

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2021 – 08:35 AM GMT

PDB ID : 6TBJ

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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as 541 be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.17.1.dev1 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

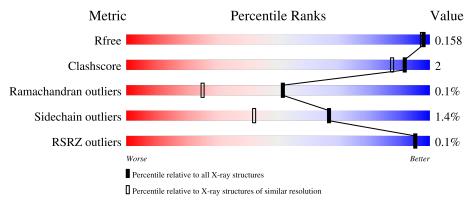
Validation Pipeline (wwPDB-VP) : 2.17.1.dev1

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
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	92%	• 5%
1	В	550	90%	5% 5%
1	С	550	91%	5% •
1	D	550	91%	5% •
1	Е	550	93%	

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Mol	Chain	Length	Quality of chain	
1	F	550	93%	
1	G	550	91%	6% •
1	Н	550	90%	5% 5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35492 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		At	oms			ZeroOcc	AltConf	Trace
1	A	ror.	Total	С	Ν	О	S	0	3	0
1	A	525	4131	2650	697	767	17	0	ე	0
1	В	524	Total	С	N	О	S	0	2	0
1	Б	324	4135	2652	699	769	15	0	Δ	
1	С	526	Total	С	N	О	S	0	1	1
1		520	4123	2641	698	769	15	0	1	1
1	D	531	Total	С	N	О	S	0	4	0
1	ש	991	4194	2691	709	779	15	0		
1	Е	532	Total	С	N	О	S	0	0	0
1	L	55∠	4156	2662	702	777	15	0	U	
1	F	531	Total	С	N	О	S	0	3	0
1	Γ	991	4186	2678	709	784	15	0)	0
1	G	532	Total	С	N	О	S	0	5	0
1	G	004	4206	2695	715	780	16)	
1	Н	523	Total	С	N	О	S	0	5	0
1	11	J23	4106	2629	691	771	15)	

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
В	26	MET	=	initiating methionine	UNP B3PBE0
В	27	GLY	-	expression tag	UNP B3PBE0
В	28	SER	-	expression tag	UNP B3PBE0



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Chain	Residue	Modelled	Actual	Comment	Reference
В	29	SER	_	expression tag	UNP B3PBE0
В	30	HIS	_	expression tag	UNP B3PBE0
В	31	HIS	-	expression tag	UNP B3PBE0
В	32	HIS	_	expression tag	UNP B3PBE0
В	33	HIS	-	expression tag	UNP B3PBE0
В	34	HIS	_	expression tag	UNP B3PBE0
В	35	HIS	_	expression tag	UNP B3PBE0
С	26	MET	-	initiating methionine	UNP B3PBE0
С	27	GLY	-	expression tag	UNP B3PBE0
С	28	SER	_	expression tag	UNP B3PBE0
С	29	SER	-	expression tag	UNP B3PBE0
С	30	HIS	_	expression tag	UNP B3PBE0
С	31	HIS	-	expression tag	UNP B3PBE0
С	32	HIS	-	expression tag	UNP B3PBE0
С	33	HIS	-	expression tag	UNP B3PBE0
С	34	HIS	_	expression tag	UNP B3PBE0
С	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
Е	26	MET	_	initiating methionine	UNP B3PBE0
Е	27	GLY	_	expression tag	UNP B3PBE0
Е	28	SER	_	expression tag	UNP B3PBE0
Е	29	SER	_	expression tag	UNP B3PBE0
Е	30	HIS	_	expression tag	UNP B3PBE0
Е	31	HIS	_	expression tag	UNP B3PBE0
Е	32	HIS	-	expression tag	UNP B3PBE0
Е	33	HIS	-	expression tag	UNP B3PBE0
Е	34	HIS		expression tag	UNP B3PBE0
Е	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
Н	26	MET	-	initiating methionine	UNP B3PBE0
Н	27	GLY	-	expression tag	UNP B3PBE0
Н	28	SER	ı	expression tag	UNP B3PBE0
Н	29	SER	-	expression tag	UNP B3PBE0
Н	30	HIS		expression tag	UNP B3PBE0
Н	31	HIS	=	expression tag	UNP B3PBE0
Н	32	HIS	-	expression tag	UNP B3PBE0
Н	33	HIS	-	expression tag	UNP B3PBE0
Н	34	HIS	ı	expression tag	UNP B3PBE0
Н	35	HIS	_	expression tag	UNP B3PBE0

