Full wwPDB X-ray Structure Validation Report (i)

Feb 23, 2022 – 07:09 pm GMT

PDB ID	:	6TBF
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 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 (i) symbol.

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

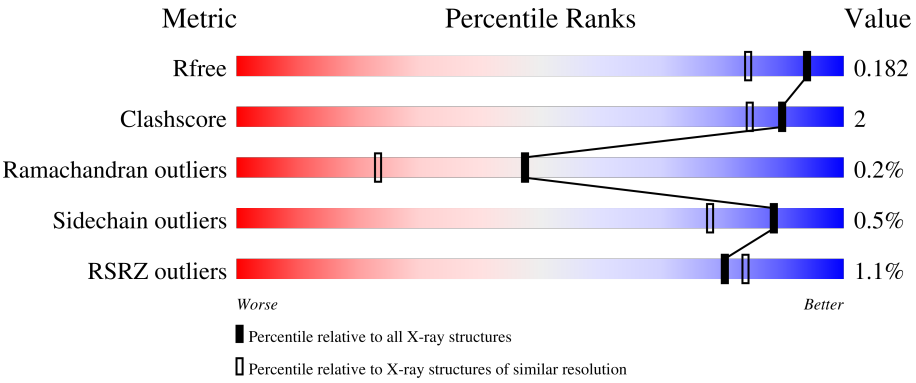
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	94%
1	B	550	93% 5%
1	C	550	94%
1	D	550	93% 5%
1	E	550	92% 6%

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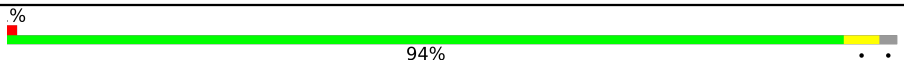
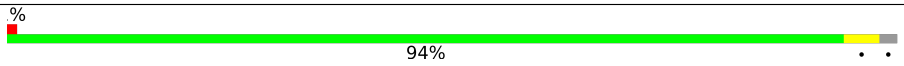
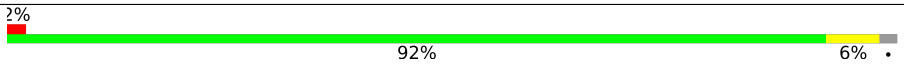
Mol	Chain	Length	Quality of chain
1	F	550	
1	G	550	
1	H	550	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39416 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	538	Total	C	N	O	S	0	8	0
			4284	2740	725	803	16			
1	B	540	Total	C	N	O	S	0	6	0
			4286	2739	731	801	15			
1	C	540	Total	C	N	O	S	0	8	0
			4292	2744	733	799	16			
1	D	539	Total	C	N	O	S	0	11	0
			4313	2759	729	809	16			
1	E	540	Total	C	N	O	S	0	9	0
			4320	2763	732	808	17			
1	F	539	Total	C	N	O	S	0	17	0
			4385	2803	747	819	16			
1	G	540	Total	C	N	O	S	0	16	0
			4379	2799	744	819	17			
1	H	539	Total	C	N	O	S	0	12	0
			4324	2765	734	809	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	6	Total Na 6 6	0	0
2	F	4	Total Na 4 4	0	0
2	G	5	Total Na 5 5	0	0

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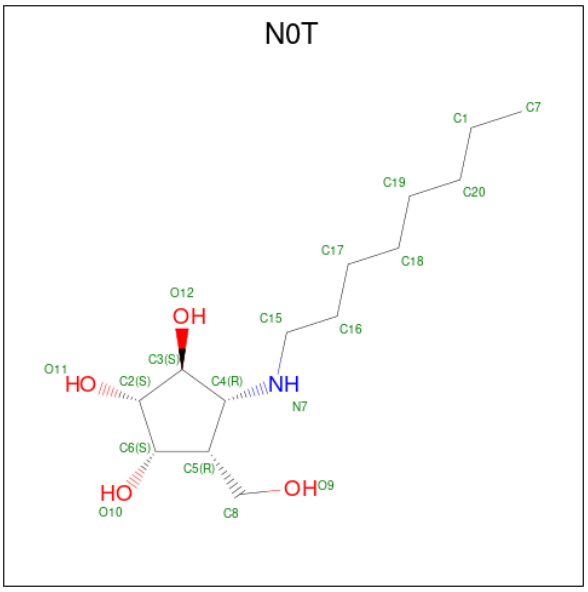
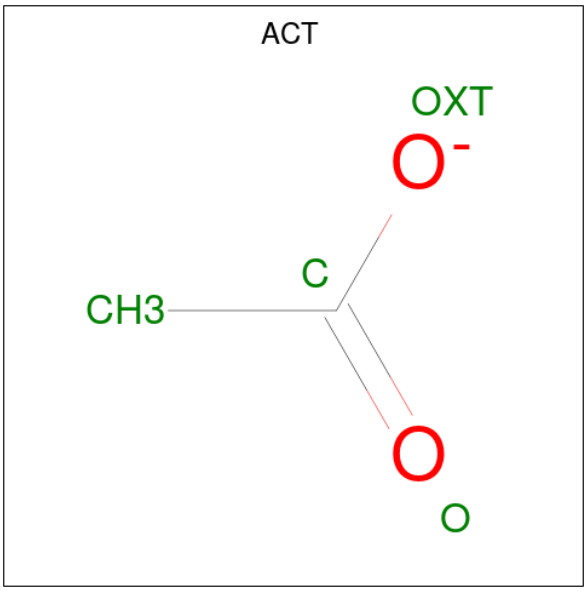
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	5	Total Na 5 5	0	0

- Molecule 3 is (1 {S},2 {S},3 {S},4 {R},5 {R})-4-(hydroxymethyl)-5-(octylamino)cyclopentane-1,2,3-triol (three-letter code: N0T) (formula: $C_{14}H_{29}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 14 1 4	0	0
3	B	1	Total C N O 19 14 1 4	0	0
3	C	1	Total C N O 19 14 1 4	0	0
3	D	1	Total C N O 19 14 1 4	0	0
3	E	1	Total C N O 19 14 1 4	0	0
3	F	1	Total C N O 19 14 1 4	0	0
3	G	1	Total C N O 19 14 1 4	0	0
3	H	1	Total C N O 19 14 1 4	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	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	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
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.

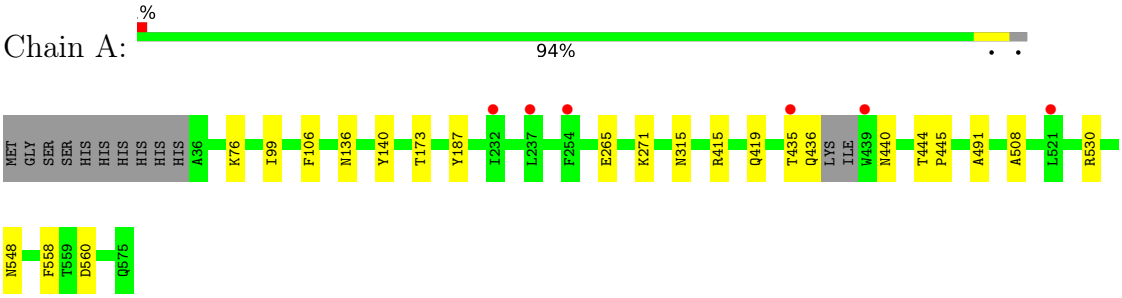
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	444	Total O 445 445	0	1
5	B	528	Total O 529 529	0	1
5	C	532	Total O 534 534	0	2
5	D	640	Total O 643 643	0	3
5	E	653	Total O 654 654	0	1
5	F	622	Total O 624 624	0	2
5	G	681	Total O 681 681	0	0
5	H	480	Total O 480 480	0	0

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.

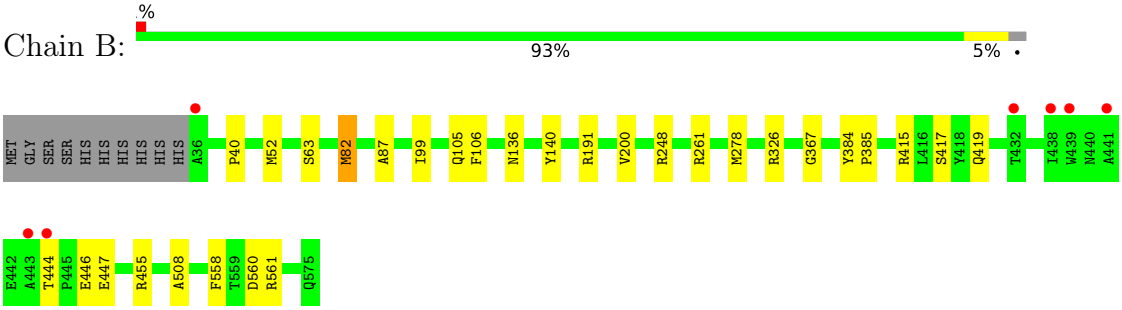
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain A:



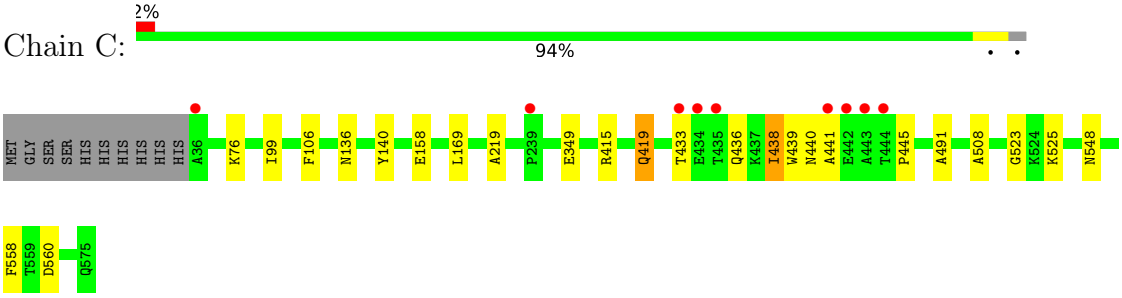
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain B:



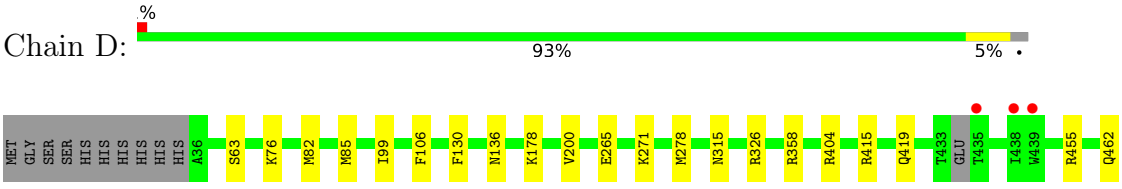
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain C:



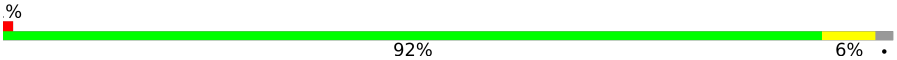
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain D:



