wwPDB X-ray Structure Validation Summary Report (i)

Feb 23, 2022 – 07:16 pm GMT

PDB ID	:	6TBG
Title	:	Structure of a beta galactosidase with inhibitor
Authors	:	Offen, W.; Davies, G.
Deposited on	:	2019-11-01
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

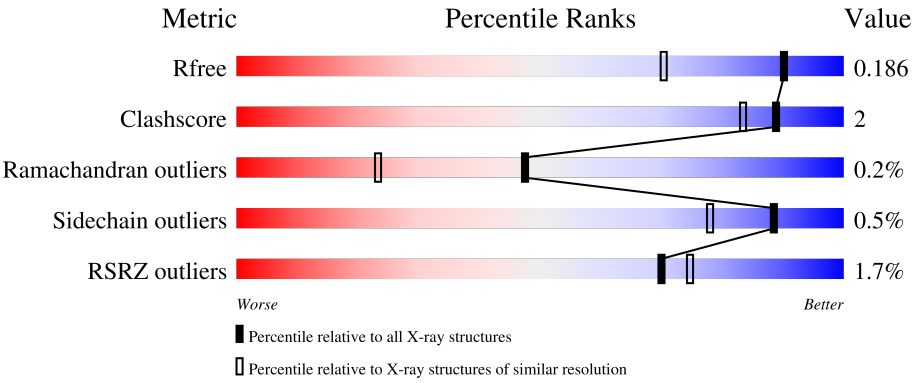
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	550	2% 95%
1	B	550	2% 93% 5%
1	C	550	% 93%
1	D	550	% 94%
1	E	550	% 95%

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Mol	Chain	Length	Quality of chain
1	F	550	2% 95%
1	G	550	% 95%
1	H	550	4% 91% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39417 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	6	0
			4252	2721	723	792	16			
1	B	540	Total	C	N	O	S	0	12	0
			4346	2783	744	803	16			
1	C	537	Total	C	N	O	S	0	9	0
			4287	2742	734	795	16			
1	D	539	Total	C	N	O	S	0	9	0
			4296	2752	726	802	16			
1	E	540	Total	C	N	O	S	0	10	0
			4334	2777	734	806	17			
1	F	539	Total	C	N	O	S	0	14	0
			4368	2801	743	808	16			
1	G	540	Total	C	N	O	S	0	17	0
			4411	2825	754	816	16			
1	H	537	Total	C	N	O	S	0	13	0
			4312	2755	734	807	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0
2	B	2	Total Na 2 2	0	0
2	C	4	Total Na 4 4	0	0
2	D	5	Total Na 5 5	0	0
2	E	5	Total Na 5 5	0	0
2	F	4	Total Na 4 4	0	0
2	G	4	Total Na 4 4	0	0

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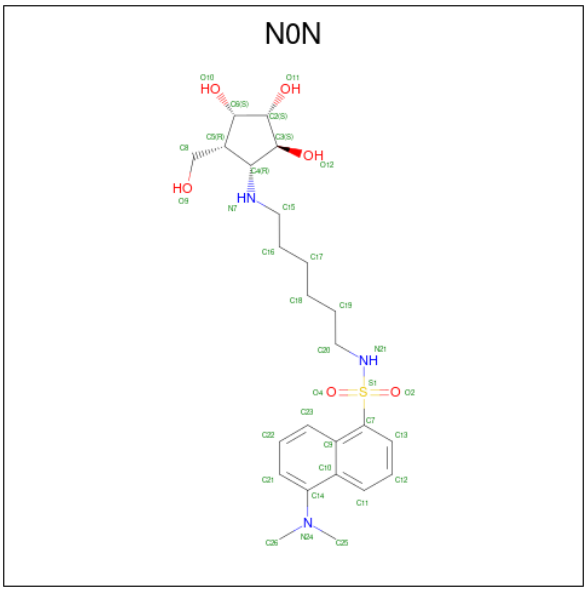
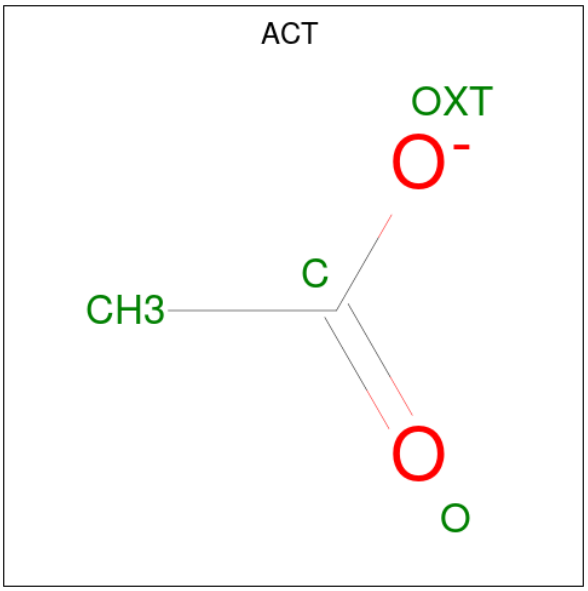
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Na 2 2	0	0

- Molecule 3 is 5-(dimethylamino)- {N}-[6-[[(1 {R},2 {R},3 {S},4 {S},5 {S})-2-(hydroxymethyl)-3,4,5-tris(oxidanyl)cyclopentyl]amino]hexyl]naphthalene-1-sulfonamide (three-letter code: N0N) (formula: $C_{24}H_{37}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 21 12 2 6 1	0	0
3	B	1	Total C N O 15 10 1 4	0	0
3	C	1	Total C N O S 21 12 2 6 1	0	0
3	D	1	Total C N O S 34 24 3 6 1	0	0
3	E	1	Total C N O S 34 24 3 6 1	0	0
3	F	1	Total C N O S 34 24 3 6 1	0	0
3	G	1	Total C N O S 34 24 3 6 1	0	0
3	H	1	Total C N O S 21 12 2 6 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

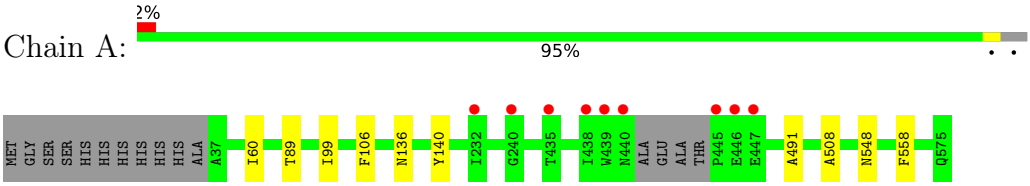
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	484	Total O 484 484	0	0
5	B	565	Total O 566 566	0	1
5	C	541	Total O 542 542	0	1
5	D	600	Total O 600 600	0	0
5	E	621	Total O 621 621	0	0
5	F	528	Total O 528 528	0	0
5	G	660	Total O 660 660	0	0
5	H	493	Total O 494 494	0	1

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.