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

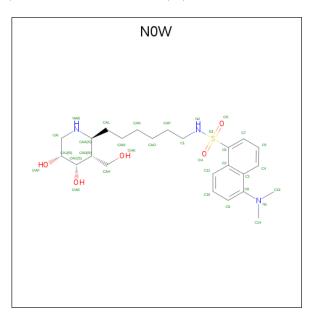
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Na 3 3	0	0
2	В	1	Total Na 1 1	0	0
2	С	3	Total Na 3 3	0	0
2	D	5	Total Na 5 5	0	0
2	E	4	Total Na 4 4	0	0
2	F	4	Total Na 4 4	0	0
2	G	3	Total Na 3 3	0	0



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Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
2	Н	4	Total Na 4 4	0	0

• Molecule 3 is 5-(dimethylamino)- $\{N\}$ -[6-[(2 $\{S\},3$ $\{R\},4$ $\{S\},5$ $\{R\}$)-3-(hydroxymethyl)-4,5-bis(oxidanyl)piperidin-2-yl]hexyl]naphthalene-1-sulfonamide (three-letter code: N0W) (formula: $C_{24}H_{37}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 21 13 2 5 1	0	0
3	В	1	Total C N O 13 9 1 3	0	0
3	С	1	Total C N O 12 8 1 3	0	0
3	D	1	Total C N O S 21 13 2 5 1	0	0
3	E	1	Total C N O 15 11 1 3	0	0
3	F	1	Total C N O S 21 13 2 5 1	0	0
3	G	1	Total C N O 15 11 1 3	0	0
3	Н	1	Total C N O 15 11 1 3	0	0

• Molecule 4 is water.



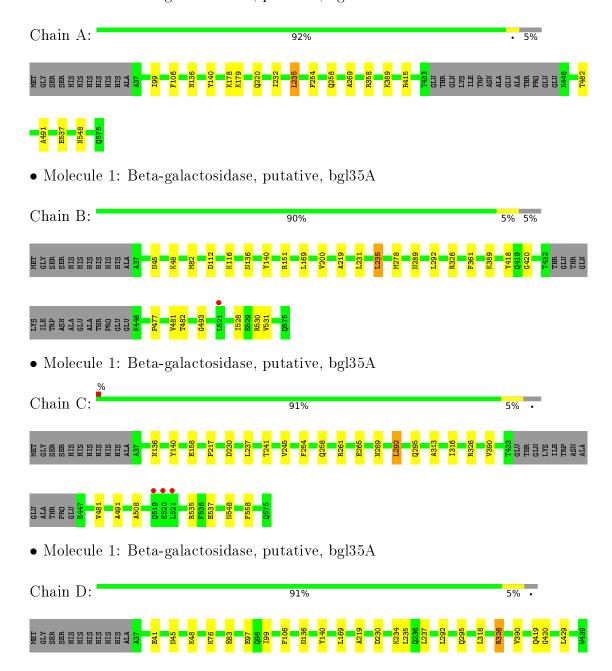
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	220	Total O 220 220	0	0
4	В	254	Total O 254 254	0	0
4	С	238	Total O 238 238	0	0
4	D	307	Total O 307 307	0	0
4	Е	301	Total O 301 301	0	0
4	F	274	Total O 274 274	0	0
4	G	291	Total O 291 291	0	0
4	Н	210	Total O 210 210	0	0



3 Residue-property plots (i)

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

• Molecule 1: Beta-galactosidase, putative, bgl35A







• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain E: 93% · ·



F558 R561

• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain F: 93% · ·



T482 E537 W541 R566 S573 V574 Q575

• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain G: 91% 6% ·



CLU
ALA
ALA
ALA
ALA
ALA
CLU
CLU
CLU
CLU
CLU
CLV
A4491
A491
A508
A508
A508
A508
A508
A508

• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H: 90% 5% 5%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	99.42Å 115.79Å 116.19Å	Danasitan
a, b, c, α , β , γ	89.93° 90.08° 89.99°	Depositor
Resolution (Å)	63.21 - 1.50	Depositor
Resolution (A)	63.21 - 1.50	EDS
% Data completeness	94.5 (63.21-1.50)	Depositor
(in resolution range)	94.5 (63.21-1.50)	EDS
R_{merge}	(Not available)	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.78 \; ({\rm at} \; 1.50 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.145 , 0.164	Depositor
10,~10 free	0.147 , 0.158	DCC
R_{free} test set	39812 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35\;,27.5$	EDS
L-test for twinning ²	$< L >=0.35, < L^2>=0.18$	Xtriage
	0.249 for h,-l,k	
	0.249 for h,l,-k	
	0.186 for h,-k,-l	
Estimated twinning fraction	0.130 for -h,k,-l	Xtriage
	0.129 for -h,-k,l	
	0.136 for -h,-l,-k	
	0.129 for -h,l,k	
	0.582 for H, K, L	
Reported twinning fraction	0.048 for h,-k,-l	Depositor
Reported twinning fraction	0.089 for H, -L, K	Depositor
	0.281 for H, L, -K	
Outliers	0 of 793059 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35492	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