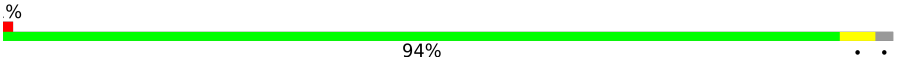
• Molecule 1: Beta-galactosidase, putative, bgl35A

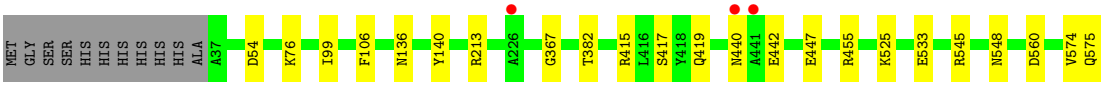
Chain E:



• Molecule 1: Beta-galactosidase, putative, bgl35A

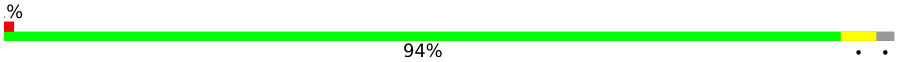
Chain F:

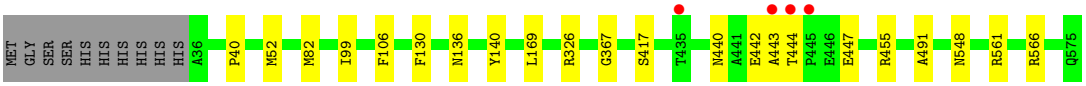




• Molecule 1: Beta-galactosidase, putative, bgl35A

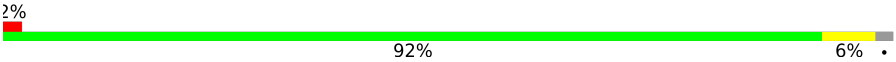
Chain G:

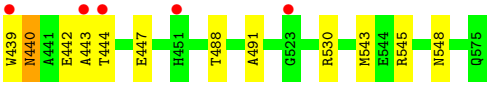




• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.42Å 115.63Å 115.94Å 90.35° 90.02° 90.16°	Depositor
Resolution (Å)	115.94 – 1.50 115.94 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (115.94-1.50) 96.6 (115.94-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.128 , 0.178 0.135 , 0.182	Depositor DCC
R_{free} test set	40201 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for h,l,-k 0.005 for h,-l,k 0.006 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,l,k 0.000 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	39416	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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: ACT, N0T, NA

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	0.84	2/4397 (0.0%)	0.97	3/5992 (0.1%)
1	B	0.86	2/4400 (0.0%)	0.98	4/6000 (0.1%)
1	C	0.88	4/4405 (0.1%)	0.96	1/6003 (0.0%)
1	D	0.88	0/4429	1.00	6/6033 (0.1%)
1	E	0.88	1/4434 (0.0%)	1.02	7/6039 (0.1%)
1	F	0.89	4/4502 (0.1%)	0.99	2/6123 (0.0%)
1	G	0.88	1/4493 (0.0%)	1.00	4/6115 (0.1%)
1	H	0.87	2/4441 (0.0%)	0.94	5/6049 (0.1%)
All	All	0.87	16/35501 (0.0%)	0.98	32/48354 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	GLU	CD-OE1	9.89	1.36	1.25
1	B	63	SER	CB-OG	-6.34	1.34	1.42
1	C	349	GLU	CD-OE1	6.07	1.32	1.25
1	C	560	ASP	CG-OD2	-6.04	1.11	1.25
1	G	442	GLU	CD-OE2	5.88	1.32	1.25
1	H	240	GLY	C-O	5.74	1.32	1.23
1	C	523	GLY	C-O	5.72	1.32	1.23
1	F	525	LYS	CG-CD	-5.66	1.33	1.52
1	F	560	ASP	CG-OD1	-5.47	1.12	1.25
1	B	560	ASP	CG-OD2	-5.19	1.13	1.25
1	F	447	GLU	CD-OE2	5.15	1.31	1.25
1	A	265	GLU	CD-OE1	5.11	1.31	1.25
1	H	237	LEU	C-O	5.05	1.32	1.23
1	A	560	ASP	CG-OD2	-5.04	1.13	1.25
1	F	533	GLU	CD-OE2	5.03	1.31	1.25
1	E	514	GLU	CD-OE1	5.01	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	H	530	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	E	455	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	E	455	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	326	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	C	433	THR	CA-CB-OG1	-6.31	95.74	109.00
1	D	404	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	H	530	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	82	MET	CG-SD-CE	-6.01	90.58	100.20
1	D	82	MET	CG-SD-CE	-5.99	90.61	100.20
1	H	82	MET	CG-SD-CE	-5.94	90.70	100.20
1	G	561	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	455	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	F	213	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	G	566	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	H	404	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	D	358	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	261	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	G	130	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	F	545	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	560	ASP	CB-CG-OD1	5.35	123.12	118.30
1	H	545	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	E	545	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	151	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	404	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	D	326	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	E	71	TYR	CB-CG-CD2	5.08	124.05	121.00
1	G	130	PHE	CB-CG-CD1	5.06	124.34	120.80
1	D	130	PHE	CB-CG-CD1	5.04	124.33	120.80
1	E	476	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	561	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	187	TYR	CB-CG-CD2	5.00	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4284	0	4096	9	0
1	B	4286	0	4105	25	0
1	C	4292	0	4108	13	0
1	D	4313	0	4130	14	0
1	E	4320	0	4154	22	0
1	F	4385	0	4222	11	0
1	G	4379	0	4204	15	0
1	H	4324	0	4146	19	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	6	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
3	F	19	0	0	0	0
3	G	19	0	0	0	0
3	H	19	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	D	12	0	9	0	0
4	E	8	0	6	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	445	0	0	2	0
5	B	529	0	0	13	0
5	C	534	0	0	0	0
5	D	643	0	0	7	0
5	E	654	0	0	8	0
5	F	624	0	0	6	0
5	G	681	0	0	5	0
5	H	480	0	0	4	0
All	All	39416	0	33207	122	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.

