



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:14 PM UTC

PDB ID : 6TBJ / pdb_00006tbj
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

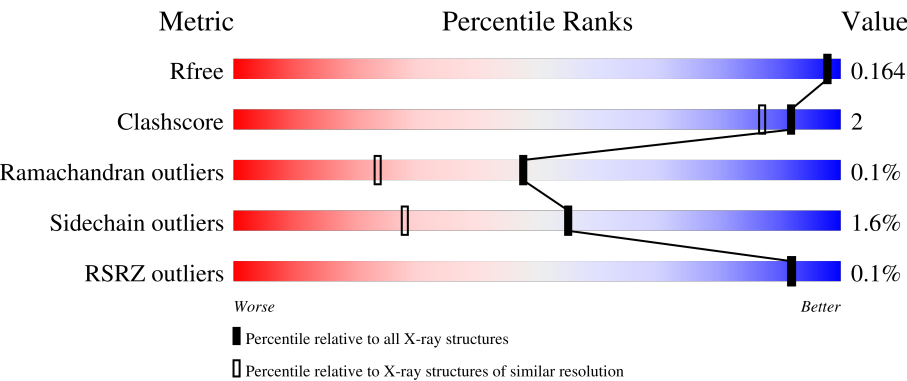
1 Overall quality at a glance i

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	91% . . 5%
1	B	550	89% 6% 5%
1	C	550	% 89% 6% . .
1	D	550	89% 7% . .
1	E	550	91% 5% .

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Mol	Chain	Length	Quality of chain
1	F	550	 91% 5% •
1	G	550	 88% 9% •
1	H	550	 88% 7% 5%

2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	3	0
			4131	2650	697	767	17			
1	B	524	Total	C	N	O	S	0	2	0
			4135	2652	699	769	15			
1	C	526	Total	C	N	O	S	0	1	1
			4123	2641	698	769	15			
1	D	531	Total	C	N	O	S	0	4	0
			4194	2691	709	779	15			
1	E	532	Total	C	N	O	S	0	0	0
			4156	2662	702	777	15			
1	F	531	Total	C	N	O	S	0	3	0
			4186	2678	709	784	15			
1	G	532	Total	C	N	O	S	0	5	0
			4206	2695	715	780	16			
1	H	523	Total	C	N	O	S	0	5	0
			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
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 (CCD ID: NA) (formula: Na).

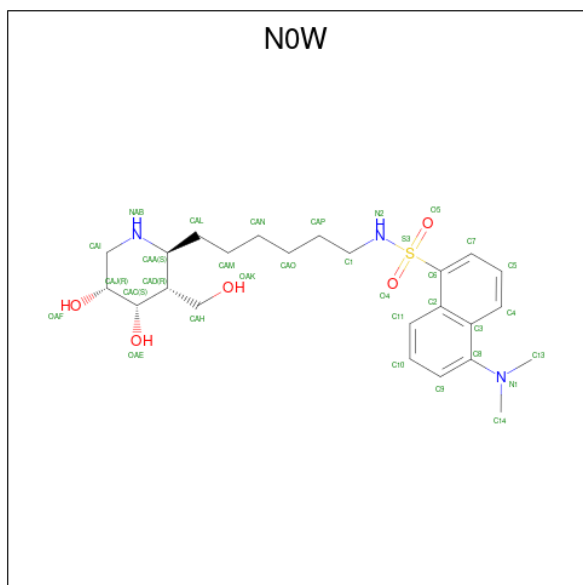
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Na 3 3	0	0
2	B	1	Total Na 1 1	0	0
2	C	3	Total Na 3 3	0	0
2	D	5	Total Na 5 5	0	0
2	E	4	Total Na 4 4	0	0
2	F	4	Total Na 4 4	0	0
2	G	3	Total Na 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	4	Total	Na	0	0
			4	4		

- 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 (CCD ID: N0W) (formula: C₂₄H₃₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