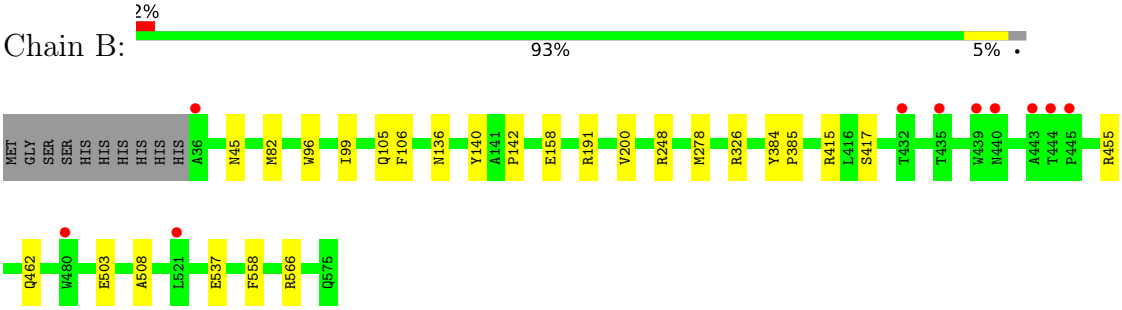
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain A:



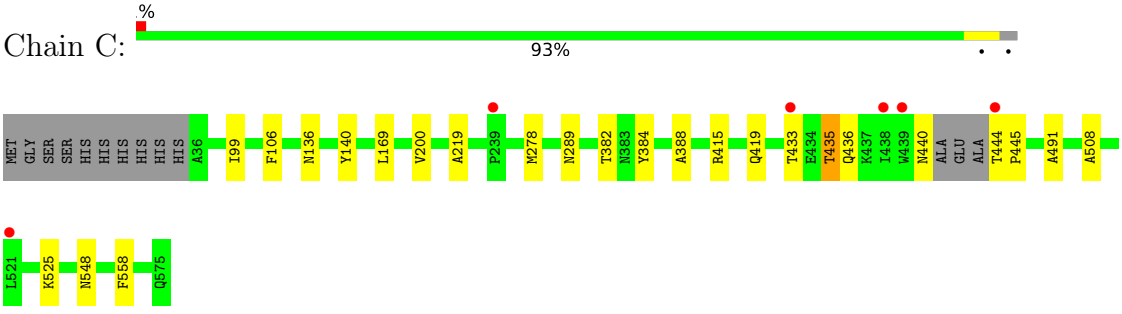
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain B:



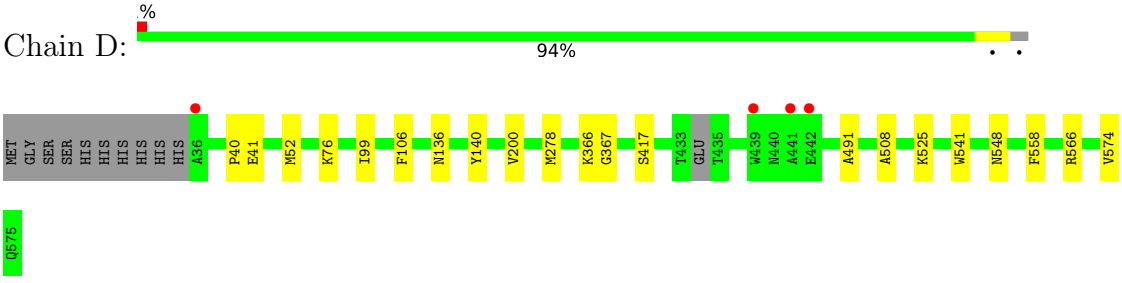
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain C:



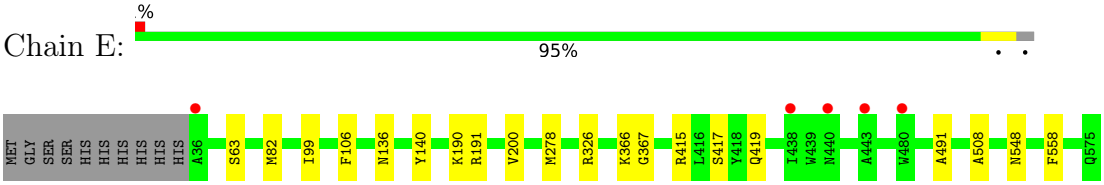
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain D:



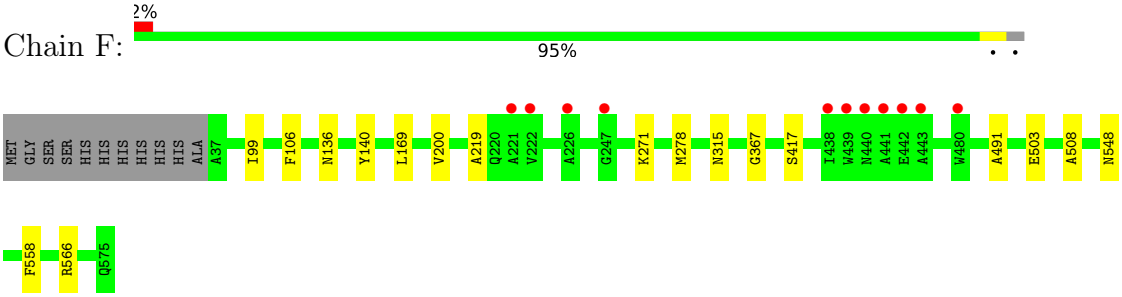
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain E:



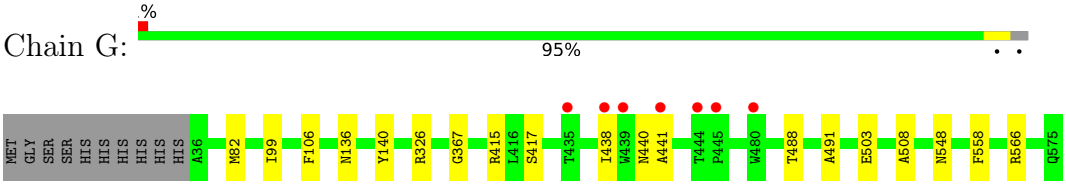
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain F:



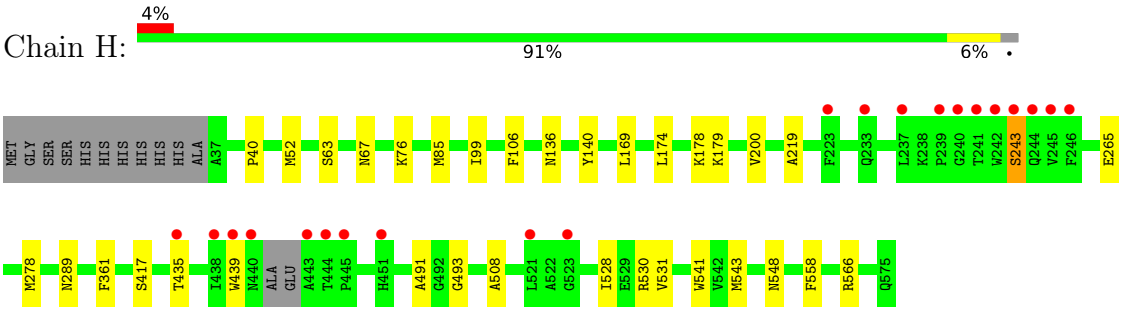
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain G:



• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.28Å 115.73Å 115.98Å 90.12° 90.00° 90.03°	Depositor
Resolution (Å)	115.98 – 1.50 115.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (115.98-1.50) 96.5 (115.98-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.138 , 0.182 0.146 , 0.186	Depositor DCC
R_{free} test set	40094 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,l,-k 0.014 for h,-l,k 0.013 for h,-k,-l 0.004 for -h,k,-l 0.004 for -h,-k,l 0.002 for -h,l,k 0.006 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	39417	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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: N0N, NA, ACT

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	0.63	0/4364	0.74	0/5945
1	B	0.62	0/4466	0.75	0/6085
1	C	0.63	0/4400	0.75	0/5994
1	D	0.63	0/4414	0.75	0/6017
1	E	0.63	0/4454	0.75	0/6067
1	F	0.63	0/4487	0.76	0/6110
1	G	0.61	0/4530	0.75	0/6169
1	H	0.63	0/4428	0.75	0/6031
All	All	0.63	0/35543	0.75	0/48418

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	4252	0	4074	5	0
1	B	4346	0	4173	25	0
1	C	4287	0	4111	19	0
1	D	4296	0	4115	11	0
1	E	4334	0	4164	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4368	0	4196	9	0
1	G	4411	0	4238	18	0
1	H	4312	0	4111	24	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	2	0	0	0	0
3	A	21	0	0	0	0
3	B	15	0	0	0	0
3	C	21	0	0	0	0
3	D	34	0	0	1	0
3	E	34	0	0	0	0
3	F	34	0	0	0	0
3	G	34	0	0	1	0
3	H	21	0	0	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	16	0	12	0	0
4	E	12	0	9	1	0
4	F	8	0	6	0	0
4	G	16	0	12	0	0
4	H	4	0	3	0	0
5	A	484	0	0	0	0
5	B	566	0	0	14	0
5	C	542	0	0	1	0
5	D	600	0	0	2	0
5	E	621	0	0	10	0
5	F	528	0	0	0	0
5	G	660	0	0	9	0
5	H	494	0	0	5	0
All	All	39417	0	33236	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 127 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191[B]:ARG:NH1	5:B:701:HOH:O	1.61	1.30
1:B:248:ARG:HD2	5:B:973:HOH:O	1.35	1.23
1:F:503:GLU:OE2	1:F:566[B]:ARG:HD3	1.51	1.08
1:E:415[B]:ARG:CZ	5:E:702:HOH:O	2.06	1.03
1:G:415[B]:ARG:CZ	5:G:703:HOH:O	2.08	1.01