 $^{^{1} {\}rm Intensities}$ estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, N0W

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	Bo	nd lengths	В	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.81	0/4247	0.94	$2/5787 \; (0.0\%)$
1	В	0.79	0/4248	0.95	$2/5786 \ (0.0\%)$
1	С	0.81	0/4233	0.96	1/5771~(0.0%)
1	D	0.85	$2/4312 \ (0.0\%)$	0.98	0/5877
1	Е	0.81	0/4266	0.95	3/5817 (0.1%)
1	F	0.84	0/4299	0.98	0/5859
1	G	0.84	$1/4325 \ (0.0\%)$	0.99	0/5891
1	Н	0.82	$1/4225 \ (0.0\%)$	0.94	$2/5768 \; (0.0\%)$
All	All	0.82	$4/34155 \ (0.0\%)$	0.96	$10/46556 \ (0.0\%)$

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	D	533	GLU	CD-OE1	-6.49	1.18	1.25
1	Н	533	GLU	CD-OE1	-5.58	1.19	1.25
1	G	205	GLU	CD-OE1	-5.45	1.19	1.25
1	D	97	GLU	CD-OE1	-5.21	1.20	1.25

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	В	530	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	С	535	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	Н	340	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	E	561	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	В	151	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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	Α	4131	0	3985	8	0
1	В	4135	0	3999	12	0
1	С	4123	0	3960	11	0
1	D	4194	0	4036	19	0
1	Ε	4156	0	3981	12	0
1	F	4186	0	4014	12	0
1	G	4206	0	4070	18	0
1	Н	4106	0	3914	14	0
2	A	3	0	0	0	0
2	В	1	0	0	0	0
2	С	3	0	0	0	0
2	D	5	0	0	0	0
2	Ε	4	0	0	0	0
2	F	4	0	0	0	0
2	G	3	0	0	0	0
2	Н	4	0	0	0	0
3	A	21	0	0	0	0
3	В	13	0	0	0	0
3	С	12	0	0	0	0
3	D	21	0	0	0	0
3	E	15	0	0	0	0
3	F	21	0	0	0	0
3	G	15	0	0	0	0
3	Н	15	0	0	0	0
4	A	220	0	0	2	0
4	В	254	0	0	1	0
4	С	238	0	0	1	0
4	D	307	0	0	3	0
4	E	301	0	0	4	0
4	F	274	0	0	1	0
4	G	291	0	0	3	0
4	Н	210	0	0	0	0
All	All	35492	0	31959	102	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 102 close contacts within the same asymmetric unit are listed below, sorted by



their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:D:528:ILE:HD13	1:D:569:MET:SD	2.02	0.99
1:D:326:ARG:HG3	1:D:326:ARG:HH21	1.24	0.98
1:A:482:THR:HG22	4:A:724:HOH:O	1.68	0.94
1:H:199:MET:HG2	1:H:277:PRO:HB2	1.52	0.92
1:E:482:THR:HG22	4:E:756:HOH:O	1.89	0.72

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	Perce	${ m ntiles}$
1	A	$524/550 \; (95\%)$	501 (96%)	22 (4%)	1 (0%)	47	23
1	В	$522/550 \; (95\%)$	499 (96%)	23 (4%)	0	100	100
1	С	$523/550 \; (95\%)$	501 (96%)	21 (4%)	1 (0%)	47	23
1	D	531/550 (96%)	511 (96%)	19 (4%)	1 (0%)	47	23
1	E	$528/550 \; (96\%)$	504 (96%)	24 (4%)	0	100	100
1	F	530/550~(96%)	509 (96%)	21 (4%)	0	100	100
1	G	$533/550 \ (97\%)$	513 (96%)	19 (4%)	1 (0%)	47	23
1	Н	$524/550 \; (95\%)$	504 (96%)	20 (4%)	0	100	100
All	All	$4215/4400 \ (96\%)$	4042 (96%)	169 (4%)	4 (0%)	51	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	491	ALA
1	A	491	ALA
1	G	491	ALA
1	D	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	Perce	ntiles
1	A	$427/461 \; (93\%)$	422 (99%)	5 (1%)	71	48
1	В	$429/461 \ (93\%)$	423 (99%)	6 (1%)	67	42
1	С	425/461 (92%)	416 (98%)	9 (2%)	53	23
1	D	432/461 (94%)	425 (98%)	7 (2%)	62	36
1	E	$427/461 \; (93\%)$	420 (98%)	7 (2%)	62	36
1	F	432/461 (94%)	426 (99%)	6 (1%)	67	42
1	G	434/461 (94%)	431 (99%)	3 (1%)	84	69
1	Н	422/461 (92%)	416 (99%)	6 (1%)	67	42
All	All	3428/3688 (93%)	3379 (99%)	49 (1%)	67	42