All (122) 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:248:ARG:HD2	5:B:1001:HOH:O	1.37	1.19
1:H:436:GLN:O	1:H:440:ASN:HB2	1.51	1.10
1:E:76:LYS:HE2	5:E:991:HOH:O	1.63	0.98
1:B:191[B]:ARG:NH1	5:B:702:HOH:O	1.61	0.92
1:D:462[B]:GLN:NE2	5:D:702:HOH:O	1.95	0.90
1:E:436:GLN:HG3	1:E:440:ASN:ND2	1.88	0.89
1:H:443:ALA:HA	1:H:447:GLU:OE1	1.73	0.87
1:D:462[B]:GLN:OE1	5:D:702:HOH:O	1.94	0.85
1:G:82[B]:MET:HG2	5:G:799:HOH:O	1.78	0.84
1:C:438:ILE:O	1:C:441:ALA:N	2.11	0.83
1:F:76:LYS:CE	5:F:856:HOH:O	2.27	0.81
1:G:444:THR:N	1:G:447:GLU:OE2	2.12	0.80
1:E:436:GLN:HG3	1:E:440:ASN:HD21	1.47	0.79
1:D:462[B]:GLN:CD	5:D:702:HOH:O	2.21	0.79
1:E:326[B]:ARG:NH1	5:E:701:HOH:O	2.19	0.75
1:B:248:ARG:CD	5:B:1001:HOH:O	2.11	0.74
1:D:76:LYS:CE	5:D:1004:HOH:O	2.35	0.73
1:E:415:ARG:NH1	5:E:703:HOH:O	2.22	0.73
1:F:415[A]:ARG:NH1	5:F:701:HOH:O	1.79	0.72
1:G:326[B]:ARG:NH1	5:G:701:HOH:O	2.24	0.70
1:E:326[B]:ARG:HH11	1:E:326[B]:ARG:HG3	1.56	0.70
1:A:436:GLN:C	1:A:440:ASN:HB2	2.11	0.69
1:B:105:GLN:HG3	5:B:1178:HOH:O	1.93	0.68
1:E:419:GLN:NE2	5:E:704:HOH:O	2.27	0.68
1:B:248:ARG:CG	5:B:1001:HOH:O	2.37	0.67
1:A:76:LYS:CE	5:A:911:HOH:O	2.44	0.66
1:B:415:ARG:CZ	5:B:708:HOH:O	2.46	0.64
1:E:415:ARG:CZ	5:E:703:HOH:O	2.45	0.64
1:D:488[B]:THR:HG23	5:D:1207:HOH:O	1.98	0.63
1:B:444:THR:HB	1:B:447:GLU:HG3	1.82	0.61
1:H:443:ALA:CA	1:H:447:GLU:OE1	2.48	0.61
1:B:444:THR:HB	1:B:447:GLU:CG	2.32	0.59
1:A:99:ILE:O	1:A:106:PHE:HA	2.04	0.58
1:B:419[B]:GLN:HG2	5:B:1012:HOH:O	2.04	0.58
1:B:191[B]:ARG:NH2	5:B:702:HOH:O	2.35	0.58
1:G:440:ASN:CB	5:G:1188:HOH:O	2.51	0.57
1:E:326[B]:ARG:HD3	5:E:1137:HOH:O	2.05	0.57
1:B:419[B]:GLN:CG	5:B:1012:HOH:O	2.52	0.57
1:D:178:LYS:HE2	1:D:265:GLU:HB3	1.87	0.57
1:G:444:THR:OG1	1:G:447:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LYS:NZ	5:H:705:HOH:O	2.38	0.56
1:H:444:THR:N	1:H:447:GLU:OE1	2.37	0.56
1:C:415[A]:ARG:O	1:C:419:GLN:HG3	2.06	0.55
1:B:191[B]:ARG:CZ	5:B:702:HOH:O	2.25	0.55
1:H:436:GLN:O	1:H:440:ASN:CB	2.41	0.54
1:C:415[B]:ARG:O	1:C:419:GLN:HG3	2.07	0.53
1:E:326[B]:ARG:HH11	1:E:326[B]:ARG:CG	2.18	0.53
1:F:382[B]:THR:OG1	5:F:702:HOH:O	2.18	0.53
1:E:436:GLN:CG	1:E:440:ASN:HD21	2.21	0.52
1:B:415:ARG:NH2	5:B:708:HOH:O	2.41	0.52
1:D:548:ASN:HB3	1:F:140:TYR:CZ	2.46	0.51
1:F:455[B]:ARG:HD3	5:F:744:HOH:O	2.10	0.51
1:G:40:PRO:HA	1:G:52:MET:O	2.10	0.51
1:G:455:ARG:NH1	5:G:705:HOH:O	2.39	0.51
1:H:99:ILE:O	1:H:106:PHE:HA	2.11	0.51
1:H:543[B]:MET:O	1:H:543[B]:MET:HG3	2.10	0.51
1:F:54:ASP:OD1	5:F:703:HOH:O	2.19	0.51
1:H:435:THR:O	1:H:439:TRP:N	2.37	0.50
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.47	0.50
1:A:415[A]:ARG:O	1:A:419:GLN:HG3	2.12	0.49
1:B:444:THR:HG22	1:B:446:GLU:N	2.27	0.49
1:D:415:ARG:NH2	5:D:707:HOH:O	2.45	0.49
1:E:394:GLU:HG3	5:E:1233:HOH:O	2.13	0.49
1:G:326[B]:ARG:HD3	5:G:1171:HOH:O	2.11	0.49
1:H:488[A]:THR:O	1:H:488[A]:THR:HG23	2.12	0.49
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.47	0.49
1:C:436:GLN:O	1:C:440:ASN:CB	2.60	0.48
1:F:575:GLN:HA	5:F:1077:HOH:O	2.12	0.48
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.49	0.48
1:F:574:VAL:O	1:F:575:GLN:OXT	2.30	0.48
1:A:271:LYS:HE3	1:A:315:ASN:O	2.14	0.48
1:H:193:LYS:NZ	5:H:703:HOH:O	2.33	0.47
1:A:444:THR:HB	1:A:445:PRO:HD2	1.96	0.47
1:H:179:LYS:CD	5:H:910:HOH:O	2.63	0.47
1:E:63[A]:SER:OG	1:E:82[A]:MET:SD	2.73	0.47
1:H:271[A]:LYS:HE3	1:H:315:ASN:O	2.14	0.46
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.51	0.46
1:B:455:ARG:NH1	5:B:709:HOH:O	2.42	0.46
1:H:435:THR:O	1:H:439:TRP:CB	2.63	0.46
1:B:200:VAL:O	1:B:278:MET:HA	2.16	0.46
1:D:99:ILE:O	1:D:106:PHE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:GLY:HA2	1:G:417[A]:SER:OG	2.16	0.46
1:B:191[B]:ARG:NH1	5:B:712:HOH:O	2.47	0.46
5:A:1054:HOH:O	1:C:525:LYS:HE2	2.15	0.45
1:C:436:GLN:O	1:C:440:ASN:N	2.48	0.45
1:B:40:PRO:HA	1:B:52:MET:O	2.17	0.45
1:F:99:ILE:O	1:F:106:PHE:HA	2.17	0.45
1:G:99:ILE:O	1:G:106:PHE:HA	2.17	0.45
1:G:82[B]:MET:HE3	1:G:82[B]:MET:HB3	1.91	0.45
1:B:99:ILE:O	1:B:106:PHE:HA	2.17	0.44
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.52	0.44
1:F:548:ASN:HB3	1:G:140:TYR:CZ	2.52	0.44
1:B:367:GLY:HA2	1:B:417[A]:SER:OG	2.17	0.44
1:D:419:GLN:NE2	5:D:713:HOH:O	2.51	0.44
1:C:436:GLN:O	1:C:440:ASN:HB2	2.17	0.44
1:D:271[A]:LYS:HE3	1:D:315:ASN:O	2.17	0.44
1:C:99:ILE:O	1:C:106:PHE:HA	2.19	0.43
1:H:63[B]:SER:OG	1:H:376:MET:HB2	2.18	0.43
1:E:200:VAL:O	1:E:278:MET:HA	2.19	0.43
1:E:140:TYR:CZ	1:G:548:ASN:HB3	2.54	0.42
1:E:191:ARG:NE	4:E:606:ACT:O	2.36	0.42
1:E:367:GLY:HA2	1:E:417[A]:SER:OG	2.20	0.42
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.55	0.42
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.54	0.42
1:C:169:LEU:HD13	1:C:219:ALA:HA	2.01	0.42
1:B:82:MET:HG2	1:B:87:ALA:HB3	2.01	0.42
1:H:384:TYR:CD1	1:H:385:PRO:HA	2.55	0.42
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.54	0.42
1:G:443:ALA:HB1	1:G:447:GLU:CB	2.50	0.41
1:E:271:LYS:HE3	1:E:315:ASN:O	2.20	0.41
1:E:462[B]:GLN:NE2	1:E:471:GLU:OE1	2.52	0.41
1:B:384:TYR:CD1	1:B:385:PRO:HA	2.55	0.41
1:D:200:VAL:O	1:D:278:MET:HA	2.19	0.41
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.95	0.41
1:C:436:GLN:O	1:C:440:ASN:CG	2.59	0.41
1:D:63[B]:SER:HB3	1:D:85:MET:SD	2.61	0.41
1:H:169:LEU:HD23	1:H:169:LEU:HA	1.91	0.41
1:E:99:ILE:O	1:E:106:PHE:HA	2.21	0.41
1:E:457:SER:O	5:E:702:HOH:O	2.22	0.41
1:B:444:THR:HG22	1:B:446:GLU:H	1.87	0.40
1:F:367:GLY:HA2	1:F:417[A]:SER:OG	2.21	0.40
1:H:415[A]:ARG:HD2	5:H:1078:HOH:O	2.21	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	542/550 (98%)	519 (96%)	21 (4%)	2 (0%)	34 13
1	B	544/550 (99%)	526 (97%)	18 (3%)	0	100 100
1	C	546/550 (99%)	521 (95%)	21 (4%)	4 (1%)	22 6
1	D	546/550 (99%)	527 (96%)	19 (4%)	0	100 100
1	E	547/550 (100%)	528 (96%)	19 (4%)	0	100 100
1	F	555/550 (101%)	534 (96%)	20 (4%)	1 (0%)	47 23
1	G	554/550 (101%)	535 (97%)	18 (3%)	1 (0%)	47 23
1	H	549/550 (100%)	527 (96%)	21 (4%)	1 (0%)	47 23
All	All	4383/4400 (100%)	4217 (96%)	157 (4%)	9 (0%)	47 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	PRO
1	A	435	THR
1	C	439	TRP
1	F	440	ASN
1	C	491	ALA
1	A	491	ALA
1	G	491	ALA
1	H	491	ALA
1	C	438	ILE

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	439/461 (95%)	437 (100%)	2 (0%)	88 78
1	B	440/461 (95%)	439 (100%)	1 (0%)	93 86
1	C	438/461 (95%)	435 (99%)	3 (1%)	84 69
1	D	443/461 (96%)	442 (100%)	1 (0%)	93 86
1	E	446/461 (97%)	445 (100%)	1 (0%)	93 86
1	F	452/461 (98%)	449 (99%)	3 (1%)	84 69
1	G	450/461 (98%)	449 (100%)	1 (0%)	93 86
1	H	444/461 (96%)	439 (99%)	5 (1%)	73 53
All	All	3552/3688 (96%)	3535 (100%)	17 (0%)	88 78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	173	THR
1	B	136	ASN
1	C	76	LYS
1	C	136	ASN
1	C	419	GLN
1	D	136	ASN
1	E	136	ASN
1	F	136	ASN
1	F	419	GLN
1	F	442	GLU
1	G	136	ASN
1	H	136	ASN
1	H	173	THR
1	H	289	ASN
1	H	440	ASN
1	H	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	421	GLN

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Mol	Chain	Res	Type
1	D	45	ASN
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 57 ligands modelled in this entry, 35 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
4	ACT	G	607	-	1,3,3	5.12	1 (100%)	0,3,3	-	-
3	N0T	C	603	-	19,19,19	1.22	3 (15%)	21,24,24	1.77	5 (23%)
4	ACT	D	604	-	1,3,3	6.01	1 (100%)	0,3,3	-	-
3	N0T	D	605	-	19,19,19	1.00	1 (5%)	21,24,24	1.52	5 (23%)
4	ACT	A	603	-	1,3,3	4.55	1 (100%)	0,3,3	-	-
3	N0T	H	602	-	19,19,19	1.28	1 (5%)	21,24,24	1.23	3 (14%)
4	ACT	F	606	-	1,3,3	3.02	1 (100%)	0,3,3	-	-
4	ACT	D	607	-	1,3,3	1.74	0	0,3,3	-	-
3	N0T	E	604	-	19,19,19	1.35	2 (10%)	21,24,24	1.27	2 (9%)
4	ACT	G	604	-	1,3,3	4.39	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	E	605	-	1,3,3	2.23	1 (100%)	0,3,3	-	-
4	ACT	B	603	-	1,3,3	2.61	1 (100%)	0,3,3	-	-
3	N0T	G	603	-	19,19,19	1.67	3 (15%)	21,24,24	1.61	6 (28%)
3	N0T	A	602	-	19,19,19	1.23	1 (5%)	21,24,24	1.25	1 (4%)
4	ACT	H	603	-	1,3,3	7.27	1 (100%)	0,3,3	-	-
4	ACT	D	606	-	1,3,3	1.10	0	0,3,3	-	-
4	ACT	F	605	-	1,3,3	7.37	1 (100%)	0,3,3	-	-
3	N0T	F	604	-	19,19,19	1.35	3 (15%)	21,24,24	1.42	4 (19%)
4	ACT	G	605	-	1,3,3	5.58	1 (100%)	0,3,3	-	-
4	ACT	G	606	-	1,3,3	7.12	1 (100%)	0,3,3	-	-
3	N0T	B	602	-	19,19,19	1.34	2 (10%)	21,24,24	1.37	3 (14%)
4	ACT	E	606	-	1,3,3	3.87	1 (100%)	0,3,3	-	-

