2
1	BBB	683	ASP	3.1
1	AAA	667	THR	3.1
1	AAA	659	LYS	3.1
1	AAA	428	ASN	3.0
1	AAA	423	ASP	3.0
1	BBB	629	LEU	3.0
1	AAA	282	GLY	2.9
1	BBB	413	PHE	2.9
1	BBB	468	GLY	2.9
1	BBB	472	LYS	2.9
1	BBB	689	CYS	2.9
1	BBB	659	LYS	2.8
1	BBB	426	HIS	2.8
1	AAA	398	PHE	2.8
1	BBB	615	GLY	2.8
1	BBB	402	PHE	2.7
1	BBB	673	LEU	2.7
1	AAA	661	MET	2.7
1	BBB	474	ILE	2.7
1	AAA	683	ASP	2.7
1	AAA	663	LYS	2.7
1	AAA	622	LEU	2.6
1	BBB	414	VAL	2.6
1	BBB	657	LYS	2.6
1	BBB	569	ASN	2.6
1	AAA	684	PRO	2.6
1	AAA	422	SER	2.5
1	AAA	472	LYS	2.5
1	BBB	672	GLU	2.5
1	BBB	705	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	412	GLY	2.5
1	AAA	660	ASP	2.4
1	AAA	279	LYS	2.4
1	BBB	421	SER	2.4
1	AAA	706	ARG	2.4
1	BBB	476	SER	2.3
1	AAA	707	HIS	2.3
1	AAA	281	SER	2.3
1	BBB	400	THR	2.3
1	AAA	682	PHE	2.3
1	BBB	719	GLY	2.3
1	AAA	321	LEU	2.3
1	BBB	662	LEU	2.2
1	BBB	399	TYR	2.1
1	BBB	224	ILE	2.1
1	AAA	657	LYS	2.1
1	AAA	402	PHE	2.1
1	BBB	703	ALA	2.1
1	BBB	410	PHE	2.1
1	BBB	415	VAL	2.1
1	AAA	629	LEU	2.0
1	AAA	366	SER	2.0
1	BBB	592	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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.

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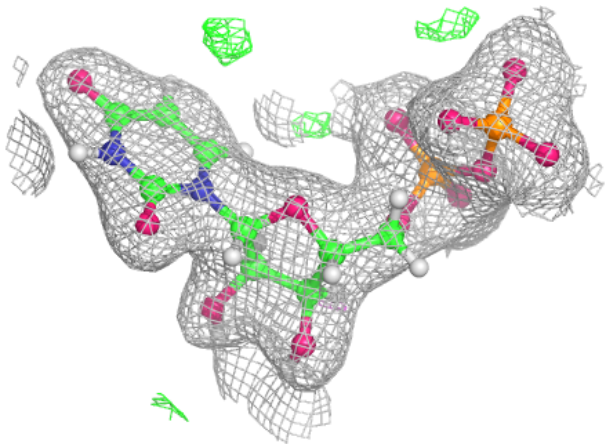
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

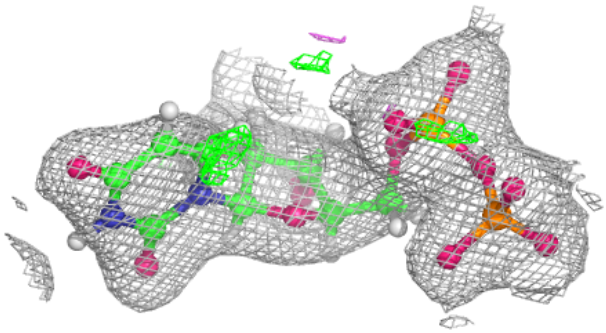
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	BBB	806	14/15	0.68	0.19	98,101,106,107	3
4	NAG	AAA	806	14/15	0.73	0.21	83,107,113,113	3
3	EDO	BBB	801	4/4	0.87	0.16	71,75,81,87	1
5	SO4	BBB	808	5/5	0.87	0.11	65,69,79,83	5
5	SO4	BBB	809	5/5	0.87	0.12	75,77,84,86	5
5	SO4	AAA	807	5/5	0.91	0.12	62,66,72,74	5
5	SO4	BBB	811	5/5	0.92	0.18	59,62,67,72	5
3	EDO	BBB	804	4/4	0.93	0.20	51,65,68,69	1
3	EDO	AAA	803	4/4	0.94	0.10	67,71,84,84	1
3	EDO	AAA	804	4/4	0.95	0.12	65,67,68,68	1
3	EDO	BBB	803	4/4	0.95	0.18	62,73,76,78	1
3	EDO	AAA	805	4/4	0.95	0.12	50,59,60,64	1
5	SO4	BBB	810	5/5	0.96	0.10	56,71,79,80	5
3	EDO	AAA	802	4/4	0.96	0.15	60,64,68,69	1
3	EDO	BBB	805	4/4	0.97	0.10	56,58,69,70	1
2	UDP	AAA	801	25/25	0.98	0.10	44,49,53,54	2
2	UDP	BBB	802	25/25	0.99	0.09	43,48,52,56	2
5	SO4	BBB	807	5/5	0.99	0.09	58,61,62,65	5