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	537/550 (98%)	517 (96%)	19 (4%)	1 (0%)	47	23
1	B	550/550 (100%)	530 (96%)	20 (4%)	0	100	100
1	C	542/550 (98%)	521 (96%)	20 (4%)	1 (0%)	47	23
1	D	544/550 (99%)	523 (96%)	20 (4%)	1 (0%)	47	23
1	E	548/550 (100%)	525 (96%)	22 (4%)	1 (0%)	47	23
1	F	551/550 (100%)	531 (96%)	19 (3%)	1 (0%)	47	23
1	G	556/550 (101%)	533 (96%)	22 (4%)	1 (0%)	47	23
1	H	547/550 (100%)	524 (96%)	22 (4%)	1 (0%)	47	23
All	All	4375/4400 (99%)	4204 (96%)	164 (4%)	7 (0%)	47	23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	ALA
1	C	491	ALA
1	E	491	ALA
1	F	491	ALA
1	G	491	ALA

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	436/461 (95%)	435 (100%)	1 (0%)	93	86
1	B	445/461 (96%)	440 (99%)	5 (1%)	73	53
1	C	439/461 (95%)	436 (99%)	3 (1%)	84	69
1	D	441/461 (96%)	439 (100%)	2 (0%)	88	78
1	E	446/461 (97%)	445 (100%)	1 (0%)	93	86
1	F	448/461 (97%)	447 (100%)	1 (0%)	93	86
1	G	453/461 (98%)	451 (100%)	2 (0%)	91	82
1	H	440/461 (95%)	437 (99%)	3 (1%)	84	69
All	All	3548/3688 (96%)	3530 (100%)	18 (0%)	88	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	136	ASN
1	H	289	ASN
1	H	243	SER
1	C	435	THR
1	G	82	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	C	289	ASN
1	D	45	ASN
1	G	307	HIS
1	H	289	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 30 are monoatomic - leaving 26 for Mogul analysis.

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	N0N	G	603	-	36,36,36	2.82	5 (13%)	48,51,51	2.20	12 (25%)
4	ACT	G	607	-	1,3,3	3.46	1 (100%)	0,3,3	-	-
4	ACT	B	604	-	1,3,3	3.34	1 (100%)	0,3,3	-	-
3	N0N	F	604	-	36,36,36	2.75	4 (11%)	48,51,51	1.74	10 (20%)
4	ACT	D	608	-	1,3,3	3.71	1 (100%)	0,3,3	-	-
4	ACT	F	605	-	1,3,3	3.83	1 (100%)	0,3,3	-	-
3	N0N	H	602	-	19,21,36	0.79	1 (5%)	20,27,51	1.04	2 (10%)
4	ACT	H	603	-	1,3,3	3.93	1 (100%)	0,3,3	-	-
4	ACT	D	606	-	1,3,3	2.93	1 (100%)	0,3,3	-	-
3	N0N	D	605	-	36,36,36	2.76	5 (13%)	48,51,51	1.95	10 (20%)
3	N0N	B	602	-	15,15,36	0.79	0	17,20,51	1.31	2 (11%)
4	ACT	E	607	-	1,3,3	3.37	1 (100%)	0,3,3	-	-
3	N0N	E	604	-	36,36,36	2.75	6 (16%)	48,51,51	1.76	9 (18%)
4	ACT	D	604	-	1,3,3	3.04	1 (100%)	0,3,3	-	-
4	ACT	F	606	-	1,3,3	3.89	1 (100%)	0,3,3	-	-
4	ACT	C	604	-	1,3,3	3.68	1 (100%)	0,3,3	-	-
4	ACT	B	603	-	1,3,3	3.62	1 (100%)	0,3,3	-	-
4	ACT	A	603	-	1,3,3	3.91	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	G	606	-	1,3,3	4.19	1 (100%)	0,3,3	-	-
4	ACT	E	606	-	1,3,3	3.50	1 (100%)	0,3,3	-	-
3	N0N	C	603	-	19,21,36	1.14	2 (10%)	20,27,51	1.25	1 (5%)
4	ACT	G	604	-	1,3,3	3.65	1 (100%)	0,3,3	-	-
4	ACT	G	605	-	1,3,3	3.67	1 (100%)	0,3,3	-	-
4	ACT	D	607	-	1,3,3	4.03	1 (100%)	0,3,3	-	-
4	ACT	E	605	-	1,3,3	3.75	1 (100%)	0,3,3	-	-
3	N0N	A	602	-	19,21,36	0.86	1 (5%)	20,27,51	1.20	2 (10%)

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	N0N	E	604	-	-	1/24/44/44	0/3/3/3
3	N0N	G	603	-	-	2/24/44/44	0/3/3/3
3	N0N	H	602	-	-	1/11/33/44	0/1/1/3
3	N0N	F	604	-	-	3/24/44/44	0/3/3/3
3	N0N	D	605	-	-	3/24/44/44	0/3/3/3
3	N0N	B	602	-	-	0/7/27/44	0/1/1/3
3	N0N	C	603	-	-	2/11/33/44	0/1/1/3
3	N0N	A	602	-	-	1/11/33/44	0/1/1/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	604	N0N	C7-S1	-14.93	1.62	1.77
3	G	603	N0N	C7-S1	-14.83	1.62	1.77
3	D	605	N0N	C7-S1	-14.55	1.62	1.77
3	E	604	N0N	C7-S1	-14.47	1.62	1.77
4	G	606	ACT	CH3-C	4.19	1.54	1.48

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	603	N0N	O2-S1-O4	-10.05	107.19	119.55
3	D	605	N0N	O2-S1-O4	-8.64	108.93	119.55
3	E	604	N0N	O2-S1-O4	-7.18	110.72	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	604	N0N	O2-S1-O4	-6.89	111.08	119.55
3	G	603	N0N	O2-S1-N21	5.52	115.67	107.04

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	604	N0N	C18-C19-C20-N21
3	C	603	N0N	C17-C18-C19-C20
3	F	604	N0N	C16-C17-C18-C19
3	F	604	N0N	C20-N21-S1-O2
3	A	602	N0N	C18-C19-C20-N21

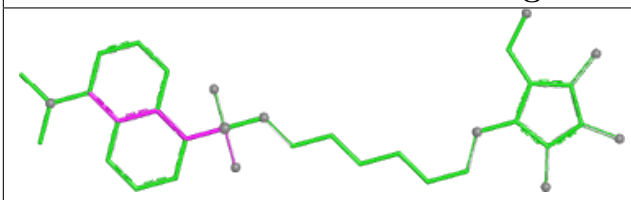
There are no ring outliers.

3 monomers are involved in 3 short contacts:

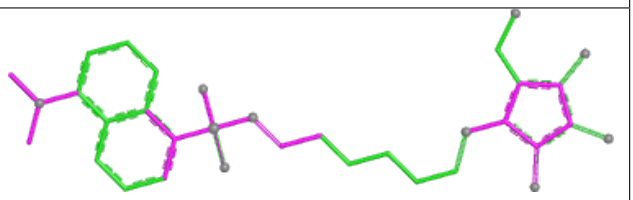
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	603	N0N	1	0
3	D	605	N0N	1	0
4	E	607	ACT	1	0

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.