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	N0T	C	603	-	-	0/11/31/31	0/1/1/1
3	N0T	F	604	-	-	1/11/31/31	0/1/1/1
3	N0T	H	602	-	-	1/11/31/31	0/1/1/1
3	N0T	D	605	-	-	1/11/31/31	0/1/1/1
3	N0T	A	602	-	-	3/11/31/31	0/1/1/1
3	N0T	E	604	-	-	1/11/31/31	0/1/1/1
3	N0T	G	603	-	-	2/11/31/31	0/1/1/1
3	N0T	B	602	-	-	2/11/31/31	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	605	ACT	CH3-C	7.37	1.58	1.48
4	H	603	ACT	CH3-C	7.27	1.58	1.48
4	G	606	ACT	CH3-C	7.12	1.57	1.48
4	D	604	ACT	CH3-C	6.01	1.56	1.48
3	G	603	N0T	C4-N7	5.70	1.57	1.47
4	G	605	ACT	CH3-C	5.58	1.55	1.48
4	G	607	ACT	CH3-C	5.12	1.55	1.48
3	H	602	N0T	C4-N7	4.70	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	604	N0T	C4-N7	4.60	1.55	1.47
4	A	603	ACT	CH3-C	4.55	1.54	1.48
4	G	604	ACT	CH3-C	4.39	1.54	1.48
3	A	602	N0T	C4-N7	4.00	1.54	1.47
4	E	606	ACT	CH3-C	3.87	1.53	1.48
3	F	604	N0T	C4-N7	3.77	1.54	1.47
3	B	602	N0T	C4-N7	3.76	1.54	1.47
3	C	603	N0T	C8-C5	3.19	1.57	1.52
4	F	606	ACT	CH3-C	3.02	1.52	1.48
3	D	605	N0T	C4-N7	2.76	1.52	1.47
4	B	603	ACT	CH3-C	2.61	1.52	1.48
3	G	603	N0T	C5-C6	-2.59	1.49	1.53
3	B	602	N0T	O12-C3	2.40	1.48	1.43
3	E	604	N0T	C15-N7	2.32	1.52	1.47
3	F	604	N0T	C15-N7	2.24	1.51	1.47
4	E	605	ACT	CH3-C	2.23	1.51	1.48
3	C	603	N0T	C17-C16	2.19	1.63	1.51
3	F	604	N0T	C5-C6	-2.09	1.50	1.53
3	C	603	N0T	C4-N7	2.01	1.51	1.47
3	G	603	N0T	C8-C5	2.00	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	N0T	C5-C6-C2	-4.69	97.77	103.81
3	A	602	N0T	C5-C6-C2	-4.04	98.61	103.81
3	D	605	N0T	C5-C6-C2	-3.51	99.29	103.81
3	E	604	N0T	C5-C6-C2	-3.29	99.57	103.81
3	C	603	N0T	C5-C4-N7	3.21	119.48	112.52
3	D	605	N0T	C3-C4-N7	-3.19	105.26	113.24
3	F	604	N0T	O12-C3-C4	3.17	118.92	111.16
3	B	602	N0T	C5-C6-C2	-3.10	99.82	103.81
3	F	604	N0T	C5-C6-C2	-3.03	99.91	103.81
3	C	603	N0T	C2-C3-C4	2.87	106.75	102.72
3	G	603	N0T	C3-C4-N7	-2.79	106.26	113.24
3	G	603	N0T	C15-N7-C4	-2.78	110.46	114.16
3	B	602	N0T	C15-N7-C4	2.73	117.79	114.16
3	G	603	N0T	C5-C6-C2	-2.65	100.40	103.81
3	E	604	N0T	C3-C4-N7	-2.44	107.14	113.24
3	H	602	N0T	C3-C2-C6	-2.41	98.75	102.64
3	G	603	N0T	C2-C3-C4	2.37	106.05	102.72
3	F	604	N0T	C19-C18-C17	-2.35	102.50	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	605	N0T	O12-C3-C4	2.26	116.70	111.16
3	G	603	N0T	C3-C2-C6	-2.15	99.17	102.64
3	H	602	N0T	C3-C4-N7	-2.13	107.91	113.24
3	D	605	N0T	C16-C15-N7	-2.12	104.11	112.02
3	G	603	N0T	C5-C4-N7	2.11	117.09	112.52
3	H	602	N0T	O12-C3-C4	2.08	116.27	111.16
3	D	605	N0T	C5-C4-N7	2.04	116.95	112.52
3	B	602	N0T	O12-C3-C4	2.04	116.17	111.16
3	C	603	N0T	O12-C3-C4	2.04	116.15	111.16
3	F	604	N0T	O10-C6-C2	-2.03	105.26	111.82
3	C	603	N0T	C3-C2-C6	-2.01	99.40	102.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	605	N0T	N7-C15-C16-C17
3	H	602	N0T	N7-C15-C16-C17
3	F	604	N0T	N7-C15-C16-C17
3	G	603	N0T	N7-C15-C16-C17
3	A	602	N0T	C15-C16-C17-C18
3	E	604	N0T	C15-C16-C17-C18
3	A	602	N0T	C18-C19-C20-C1
3	B	602	N0T	N7-C15-C16-C17
3	G	603	N0T	C15-C16-C17-C18
3	B	602	N0T	C15-C16-C17-C18
3	A	602	N0T	C17-C18-C19-C20

There are no ring outliers.

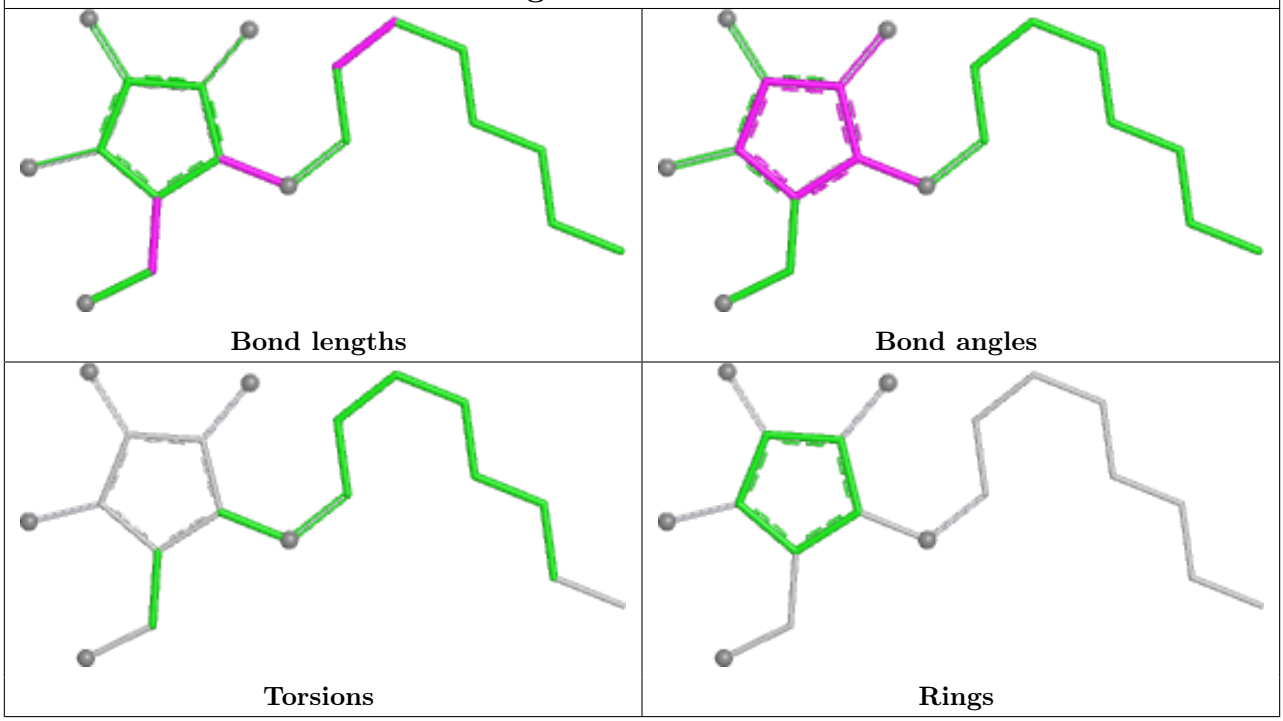
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	606	ACT	1	0

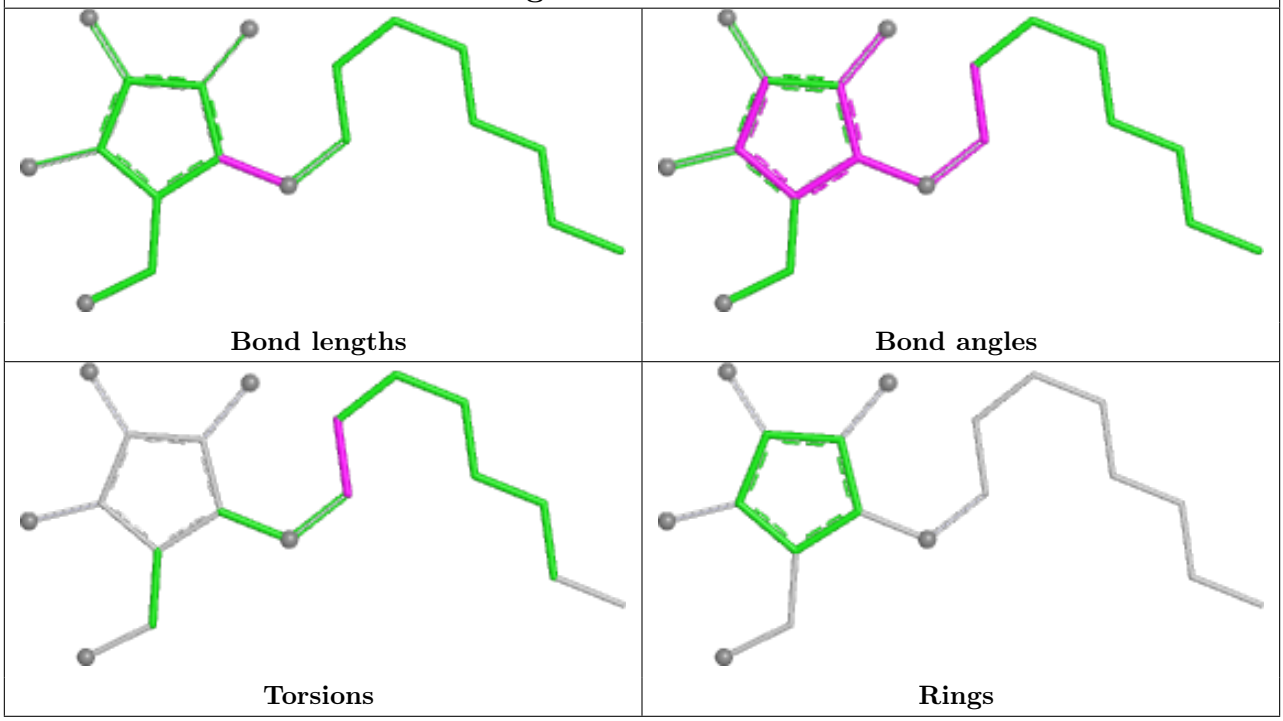
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