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

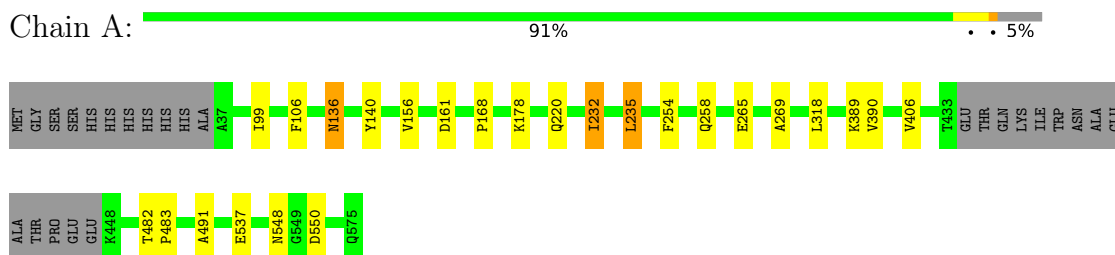
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total 220	O 220	0	0
4	B	254	Total 254	O 254	0	0
4	C	238	Total 238	O 238	0	0
4	D	307	Total 307	O 307	0	0
4	E	301	Total 301	O 301	0	0
4	F	274	Total 274	O 274	0	0
4	G	291	Total 291	O 291	0	0
4	H	210	Total 210	O 210	0	0

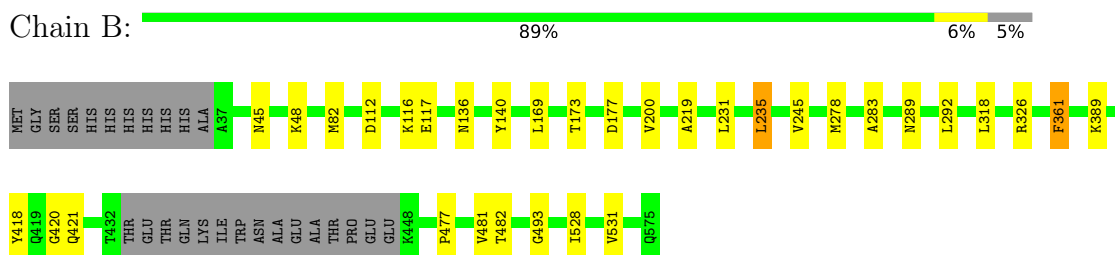
3 Residue-property plots

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.

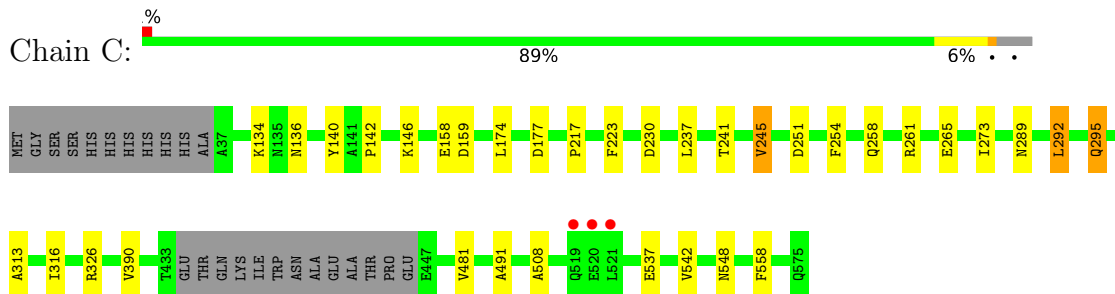
- Molecule 1: Beta-galactosidase, putative, bgl35A



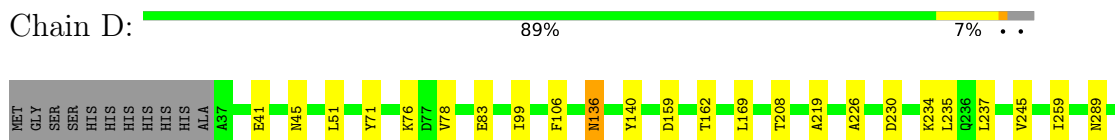
- Molecule 1: Beta-galactosidase, putative, bgl35A

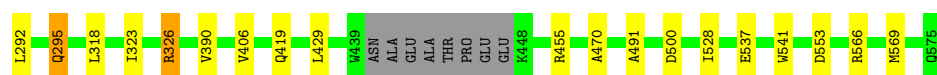


- Molecule 1: Beta-galactosidase, putative, bgl35A



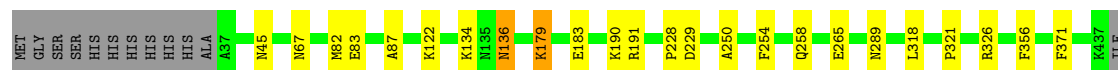
- Molecule 1: Beta-galactosidase, putative, bgl35A





- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain E: 91% 5% .



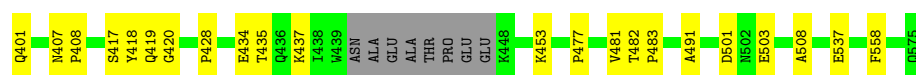
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain F: 91% 5% .



- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain G: 88% 9% .



- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H: 88% 7% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.42Å 115.79Å 116.19Å 89.93° 90.08° 89.99°	Depositor
Resolution (Å)	63.21 – 1.50 63.21 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (63.21-1.50) 94.5 (63.21-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.145 , 0.164 0.152 , 0.164	Depositor DCC
R_{free} test set	39812 reflections (4.55%)	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)	0.38 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.249 for h,-l,k 0.249 for h,l,-k 0.186 for h,-k,-l 0.130 for -h,k,-l 0.129 for -h,-k,l 0.136 for -h,-l,-k 0.129 for -h,l,k	Xtriage
Reported twinning fraction	0.582 for H, K, L 0.048 for h,-k,-l 0.089 for H, -L, K 0.281 for H, L, -K	Depositor
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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: N0W, 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	1.15	6/4247 (0.1%)	1.33	2/5787 (0.0%)
1	B	1.14	2/4248 (0.0%)	1.29	3/5786 (0.1%)
1	C	1.17	4/4233 (0.1%)	1.33	8/5771 (0.1%)
1	D	1.19	7/4312 (0.2%)	1.32	10/5877 (0.2%)
1	E	1.16	4/4266 (0.1%)	1.34	9/5817 (0.2%)
1	F	1.18	2/4299 (0.0%)	1.34	4/5859 (0.1%)
1	G	1.20	7/4325 (0.2%)	1.34	13/5891 (0.2%)
1	H	1.17	2/4225 (0.0%)	1.34	11/5768 (0.2%)
All	All	1.17	34/34155 (0.1%)	1.33	60/46556 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	390	VAL	C-O	7.38	1.32	1.24
1	G	255	HIS	C-O	7.28	1.32	1.24
1	A	406	VAL	C-O	6.46	1.30	1.23
1	E	122	LYS	C-O	6.45	1.32	1.23
1	C	223	PHE	C-O	6.43	1.31	1.24
1	A	265	GLU	C-O	6.28	1.31	1.24
1	A	156	VAL	C-O	6.12	1.31	1.24
1	G	91	SER	C-O	-6.05	1.16	1.24
1	A	168	PRO	C-O	-6.00	1.16	1.24
1	B	361	PHE	C-O	-5.91	1.19	1.24
1	E	321	PRO	C-O	5.90	1.30	1.23
1	C	146	LYS	C-O	5.67	1.31	1.24
1	G	503	GLU	C-O	-5.63	1.17	1.23
1	H	369	ILE	C-O	5.62	1.30	1.24
1	E	574	VAL	C-O	5.48	1.30	1.24
1	D	470	ALA	C-O	-5.47	1.17	1.24
1	G	90	LEU	C-O	5.47	1.30	1.24
1	D	162	THR	C-O	5.40	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	553	ASP	C-O	5.40	1.30	1.24
1	E	265	GLU	C-O	-5.39	1.17	1.24
1	F	51	LEU	C-O	-5.34	1.17	1.24
1	H	138	PRO	C-O	-5.33	1.17	1.24
1	D	51	LEU	C-O	-5.31	1.17	1.24
1	D	323	ILE	C-O	-5.29	1.17	1.23
1	B	117	GLU	C-O	-5.27	1.17	1.24
1	A	550	ASP	C-O	5.26	1.30	1.24
1	A	483	PRO	C-O	-5.26	1.20	1.25
1	C	542	VAL	C-O	5.23	1.29	1.24
1	G	417	SER	C-O	5.18	1.30	1.24
1	D	71	TYR	C-O	-5.16	1.18	1.24
1	G	428	PRO	C-O	-5.13	1.18	1.24
1	C	251	ASP	C-O	5.10	1.29	1.24
1	D	208	THR	C-O	5.06	1.29	1.23
1	G	501	ASP	C-O	-5.05	1.18	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	483	PRO	N-CA-C	9.56	119.65	110.47
1	E	87	ALA	CA-C-O	-6.96	113.98	121.56
1	H	550	ASP	CA-CB-CG	6.40	119.00	112.60
1	E	136	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	289	ASN	CA-CB-CG	6.20	118.80	112.60
1	H	295	GLN	N-CA-C	-6.16	104.12	111.69
1	D	289	ASN	CA-CB-CG	5.89	118.49	112.60
1	H	289	ASN	CA-CB-CG	5.87	118.47	112.60
1	G	46	ASN	CB-CA-C	-5.87	103.56	111.89