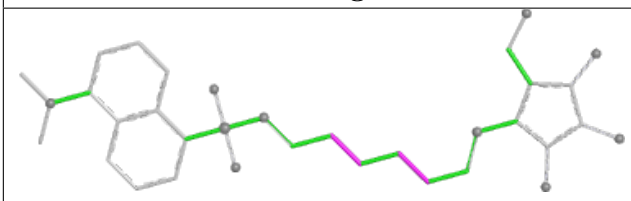
Ligand N0N G 603



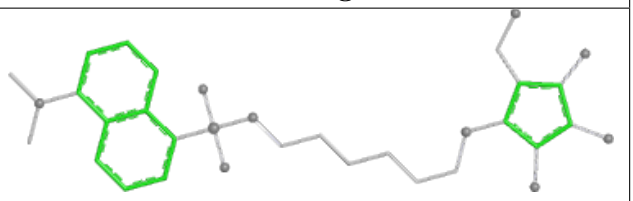
Bond lengths



Bond angles

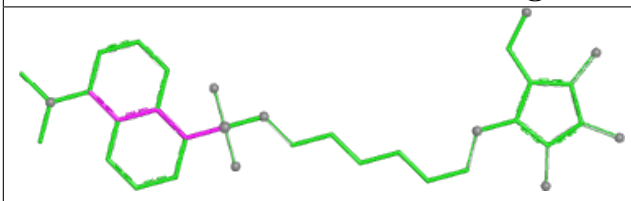


Torsions



Rings

Ligand N0N F 604



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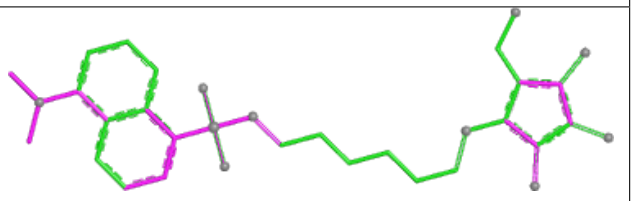

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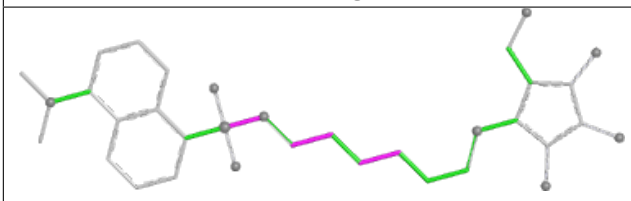

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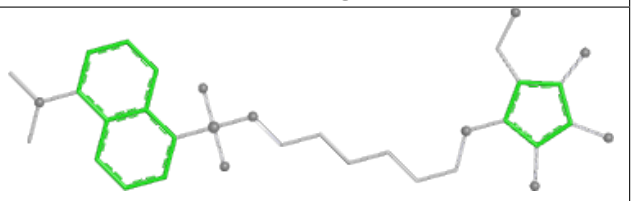
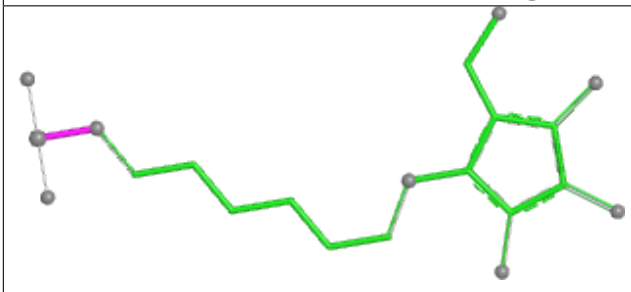
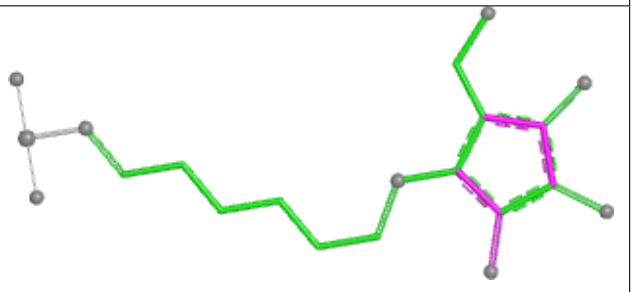


Rings

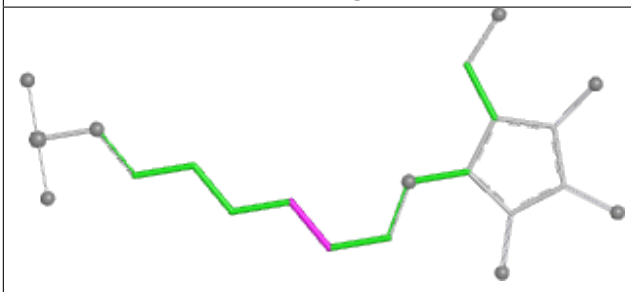
Ligand N0N H 602



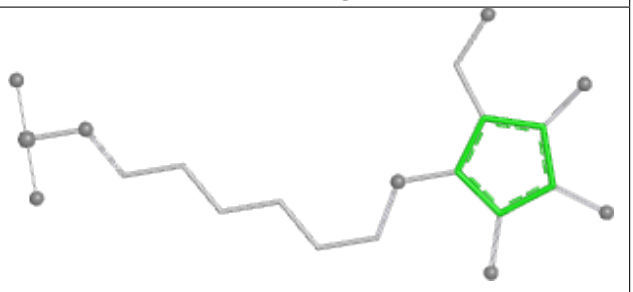
Bond lengths



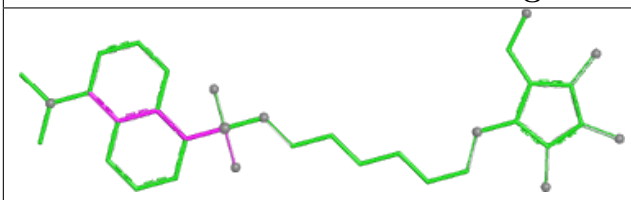
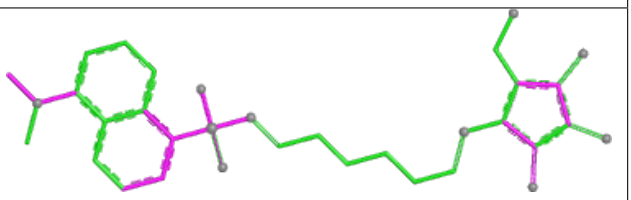
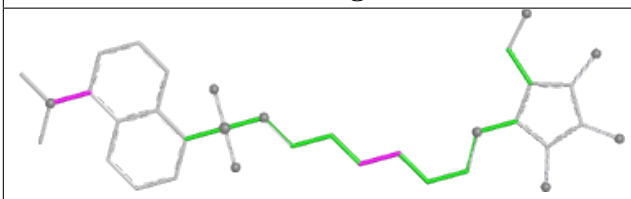
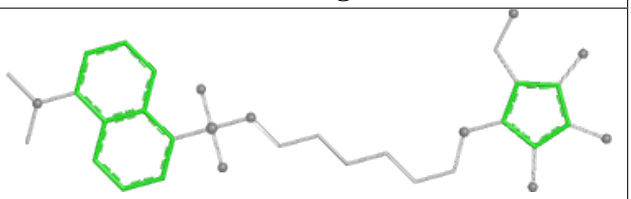
Bond angles