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	83	GLU
1	F	292	LEU
1	E	136	ASN
1	E	289	ASN
1	F	449	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	419	GLN
1	Н	64	GLN
1	Н	289	ASN
1	С	451	HIS
1	D	45	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 35 ligands modelled in this entry, 27 are monoatomic - leaving 8 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	T	Chain	Res	Link	Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	NoW	В	602	_	13,13,35	1.26	1 (7%)	11,17,49	1.19	2 (18%)	
3	NoW	D	606	-	21,21,35	1.94	4 (19%)	21,28,49	1.51	4 (19%)	
3	NoW	G	604	_	15,15,35	1.20	2 (13%)	13,19,49	1.26	1 (7%)	
3	NoW	A	604	_	21,21,35	1.69	2 (9%)	21,28,49	3.00	3 (14%)	
3	NoW	С	604	_	12,12,35	1.63	1 (8%)	11,16,49	1.69	2 (18%)	
3	NoW	F	605	-	21,21,35	1.69	3 (14%)	21,28,49	1.73	4 (19%)	
3	NoW	Н	605	_	15,15,35	1.04	1 (6%)	13,19,49	1.12	1 (7%)	
3	NoW	E	605	_	15,15,35	1.77	5 (33%)	13,19,49	1.03	1 (7%)	

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	N0W	В	602	-	-	2/5/22/40	0/1/1/3
3	N0W	D	606	-	-	3/13/30/40	0/1/1/3
3	NoW	G	604	-	-	4/7/24/40	0/1/1/3
3	NoW	A	604	_	-	4/13/30/40	0/1/1/3



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NoW	С	604	-	-	2/4/21/40	0/1/1/3
3	NoW	F	605	-	-	3/13/30/40	0/1/1/3
3	NoW	Н	605	-	-	3/7/24/40	0/1/1/3
3	N0W	E	605	-	-	2/7/24/40	0/1/1/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	Α	604	N0W	C6-S3	-6.61	1.59	1.75
3	F	605	N0W	C6-S3	-5.92	1.61	1.75
3	D	606	N0W	C6-S3	-5.54	1.62	1.75
3	E	605	NoW	CAD-CAC	-4.19	1.48	1.53
3	С	604	N0W	CAI-CAJ	3.95	1.56	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	604	N0W	C6-S3-N2	9.53	113.59	107.76
3	A	604	N0W	O5-S3-O4	-8.97	105.96	118.85
3	F	605	N0W	CAI-CAJ-CAC	5.40	116.66	110.33
3	С	604	N0W	CAL-CAA-NAB	-4.98	105.02	110.60
3	D	606	NoW	O5-S3-N2	-3.93	101.71	107.31

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	N0W	C1-N2-S3-O5
3	A	604	N0W	N2-C1-CAP-CAO
3	A	604	N0W	NAB-CAA-CAL-CAM
3	A	604	NoW	CAD-CAA-CAL-CAM
3	В	602	NoW	NAB-CAA-CAL-CAM

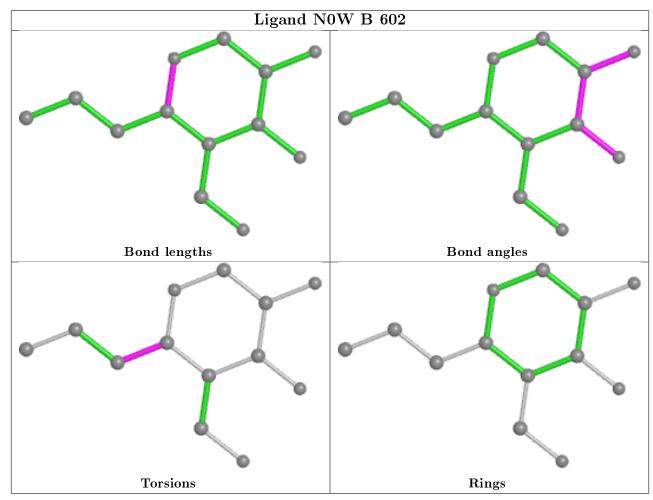
There are no ring outliers.