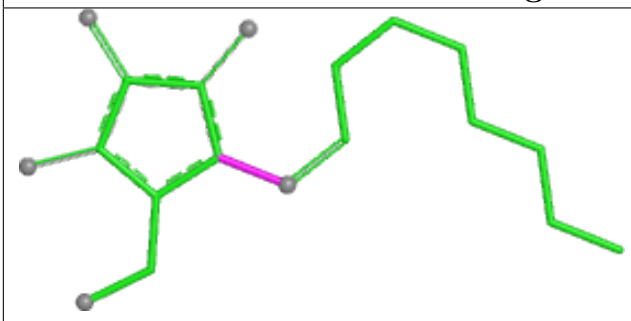
Ligand N0T C 603



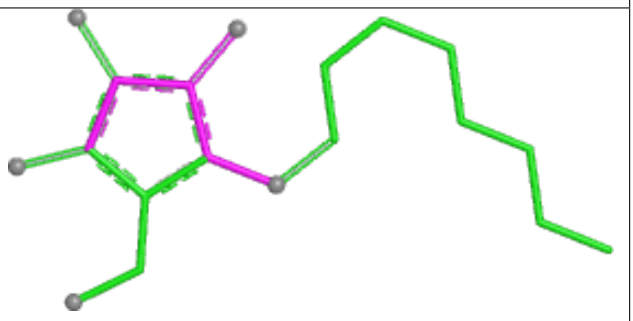
Ligand N0T D 605



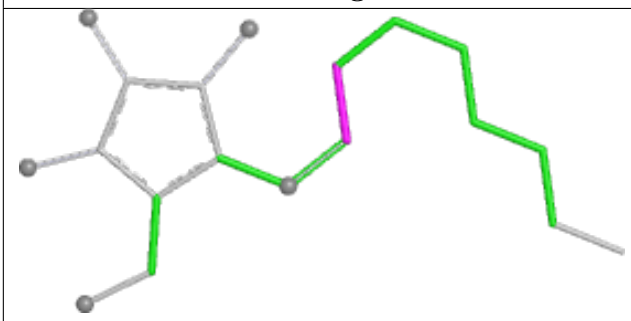
Ligand N0T H 602



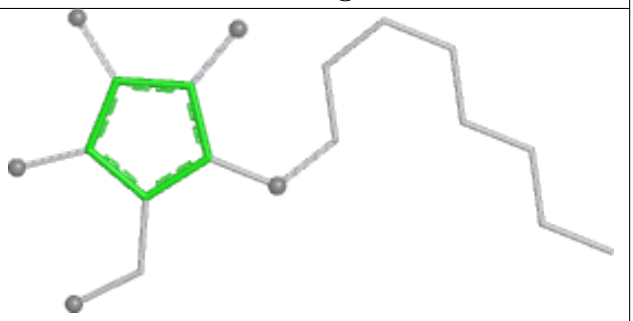
Bond lengths



Bond angles

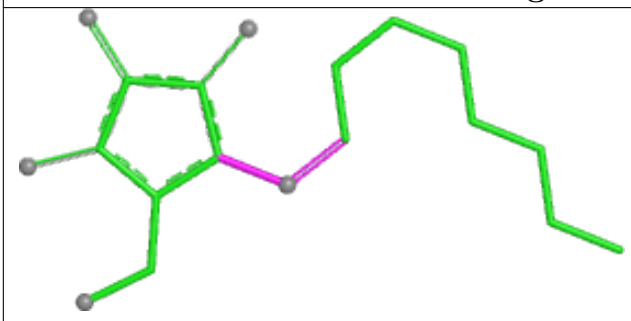


Torsions

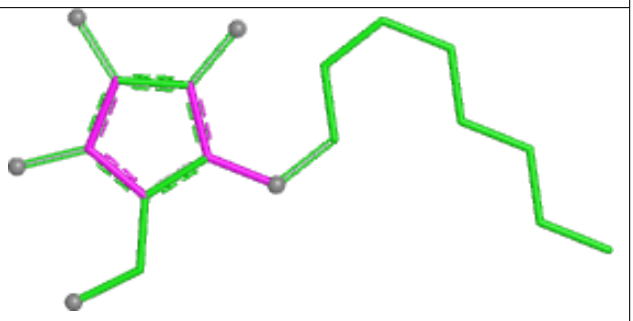


Rings

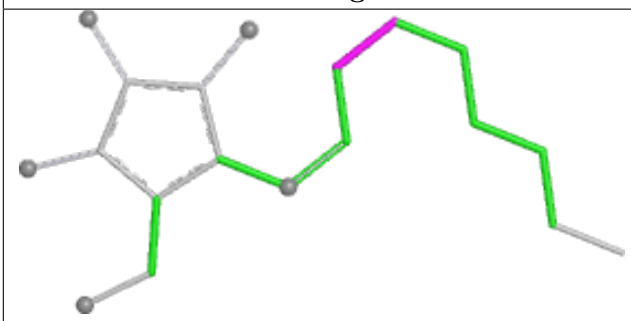
Ligand N0T E 604



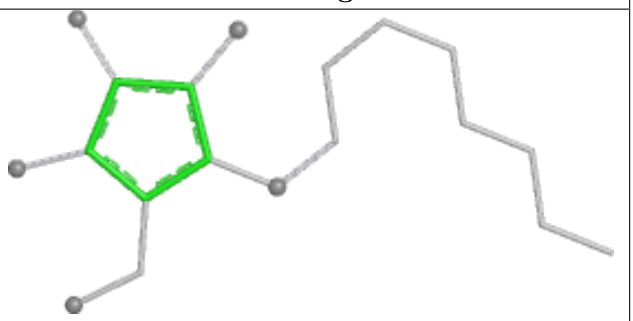
Bond lengths



Bond angles

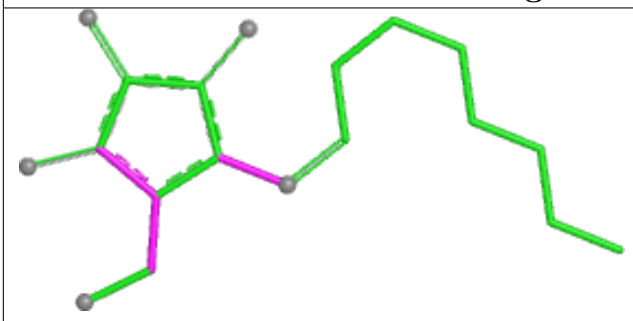


Torsions

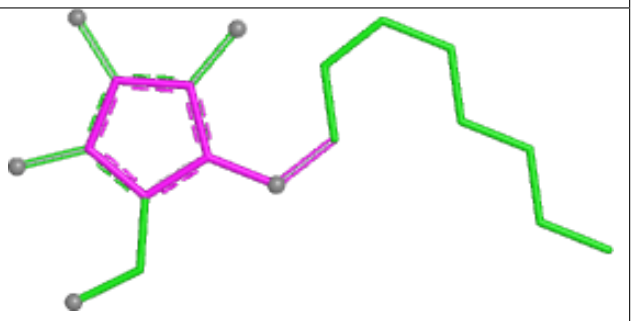


Rings

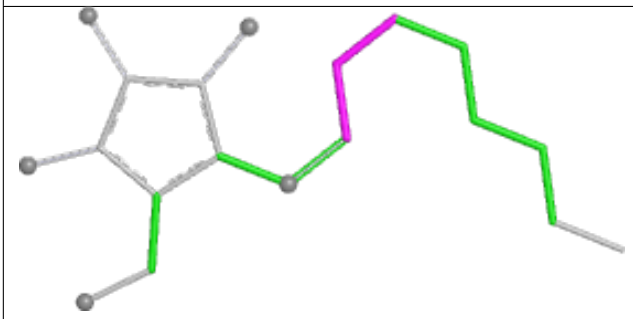
Ligand N0T G 603



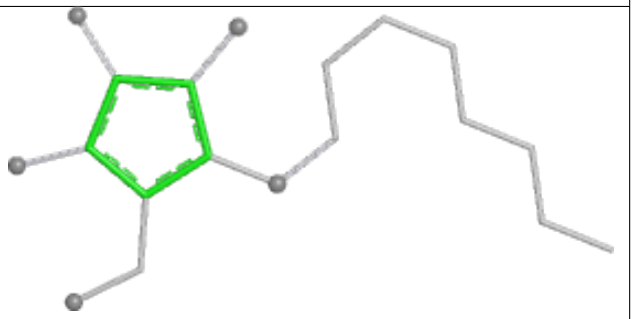
Bond lengths



Bond angles

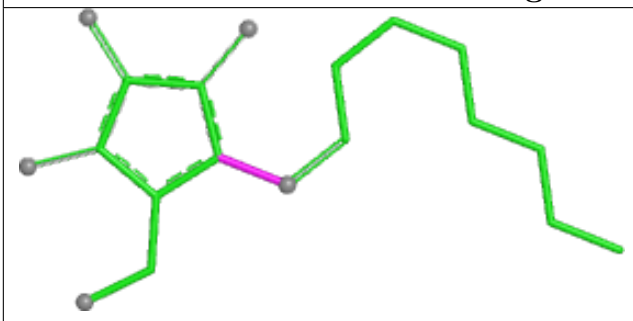


Torsions

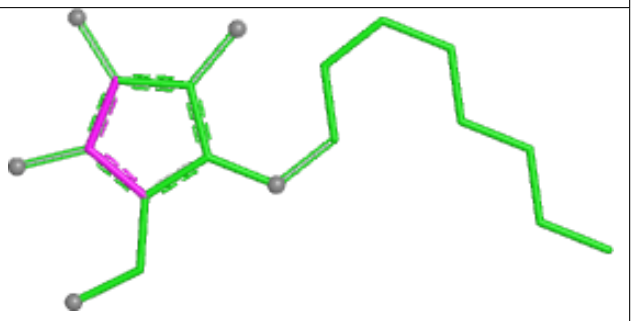


Rings

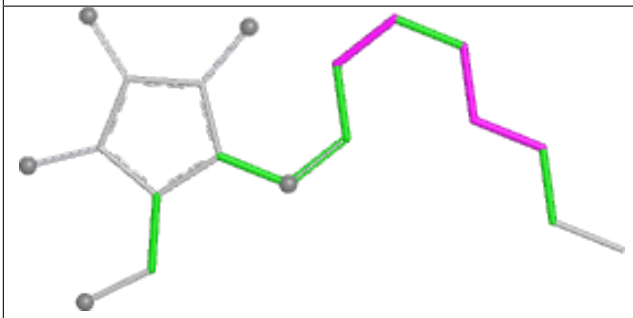
Ligand N0T A 602



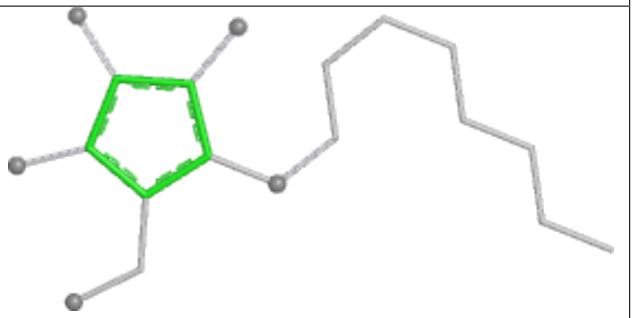
Bond lengths



Bond angles

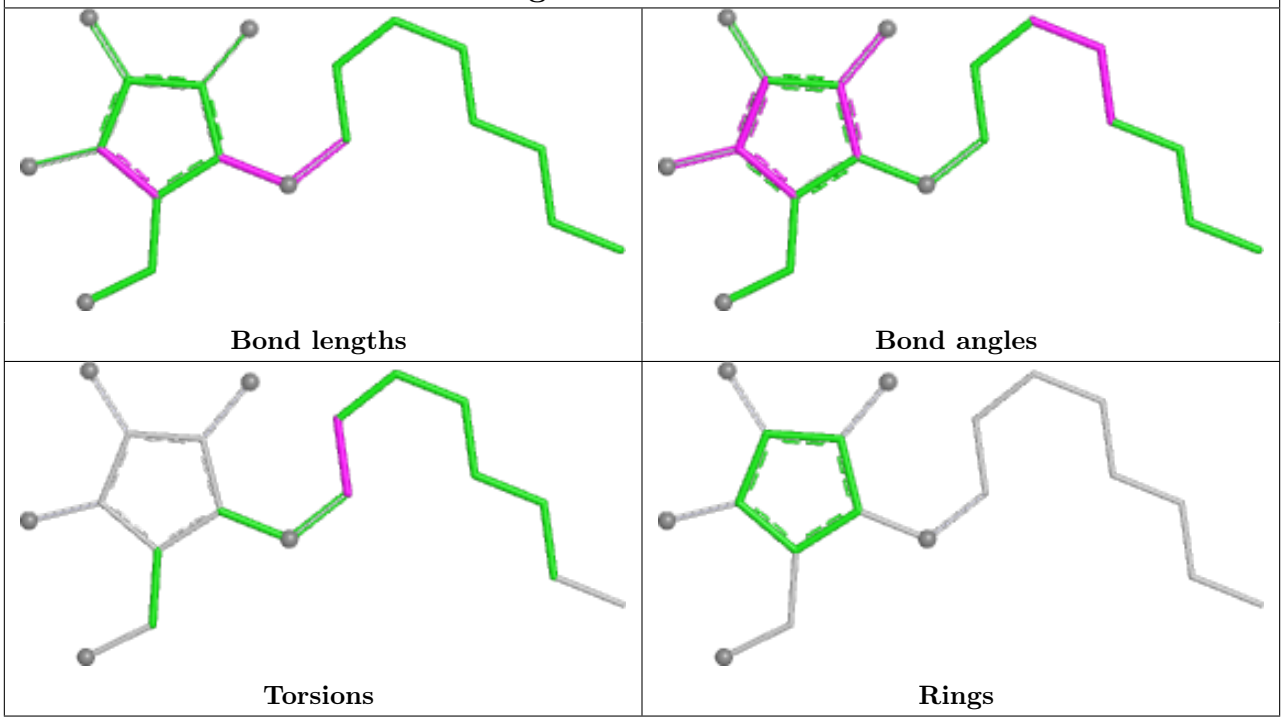


Torsions

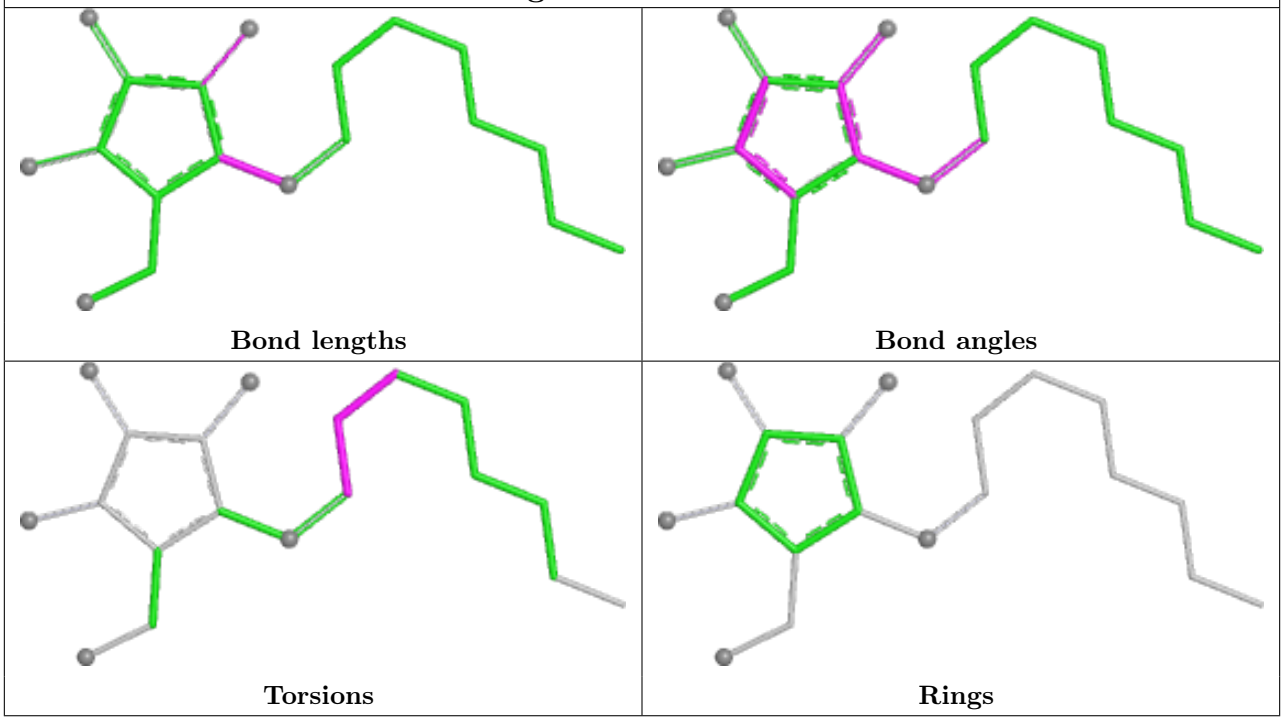


Rings

Ligand N0T F 604



Ligand N0T B 602



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, 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	538/550 (97%)	-0.21	6 (1%)	80	84	18, 27, 51, 86	41 (7%)
1	B	540/550 (98%)	-0.32	7 (1%)	77	81	18, 24, 42, 64	23 (4%)
1	C	540/550 (98%)	-0.26	9 (1%)	70	75	17, 23, 44, 66	29 (5%)
1	D	539/550 (98%)	-0.30	3 (0%)	89	91	14, 20, 39, 68	25 (4%)
1	E	540/550 (98%)	-0.31	7 (1%)	77	81	14, 21, 40, 60	28 (5%)
1	F	539/550 (98%)	-0.28	3 (0%)	89	91	14, 22, 43, 77	24 (4%)
1	G	540/550 (98%)	-0.29	4 (0%)	87	90	14, 20, 40, 76	26 (4%)
1	H	539/550 (98%)	-0.25	9 (1%)	70	75	18, 27, 50, 68	39 (7%)
All	All	4315/4400 (98%)	-0.28	48 (1%)	80	84	14, 23, 45, 86	235 (5%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	TRP	5.3
1	D	439	TRP	5.2
1	H	444	THR	5.0
1	C	441	ALA	4.5
1	G	435	THR	4.4
1	E	439	TRP	4.4
1	B	36	ALA	4.1
1	G	444	THR	4.0
1	H	439	TRP	4.0
1	B	443	ALA	3.8
1	E	441	ALA	3.8
1	C	433	THR	3.7
1	H	523	GLY	3.3
1	E	36	ALA	3.2
1	G	443	ALA	3.2