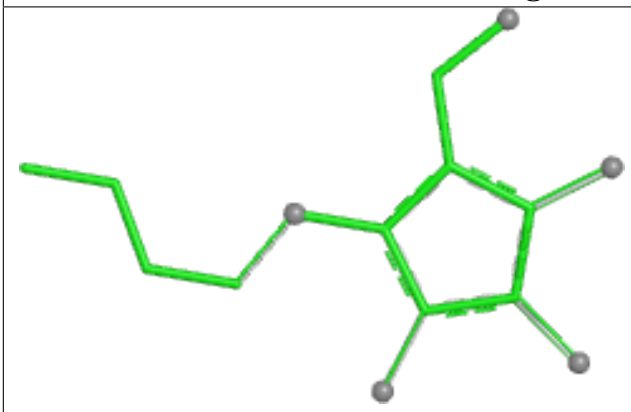
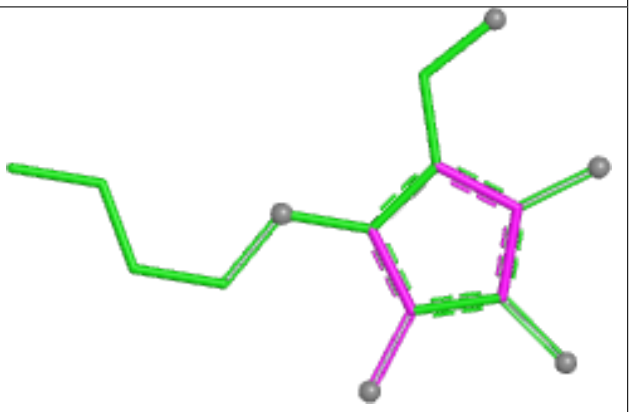
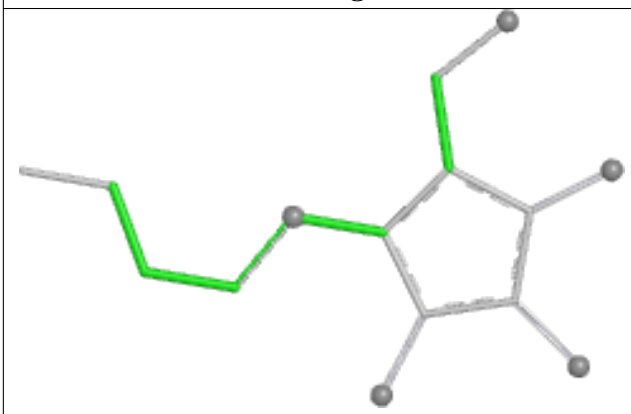
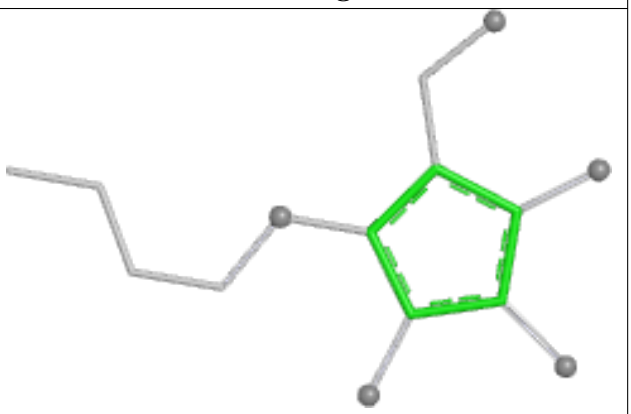


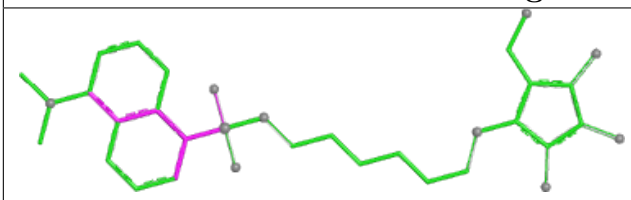
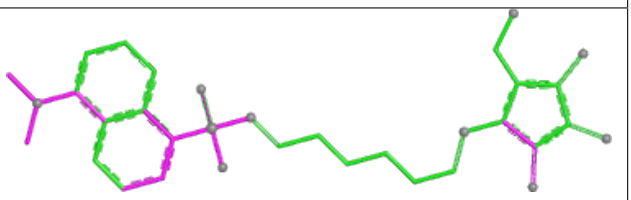
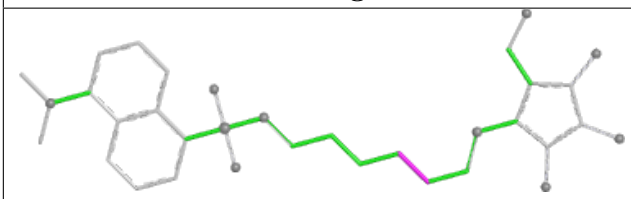
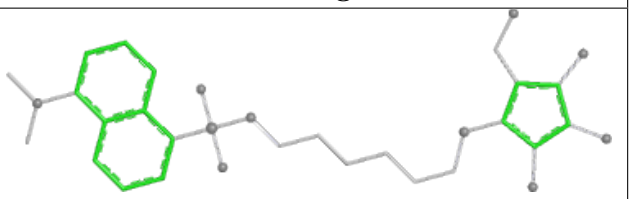
Torsions

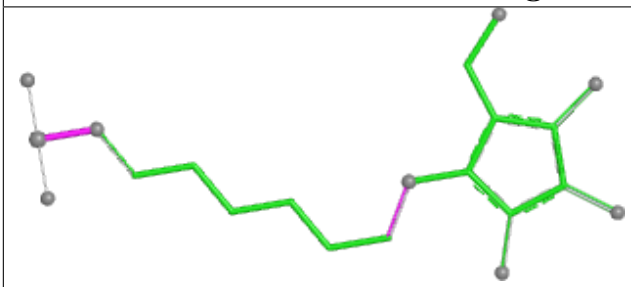
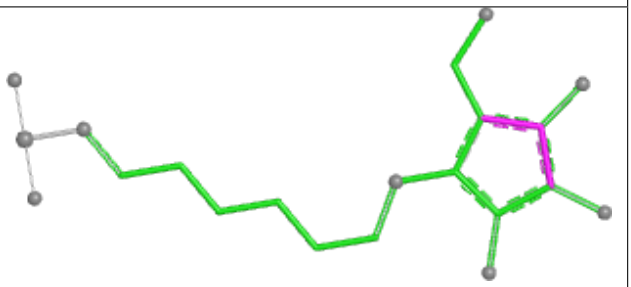
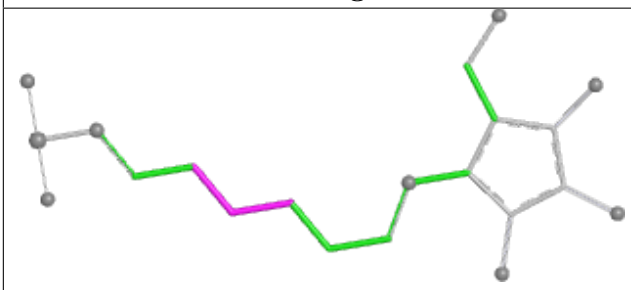
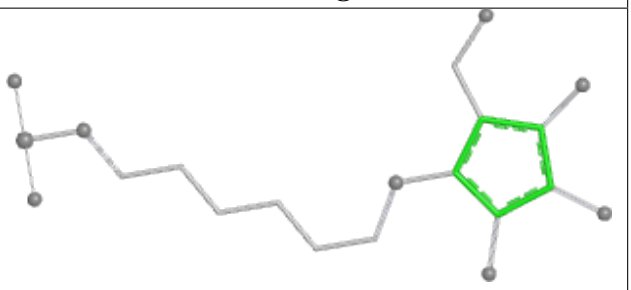