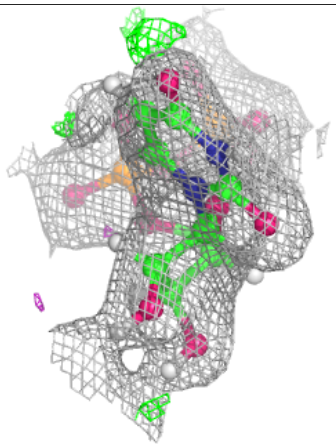
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP AAA 801:

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

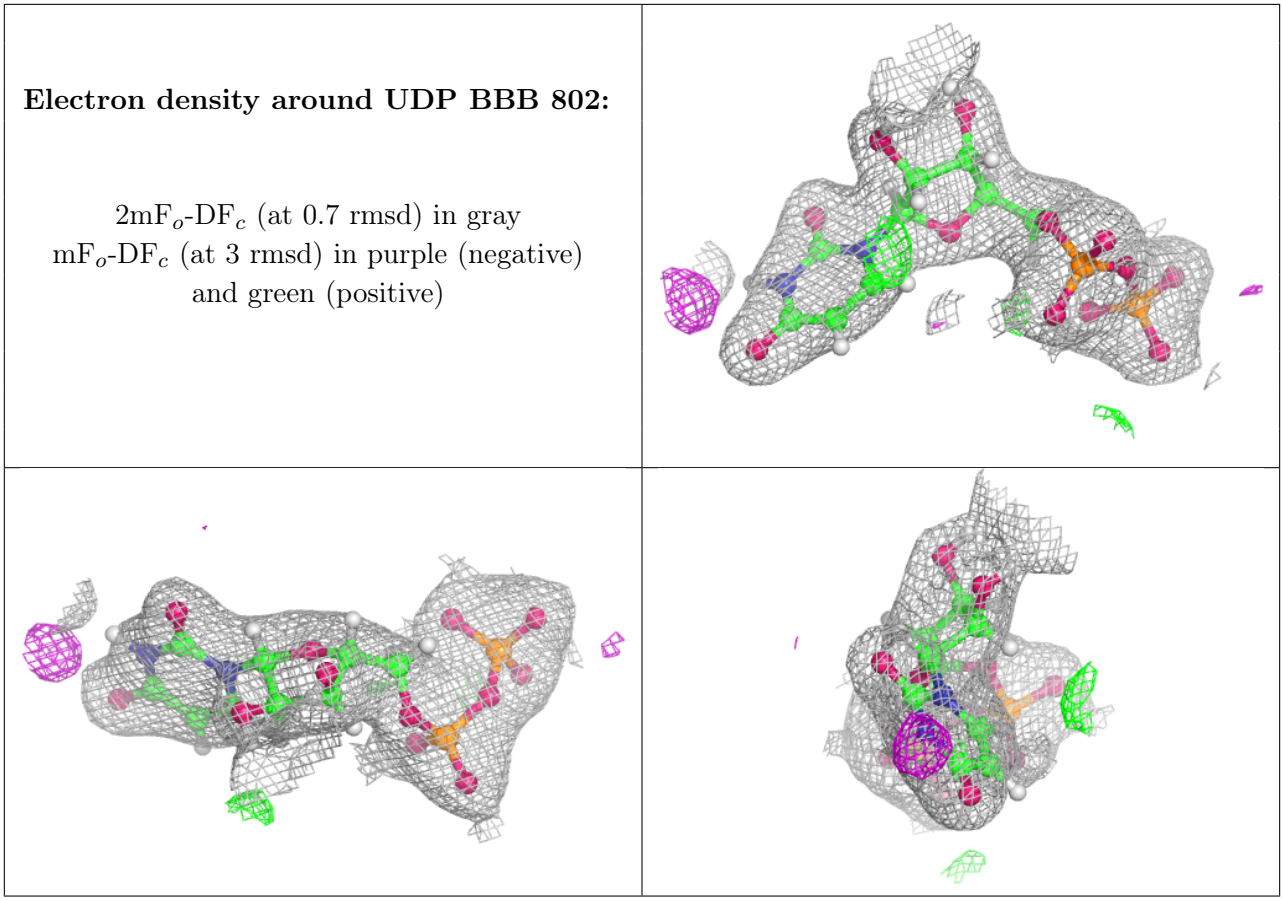






Electron density around UDP BBB 802:

$2mF_o$-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

There are no such residues in this entry.