No monomer is involved in short contacts.

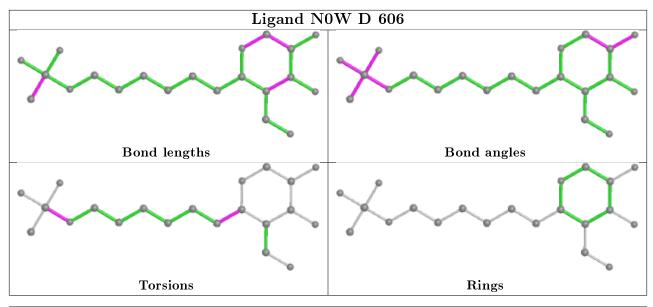
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

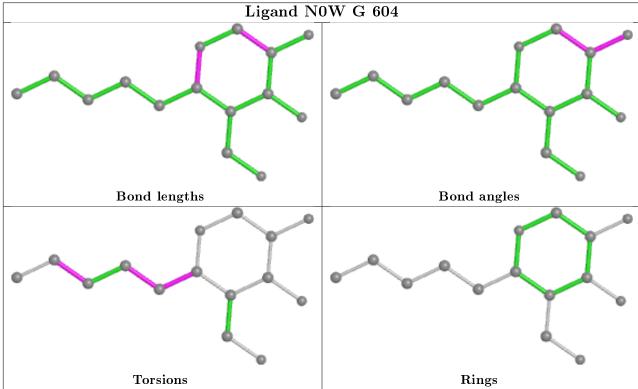


Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

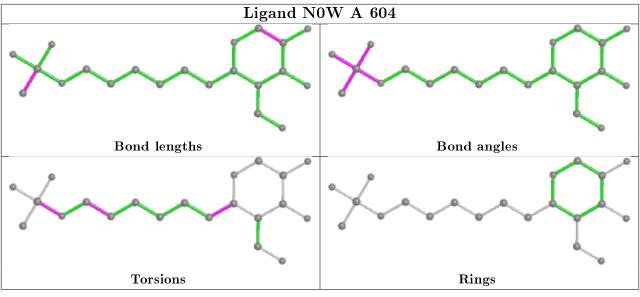


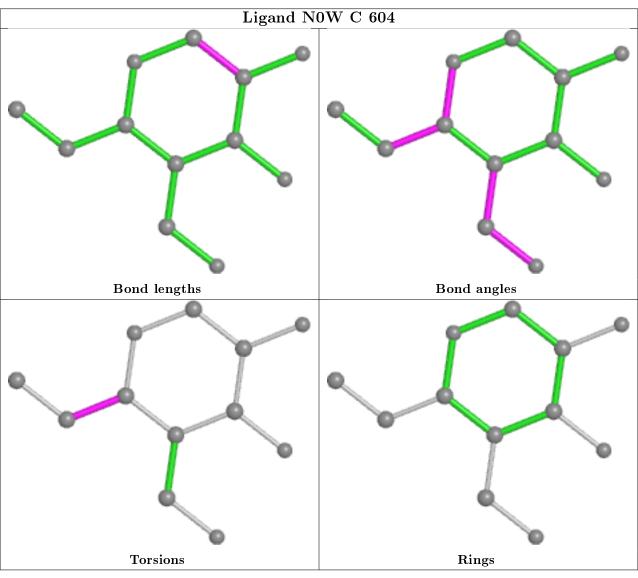




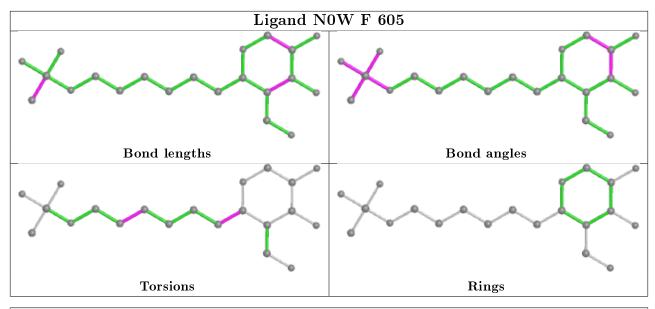


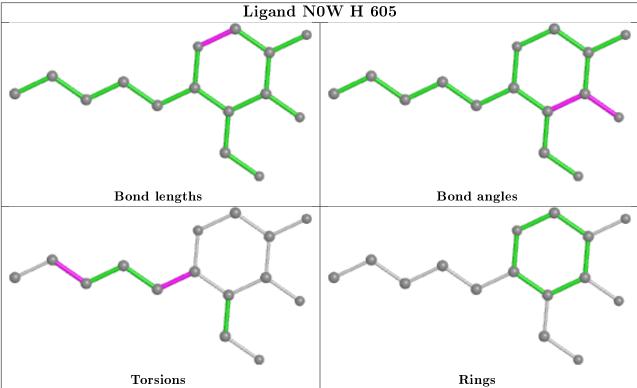




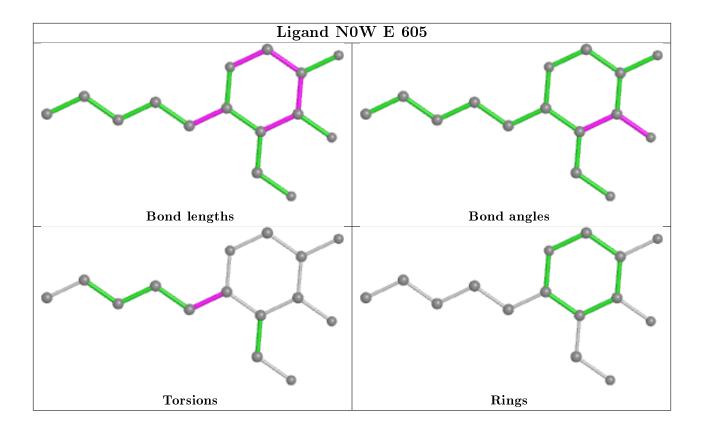












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	525/550 (95%)	-0.49	0 100 100	15, 22, 37, 53	3 (0%)
1	В	$524/550 \; (95\%)$	-0.57	1 (0%) 95 95	15, 21, 31, 45	6 (1%)
1	С	$526/550 \; (95\%)$	-0.52	3 (0%) 89 91	14, 21, 33, 46	7 (1%)
1	D	531/550 (96%)	-0.55	0 100 100	13, 19, 33, 52	2 (0%)
1	E	$532/550 \; (96\%)$	-0.56	0 100 100	14, 20, 33, 46	4 (0%)
1	F	531/550 (96%)	-0.51	1 (0%) 95 95	13, 20, 35, 43	2 (0%)
1	G	$532/550 \; (96\%)$	-0.51	1 (0%) 95 95	13, 19, 34, 47	4 (0%)
1	Н	$523/550 \; (95\%)$	-0.51	0 100 100	15, 22, 34, 49	4 (0%)
All	All	4224/4400 (96%)	-0.53	6 (0%) 95 95	13, 20, 34, 53	32 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	521	LEU	5.0
1	G	36	ALA	4.1
1	В	521	LEU	3.3
1	С	519	GLN	2.2
1	С	520	GLU	2.2

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)