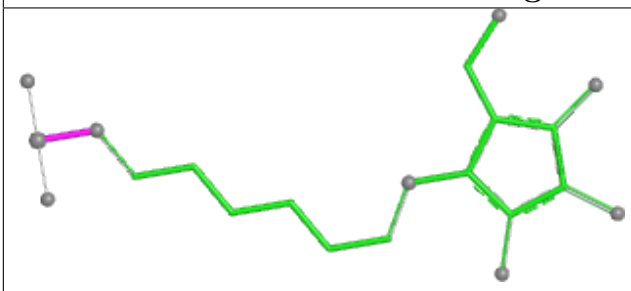
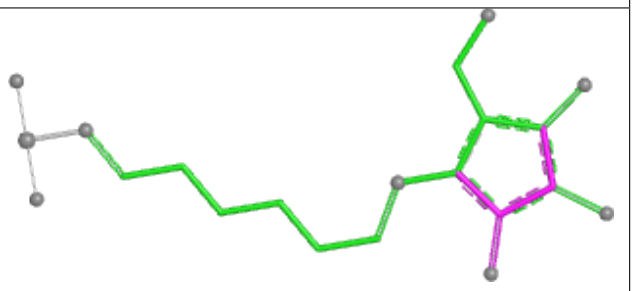
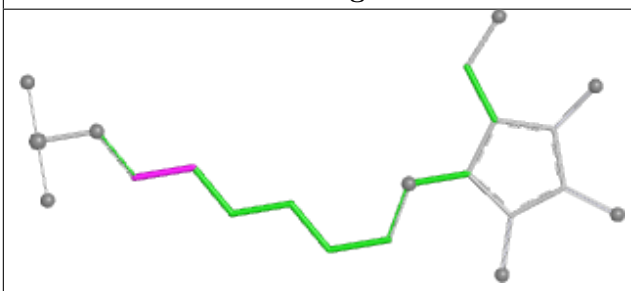
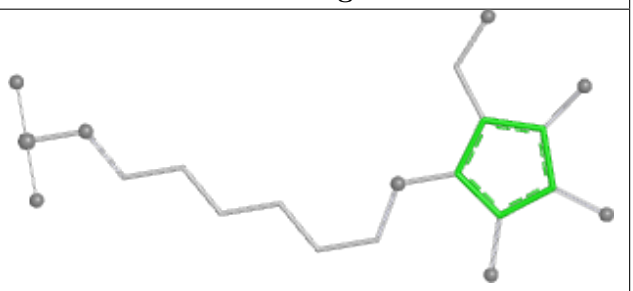
Rings

Ligand N0N D 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand N0N B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand N0N E 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand N0N C 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand N0N A 602	
 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	535/550 (97%)	-0.30	9 (1%)	70	75	18, 27, 47, 60	37 (6%)
1	B	540/550 (98%)	-0.39	10 (1%)	66	71	19, 24, 44, 61	28 (5%)
1	C	537/550 (97%)	-0.31	6 (1%)	80	84	17, 24, 45, 64	26 (4%)
1	D	539/550 (98%)	-0.38	4 (0%)	87	90	16, 23, 42, 61	27 (5%)
1	E	540/550 (98%)	-0.40	5 (0%)	84	87	16, 22, 40, 59	26 (4%)
1	F	539/550 (98%)	-0.29	11 (2%)	65	70	16, 25, 48, 61	28 (5%)
1	G	540/550 (98%)	-0.38	7 (1%)	77	81	16, 23, 45, 59	27 (5%)
1	H	537/550 (97%)	-0.30	21 (3%)	39	44	18, 26, 47, 63	39 (7%)
All	All	4307/4400 (97%)	-0.34	73 (1%)	70	75	16, 24, 45, 64	238 (5%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	TRP	7.0
1	D	439	TRP	7.0
1	A	445	PRO	6.4
1	C	444	THR	6.4
1	H	444	THR	5.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	H	603	4/4	0.76	0.13	29,33,34,40	4
4	ACT	B	604	4/4	0.81	0.20	42,43,45,46	4
4	ACT	G	605	4/4	0.82	0.14	38,38,41,45	4
4	ACT	F	605	4/4	0.83	0.14	28,31,34,37	4
4	ACT	B	603	4/4	0.85	0.14	35,37,37,38	4
4	ACT	G	607	4/4	0.88	0.16	24,30,32,35	4
4	ACT	G	606	4/4	0.88	0.13	29,31,32,35	4
4	ACT	D	604	4/4	0.89	0.11	32,35,35,37	0
4	ACT	E	605	4/4	0.90	0.17	22,23,25,26	4
4	ACT	E	607	4/4	0.90	0.14	33,38,41,43	4
4	ACT	C	604	4/4	0.90	0.13	31,39,39,40	0
4	ACT	F	606	4/4	0.90	0.15	28,33,35,36	4
4	ACT	D	607	4/4	0.91	0.10	30,37,39,40	4
4	ACT	D	608	4/4	0.91	0.14	25,28,28,29	4
4	ACT	D	606	4/4	0.92	0.14	29,37,39,44	4
4	ACT	E	606	4/4	0.94	0.15	34,38,41,44	4
2	NA	C	602	1/1	0.94	0.12	39,39,39,39	0
4	ACT	A	603	4/4	0.95	0.07	28,29,32,33	4
2	NA	F	601	1/1	0.96	0.08	30,30,30,30	0
4	ACT	G	604	4/4	0.96	0.10	23,23,24,25	4
3	N0N	F	604	34/34	0.96	0.11	18,28,33,34	20
3	N0N	G	603	34/34	0.97	0.10	15,25,36,40	19
3	N0N	H	602	21/34	0.97	0.07	16,20,32,35	6
3	N0N	C	603	21/34	0.97	0.08	16,19,34,39	4
3	N0N	D	605	34/34	0.97	0.09	15,26,38,40	19
3	N0N	B	602	15/34	0.97	0.07	17,19,26,36	0
2	NA	D	601	1/1	0.98	0.07	28,28,28,28	0
2	NA	D	610	1/1	0.98	0.07	31,31,31,31	0
3	N0N	E	604	34/34	0.98	0.09	15,29,35,38	20
2	NA	C	601	1/1	0.98	0.15	45,45,45,45	0
3	N0N	A	602	21/34	0.98	0.07	17,19,35,38	6
2	NA	B	601	1/1	0.98	0.09	34,34,34,34	0
2	NA	F	607	1/1	0.99	0.05	32,32,32,32	0
2	NA	G	608	1/1	0.99	0.07	25,25,25,25	0
2	NA	G	609	1/1	0.99	0.10	28,28,28,28	0
2	NA	H	604	1/1	0.99	0.05	26,26,26,26	0
2	NA	A	606	1/1	0.99	0.13	39,39,39,39	0

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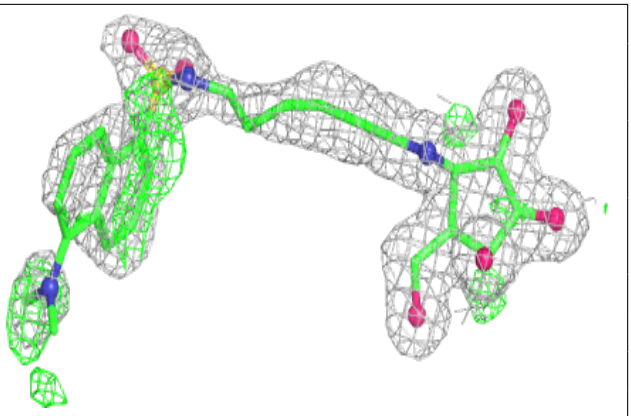
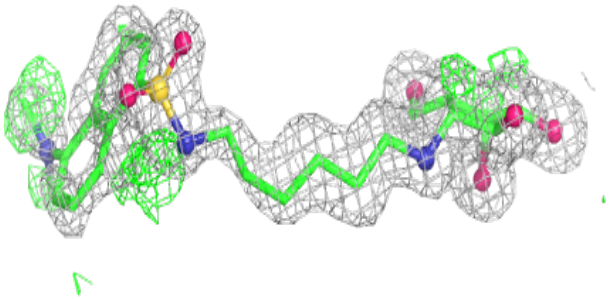
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	C	606	1/1	0.99	0.06	31,31,31,31	0
2	NA	A	604	1/1	0.99	0.06	27,27,27,27	0
2	NA	D	609	1/1	0.99	0.05	26,26,26,26	0
2	NA	B	605	1/1	0.99	0.07	27,27,27,27	1
2	NA	E	601	1/1	0.99	0.07	25,25,25,25	0
2	NA	E	603	1/1	0.99	0.08	27,27,27,27	0
2	NA	E	608	1/1	0.99	0.07	31,31,31,31	0
2	NA	E	609	1/1	0.99	0.07	23,23,23,23	0
2	NA	A	605	1/1	0.99	0.06	32,32,32,32	0
2	NA	F	603	1/1	0.99	0.05	25,25,25,25	0
2	NA	D	602	1/1	1.00	0.07	27,27,27,27	0
2	NA	F	602	1/1	1.00	0.06	28,28,28,28	0
2	NA	E	602	1/1	1.00	0.08	23,23,23,23	0
2	NA	D	603	1/1	1.00	0.09	24,24,24,24	0
2	NA	G	601	1/1	1.00	0.11	30,30,30,30	0
2	NA	G	602	1/1	1.00	0.07	23,23,23,23	0
2	NA	A	601	1/1	1.00	0.11	33,33,33,33	0
2	NA	C	605	1/1	1.00	0.05	25,25,25,25	0
2	NA	H	601	1/1	1.00	0.12	35,35,35,35	0