1	B	439	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	435	THR	2.9
1	H	443	ALA	2.9
1	E	438	ILE	2.8
1	E	435	THR	2.8
1	C	443	ALA	2.8
1	D	435	THR	2.8
1	A	232	ILE	2.7
1	E	443	ALA	2.7
1	D	438	ILE	2.6
1	H	438	ILE	2.6
1	C	239	PRO	2.6
1	B	438	ILE	2.6
1	H	435	THR	2.5
1	A	237	LEU	2.5
1	C	444	THR	2.5
1	A	521	LEU	2.5
1	F	441	ALA	2.5
1	G	445	PRO	2.4
1	F	226	ALA	2.4
1	C	435	THR	2.3
1	F	440	ASN	2.3
1	C	442	GLU	2.3
1	B	444	THR	2.2
1	B	441	ALA	2.2
1	H	226	ALA	2.2
1	B	432	THR	2.1
1	C	36	ALA	2.1
1	C	434	GLU	2.1
1	A	254	PHE	2.1
1	E	442	GLU	2.1
1	H	451	HIS	2.0
1	H	232	ILE	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	H	603	4/4	0.82	0.12	29,32,34,39	4
4	ACT	F	605	4/4	0.86	0.13	28,28,31,33	4
4	ACT	D	604	4/4	0.86	0.18	28,29,32,38	0
4	ACT	G	606	4/4	0.87	0.14	27,27,30,33	4
4	ACT	E	606	4/4	0.87	0.17	30,30,32,33	4
4	ACT	D	607	4/4	0.88	0.11	26,31,36,39	4
4	ACT	G	607	4/4	0.91	0.09	30,30,33,34	4
4	ACT	F	606	4/4	0.91	0.17	23,27,27,30	4
2	NA	C	602	1/1	0.92	0.08	36,36,36,36	0
4	ACT	B	603	4/4	0.93	0.10	31,34,36,37	4
4	ACT	D	606	4/4	0.93	0.19	28,34,36,37	4
4	ACT	G	605	4/4	0.93	0.15	36,38,44,47	4
4	ACT	E	605	4/4	0.94	0.14	22,23,23,29	4
3	N0T	C	603	19/19	0.94	0.09	15,19,31,38	5
4	ACT	A	603	4/4	0.95	0.07	27,27,30,32	4
4	ACT	G	604	4/4	0.95	0.14	23,24,24,26	4
2	NA	C	601	1/1	0.95	0.10	47,47,47,47	0
3	N0T	D	605	19/19	0.96	0.08	14,15,36,36	0
3	N0T	H	602	19/19	0.96	0.08	17,19,32,37	5
3	N0T	B	602	19/19	0.97	0.07	17,19,38,46	0
2	NA	A	605	1/1	0.97	0.12	36,36,36,36	0
2	NA	E	608	1/1	0.97	0.06	41,41,41,41	0
3	N0T	E	604	19/19	0.97	0.09	14,15,34,40	5
3	N0T	F	604	19/19	0.97	0.09	14,17,36,37	4
3	N0T	G	603	19/19	0.97	0.09	13,15,29,33	5
3	N0T	A	602	19/19	0.97	0.07	17,20,48,49	2
2	NA	D	609	1/1	0.98	0.06	27,27,27,27	0
2	NA	H	601	1/1	0.98	0.09	33,33,33,33	0
2	NA	E	603	1/1	0.99	0.09	22,22,22,22	0
2	NA	E	607	1/1	0.99	0.06	30,30,30,30	0
2	NA	B	604	1/1	0.99	0.07	30,30,30,30	0
2	NA	E	609	1/1	0.99	0.08	22,22,22,22	0
2	NA	F	601	1/1	0.99	0.05	26,26,26,26	0
2	NA	F	607	1/1	0.99	0.06	28,28,28,28	0
2	NA	G	608	1/1	0.99	0.06	30,30,30,30	0
2	NA	G	610	1/1	0.99	0.09	27,27,27,27	0
2	NA	A	601	1/1	0.99	0.15	33,33,33,33	0