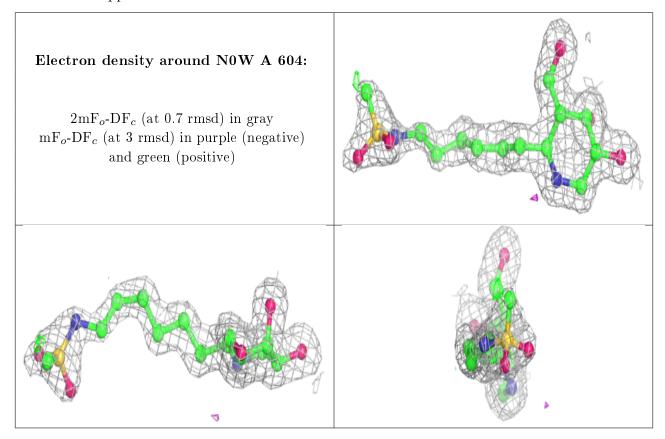
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	NA	A	602	1/1	0.97	0.07	27,27,27,27	0
2	NA	A	603	1/1	0.97	0.06	28,28,28,28	0
3	N0W	A	604	21/33	0.97	0.08	18,20,30,33	7
3	N0W	В	602	13/33	0.97	0.06	17,18,20,25	0
3	NoW	D	606	21/33	0.97	0.07	16,19,32,45	5
3	NoW	F	605	21/33	0.97	0.09	17,19,29,34	7
3	N0W	Н	605	15/33	0.97	0.07	16,18,20,24	3
2	NA	F	603	1/1	0.98	0.08	27,27,27,27	0
2	NA	F	604	1/1	0.98	0.05	28,28,28,28	0
2	NA	G	603	1/1	0.98	0.04	27,27,27,27	0
2	NA	С	601	1/1	0.98	0.06	26,26,26,26	0
2	NA	С	602	1/1	0.98	0.06	29,29,29,29	0
3	NoW	С	604	12/33	0.98	0.07	17,18,21,22	0
2	NA	D	605	1/1	0.98	0.08	28,28,28,28	0
3	NoW	E	605	15/33	0.98	0.07	15,16,21,23	3
2	NA	Ε	603	1/1	0.98	0.04	28,28,28,28	0
3	N0W	G	604	15/33	0.98	0.07	14,17,20,25	3
2	NA	F	602	1/1	0.98	0.03	26,26,26,26	0
2	NA	A	601	1/1	0.99	0.03	30,30,30,30	0
2	NA	Н	601	1/1	0.99	0.07	25,25,25,25	0
2	NA	Н	603	1/1	0.99	0.03	32,32,32,32	0
2	NA	Н	604	1/1	0.99	0.06	29,29,29,29	0
2	NA	В	601	1/1	0.99	0.03	28,28,28,28	0
2	NA	E	604	1/1	0.99	0.06	25,25,25,25	0
2	NA	F	601	1/1	0.99	0.09	21,21,21,21	0
2	NA	С	603	1/1	0.99	0.06	31,31,31,31	0
2	NA	D	601	1/1	0.99	0.04	22,22,22,22	0
2	NA	D	604	1/1	0.99	0.06	26,26,26,26	0
2	NA	G	601	1/1	0.99	0.04	20,20,20,20	0
2	NA	G	602	1/1	0.99	0.05	28,28,28,28	0
2	NA	Ε	601	1/1	1.00	0.05	21,21,21,21	0
2	NA	Ε	602	1/1	1.00	0.05	23,23,23,23	0
2	NA	D	602	1/1	1.00	0.05	20,20,20,20	0
2	NA	D	603	1/1	1.00	0.06	24,24,24,24	0
2	NA	Н	602	1/1	1.00	0.03	29,29,29,29	0

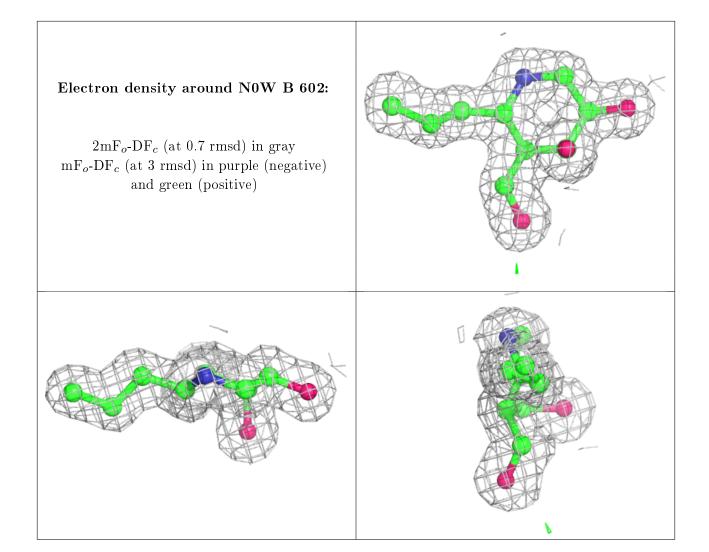
The following is a graphical depiction of the model fit to experimental electron density of all



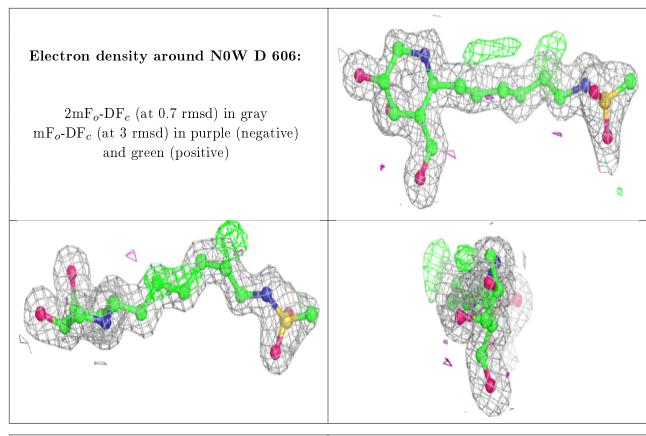
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