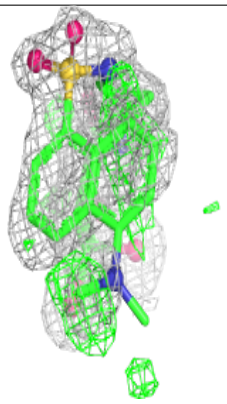
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N0N F 604:

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

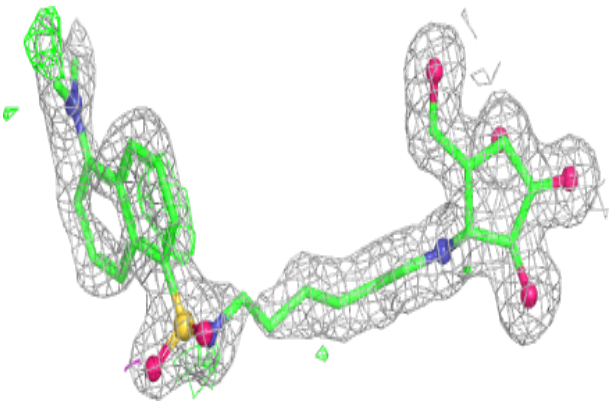


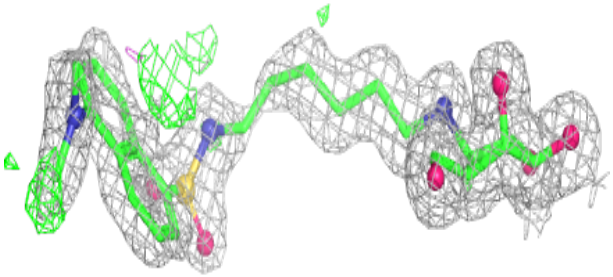


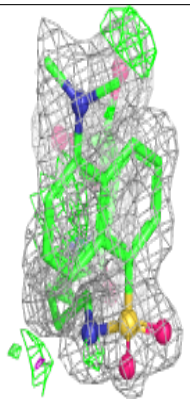


Electron density around N0N G 603:

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

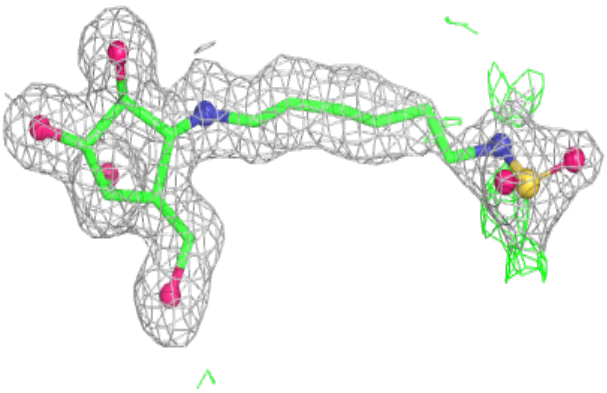


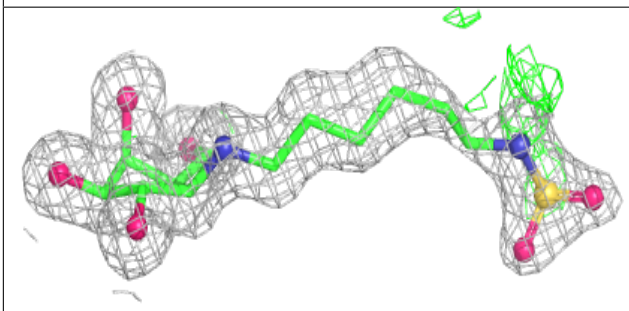


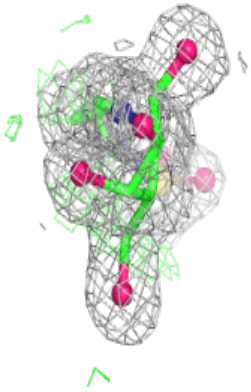


Electron density around N0N H 602:

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

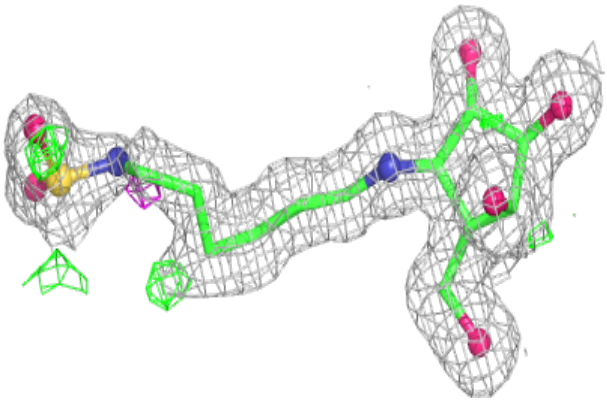


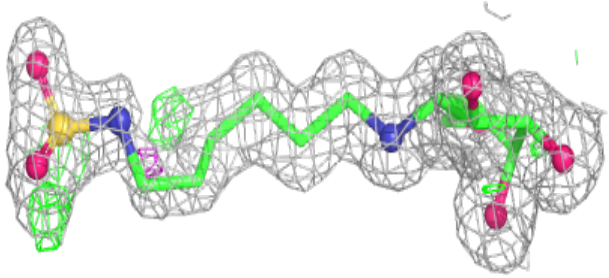


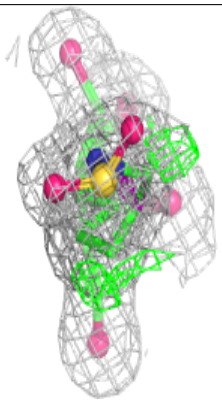


Electron density around N0N C 603:

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

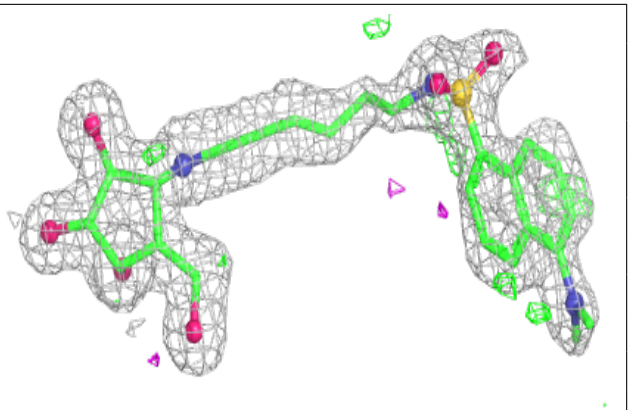


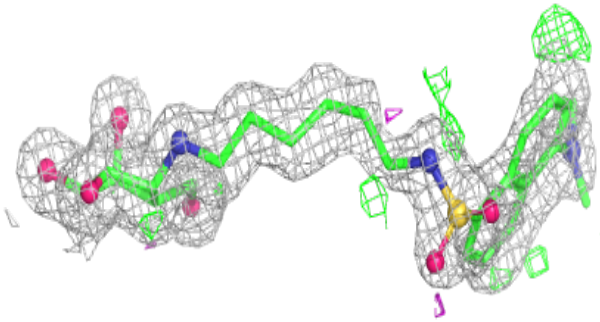


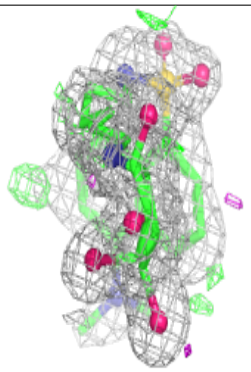


Electron density around N0N D 605:

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

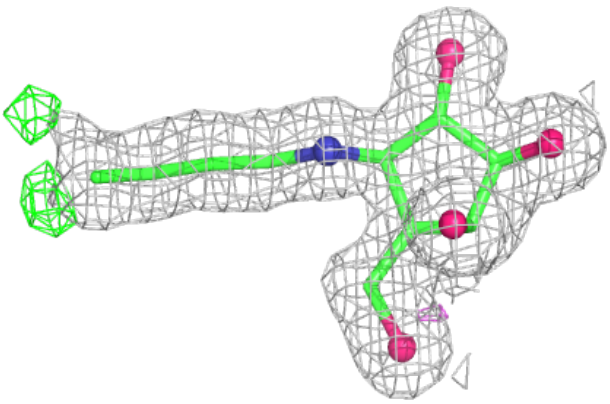


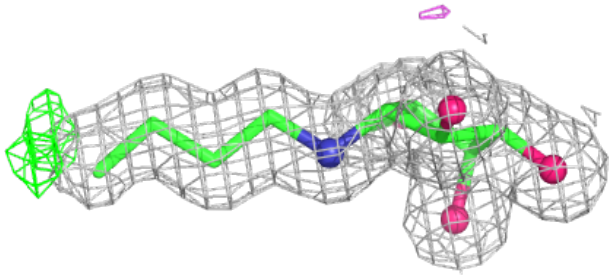




Electron density around N0N B 602:

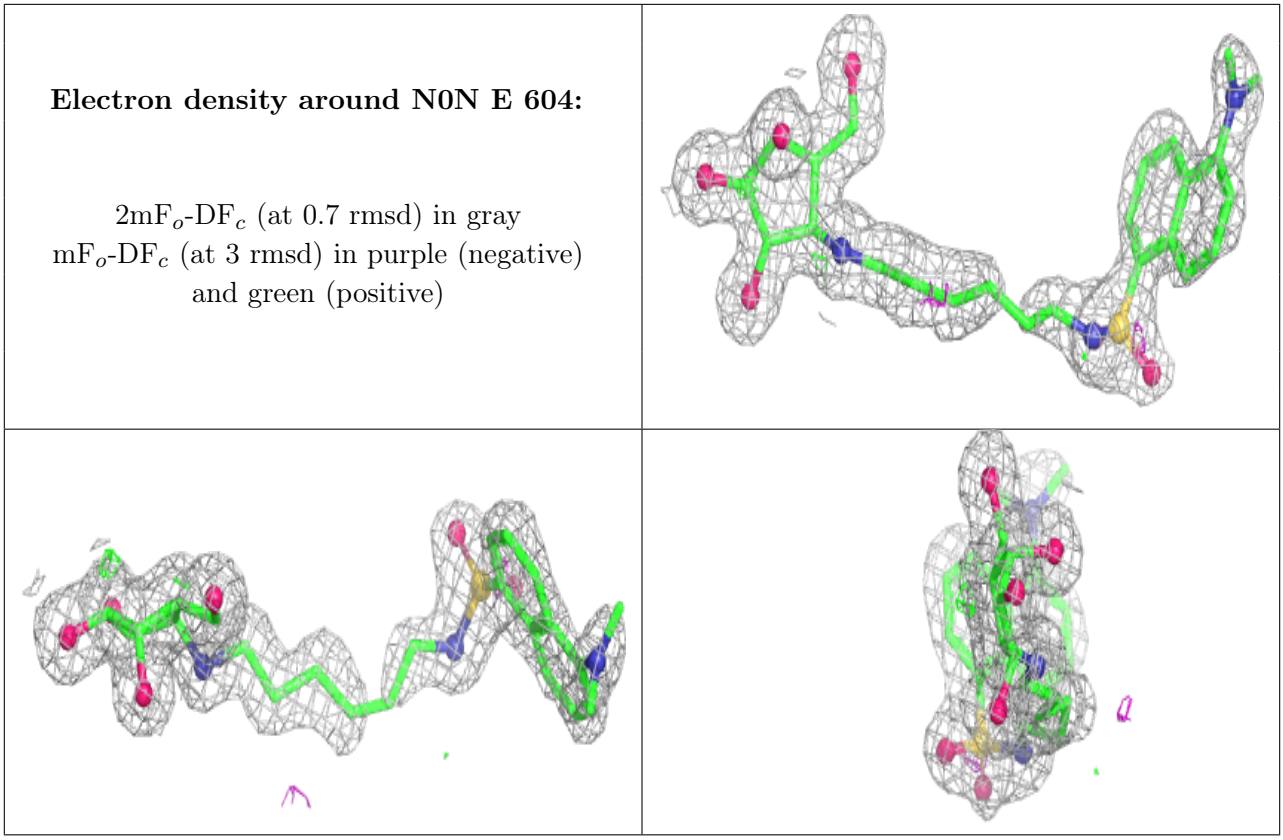
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





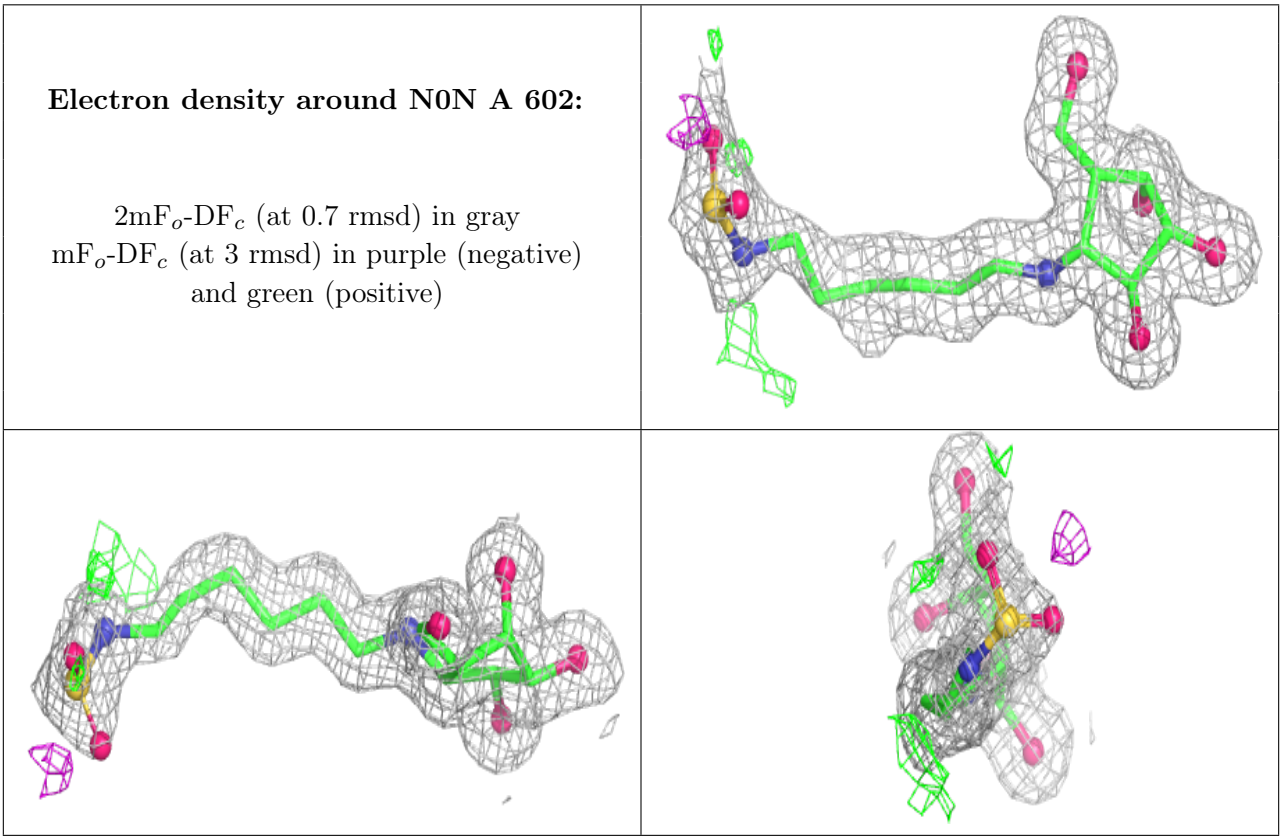
Electron density around N0N E 604:

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



Electron density around N0N A 602:

$2mF_o$-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.