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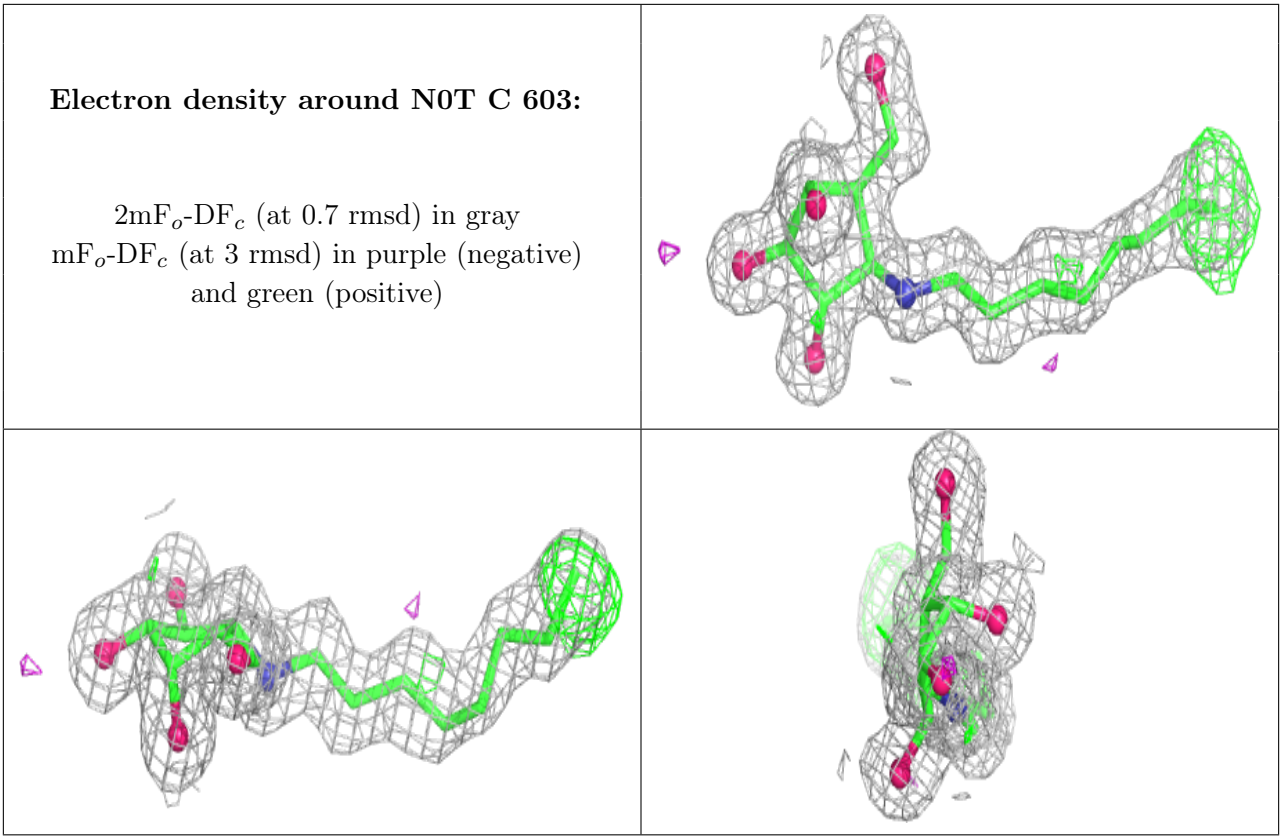
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	H	604	1/1	0.99	0.07	26,26,26,26	0
2	NA	H	606	1/1	0.99	0.04	35,35,35,35	1
2	NA	H	607	1/1	0.99	0.12	38,38,38,38	0
2	NA	A	606	1/1	0.99	0.06	34,34,34,34	0
2	NA	D	601	1/1	0.99	0.06	24,24,24,24	0
2	NA	D	602	1/1	0.99	0.07	24,24,24,24	0
2	NA	B	601	1/1	0.99	0.11	35,35,35,35	0
2	NA	E	602	1/1	0.99	0.08	21,21,21,21	0
2	NA	E	601	1/1	1.00	0.05	23,23,23,23	0
2	NA	F	602	1/1	1.00	0.07	25,25,25,25	0
2	NA	F	603	1/1	1.00	0.06	22,22,22,22	0
2	NA	A	604	1/1	1.00	0.08	27,27,27,27	0
2	NA	G	601	1/1	1.00	0.10	28,28,28,28	0
2	NA	G	602	1/1	1.00	0.07	22,22,22,22	0
2	NA	C	604	1/1	1.00	0.05	26,26,26,26	0
2	NA	G	609	1/1	1.00	0.06	24,24,24,24	0
2	NA	D	603	1/1	1.00	0.07	21,21,21,21	0
2	NA	D	608	1/1	1.00	0.06	24,24,24,24	0
2	NA	C	605	1/1	1.00	0.06	29,29,29,29	0
2	NA	H	605	1/1	1.00	0.05	30,30,30,30	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.

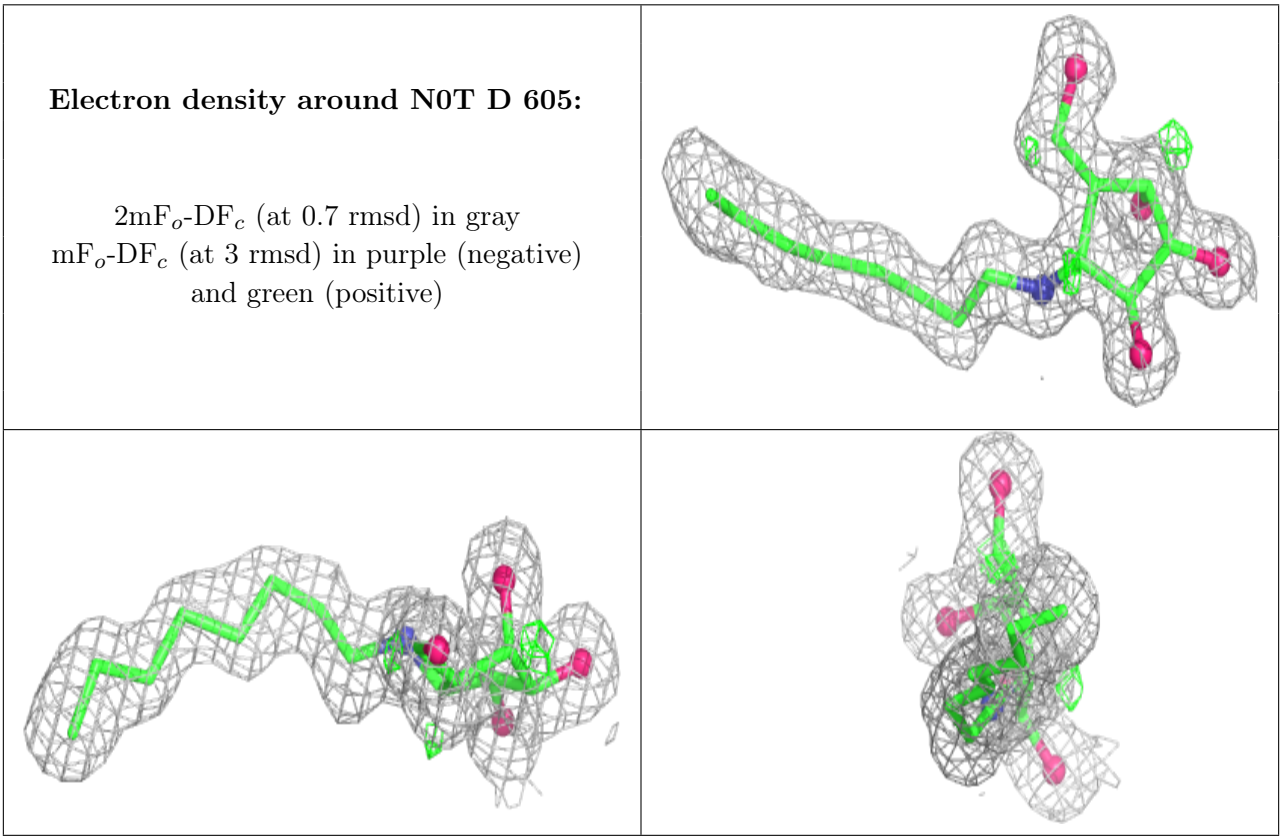
Electron density around N0T C 603:

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



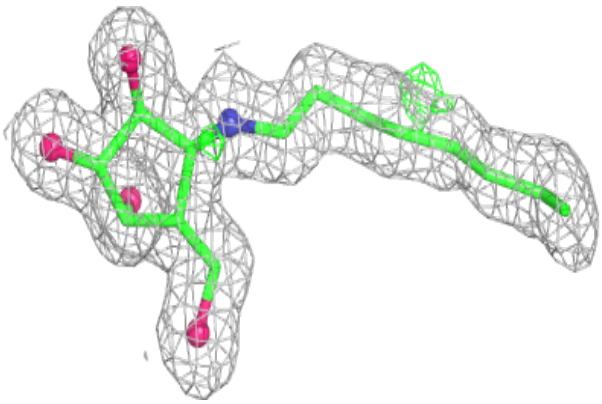
Electron density around N0T D 605:

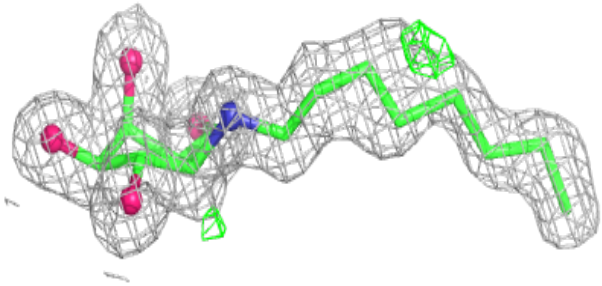
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

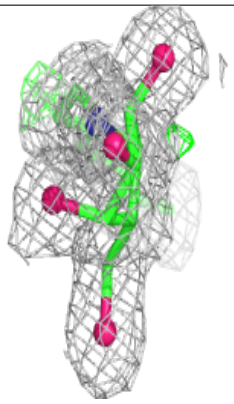


Electron density around N0T H 602:

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

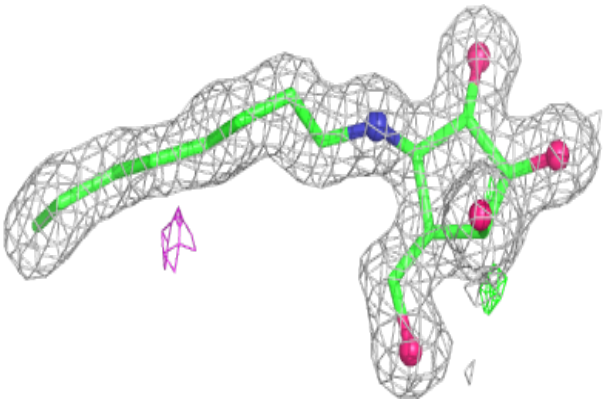


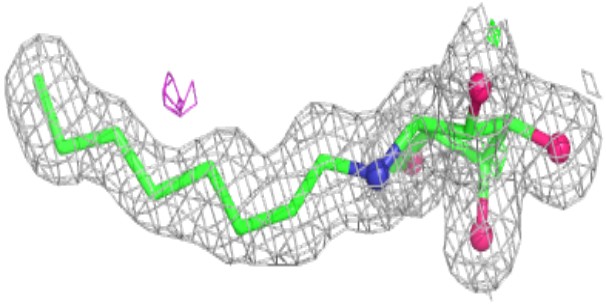


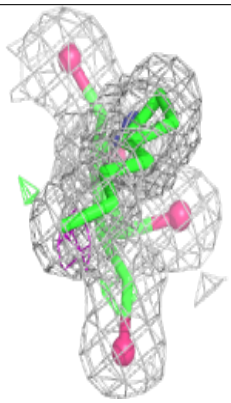


Electron density around N0T B 602:

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

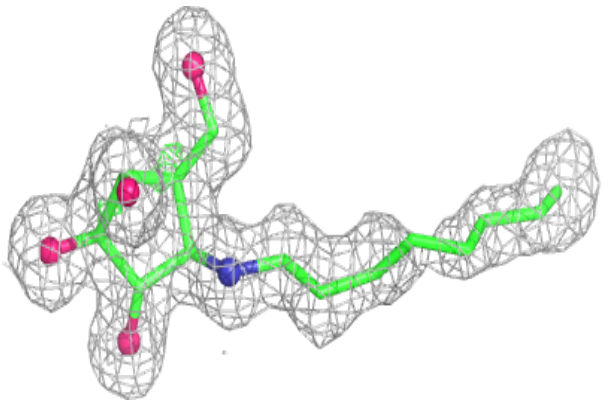


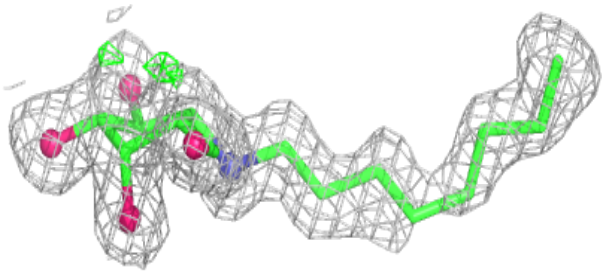


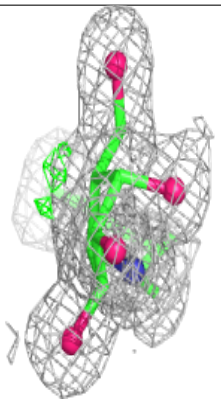


Electron density around N0T E 604:

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

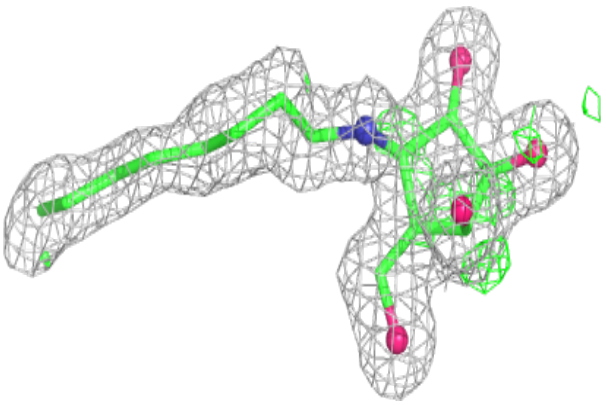


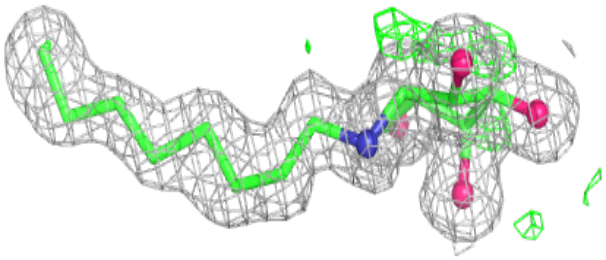


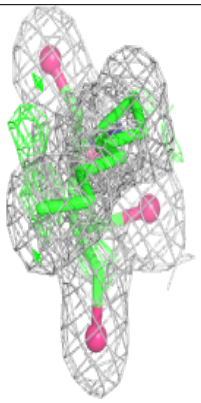


Electron density around N0T F 604:

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

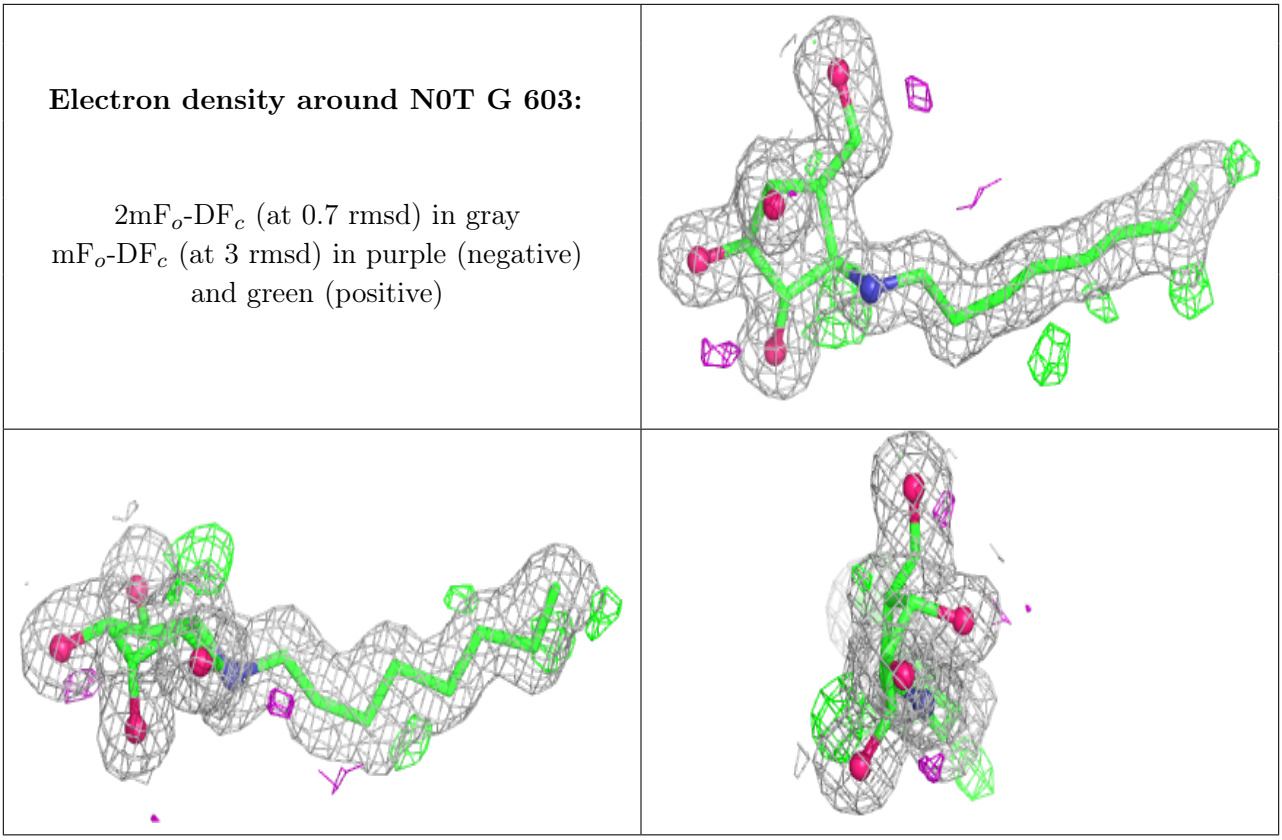






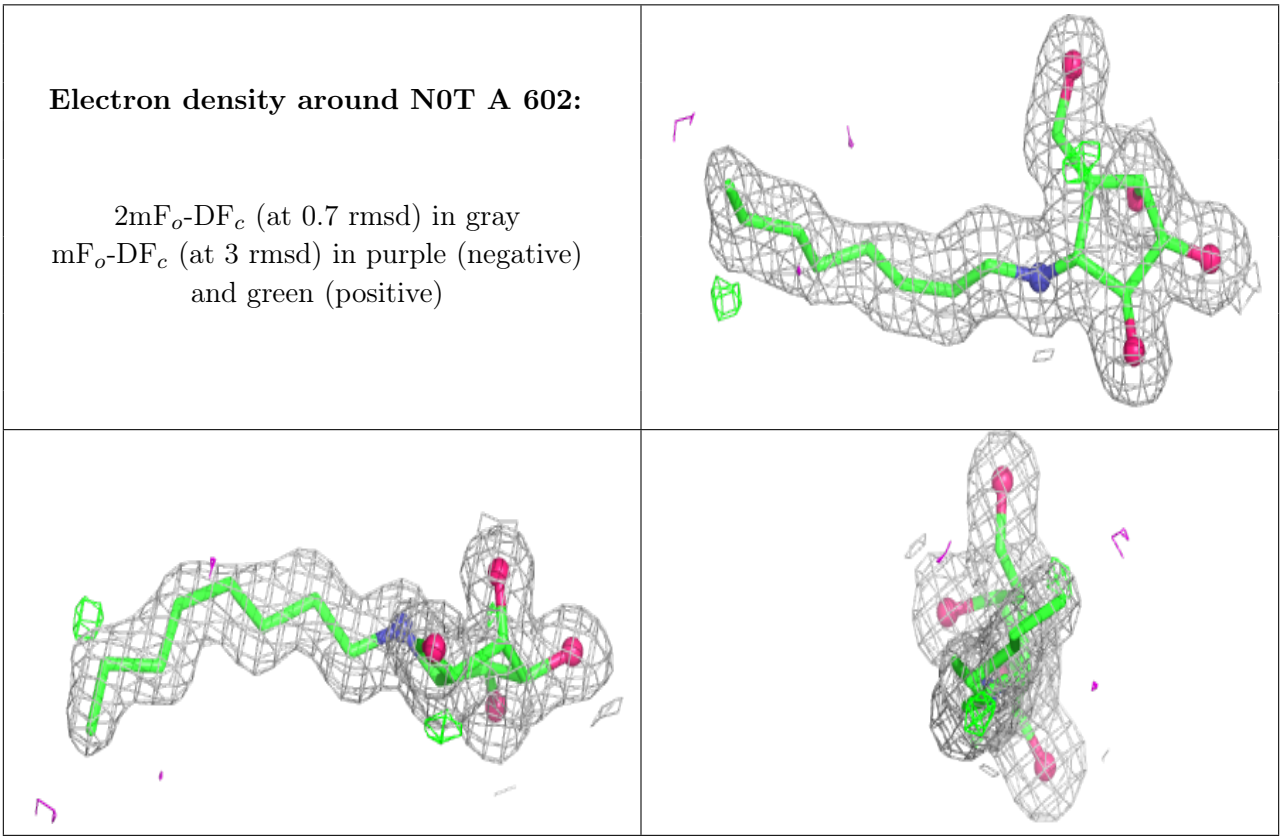
Electron density around N0T G 603:

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



Electron density around N0T 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.