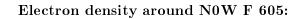




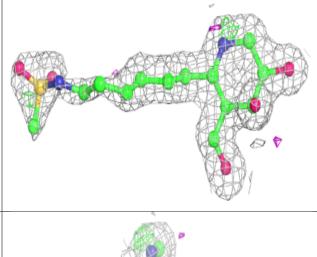


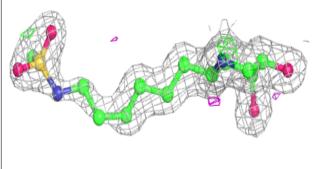


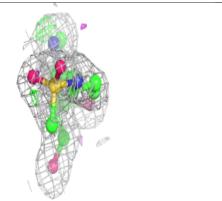




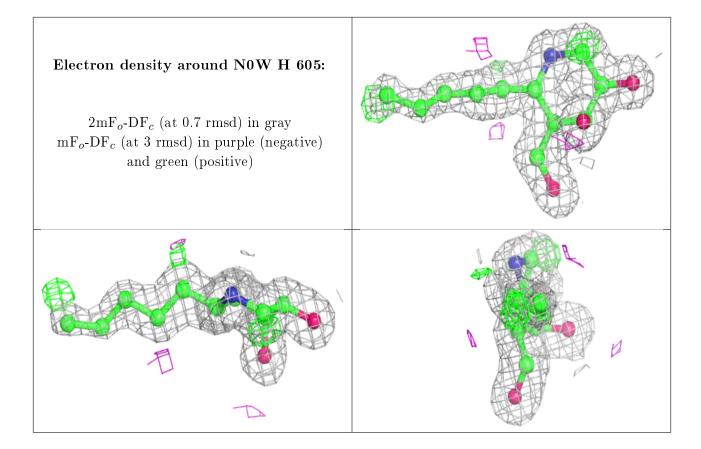
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



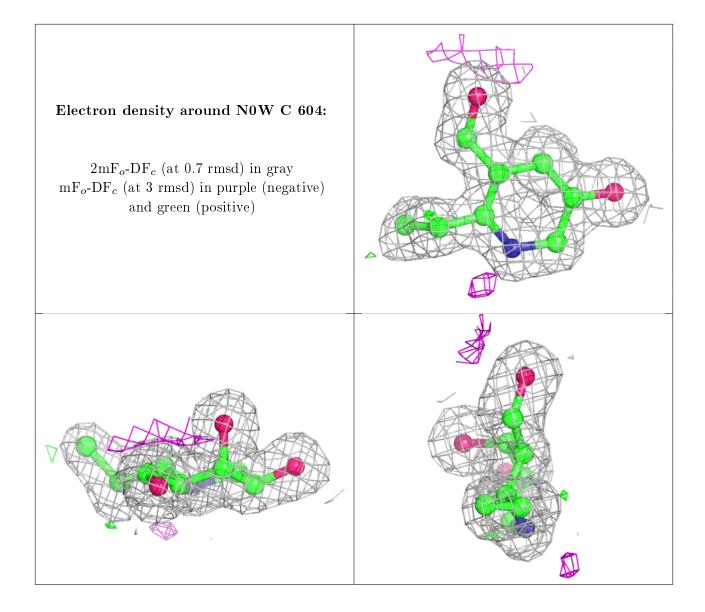




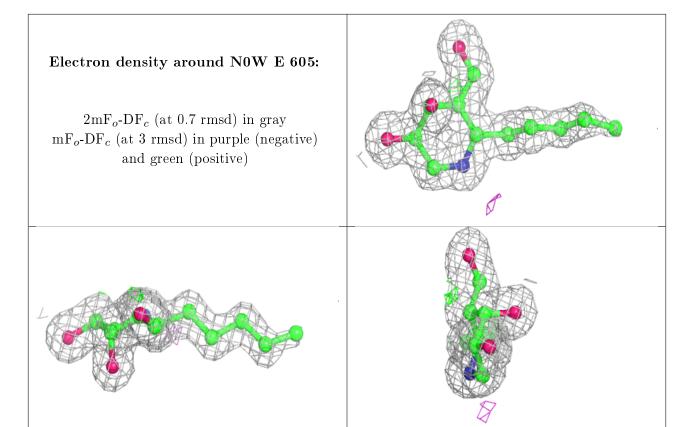












Electron density around NOW G 604: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