1	E	289	ASN	CA-CB-CG	5.83	118.43	112.60
1	E	67	ASN	CA-CB-CG	5.82	118.42	112.60
1	H	432	THR	CA-CB-OG1	-5.82	100.88	109.60
1	E	371	PHE	CA-CB-CG	5.74	119.54	113.80
1	G	135	ASN	CA-CB-CG	5.74	118.34	112.60
1	C	289	ASN	CA-CB-CG	5.72	118.32	112.60
1	C	273	ILE	N-CA-C	-5.70	106.15	111.45
1	G	46	ASN	CA-C-O	-5.67	115.27	121.84
1	G	434	GLU	CA-C-N	5.63	128.09	120.44
1	G	434	GLU	C-N-CA	5.63	128.09	120.44
1	E	250	ALA	CA-C-O	-5.59	114.95	120.82
1	H	560[A]	ASP	CA-CB-CG	5.57	118.17	112.60
1	H	560[B]	ASP	CA-CB-CG	5.57	118.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	PRO	CA-C-N	5.56	128.05	120.54
1	E	228	PRO	C-N-CA	5.56	128.05	120.54
1	G	437	LYS	CA-C-N	5.53	127.53	120.56
1	G	437	LYS	C-N-CA	5.53	127.53	120.56
1	C	142	PRO	CB-CA-C	-5.53	103.99	111.12
1	D	226	ALA	CA-C-O	-5.45	115.20	121.19
1	D	136	ASN	CA-CB-CG	5.42	118.02	112.60
1	F	500	ASP	CA-CB-CG	5.38	117.98	112.60
1	H	67	ASN	CA-CB-CG	5.35	117.95	112.60
1	C	295	GLN	N-CA-C	-5.35	104.88	111.40
1	B	177	ASP	N-CA-C	-5.34	105.15	110.97
1	F	64	GLN	CB-CG-CD	5.31	121.62	112.60
1	D	406	VAL	N-CA-C	-5.29	107.26	111.81
1	F	289	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	230	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	161	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	500	ASP	CA-CB-CG	5.25	117.85	112.60
1	G	212	VAL	N-CA-C	-5.22	106.04	111.58
1	H	484	PRO	CA-C-O	-5.21	115.40	121.34
1	G	289	ASN	CA-CB-CG	5.20	117.80	112.60
1	B	283	ALA	CA-C-O	-5.19	115.05	121.02
1	H	353	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	295	GLN	N-CA-C	-5.17	105.29	111.03
1	G	435	THR	CA-C-N	5.15	127.43	120.38
1	G	435	THR	C-N-CA	5.15	127.43	120.38
1	D	159	ASP	CA-CB-CG	5.13	117.73	112.60
1	G	272	ALA	N-CA-C	-5.13	105.81	111.71
1	A	136	ASN	CA-C-O	-5.09	113.91	119.00
1	C	177	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	78	VAL	N-CA-C	-5.08	107.19	111.56
1	D	455	ARG	CB-CG-CD	5.07	122.97	111.30
1	F	472	VAL	CA-C-O	-5.07	115.11	120.48
1	C	174	LEU	N-CA-C	-5.06	105.65	111.07
1	E	229	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	259	ILE	N-CA-C	-5.04	105.63	110.72
1	C	159	ASP	CA-CB-CG	5.03	117.63	112.60
1	H	179	LYS	N-CA-C	-5.03	105.69	111.07
1	H	574	VAL	CA-C-O	-5.01	115.41	119.97

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	4131	0	3985	8	0
1	B	4135	0	3999	13	0
1	C	4123	0	3960	12	0
1	D	4194	0	4036	18	0
1	E	4156	0	3981	13	0
1	F	4186	0	4014	13	0
1	G	4206	0	4070	18	0
1	H	4106	0	3914	15	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
3	A	21	0	0	0	0
3	B	13	0	0	0	0
3	C	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	H	15	0	0	0	0
4	A	220	0	0	1	0
4	B	254	0	0	1	0
4	C	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	H	210	0	0	0	0
All	All	35492	0	31959	106	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 (106) 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: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
1:E:179:LYS:HE3	4:E:953:HOH:O	1.90	0.71
1:G:48:LYS:NZ	1:G:420:GLY:O	2.24	0.70
1:B:326:ARG:NH1	4:B:701:HOH:O	2.26	0.69
1:F:482:THR:HG22	4:F:792:HOH:O	1.94	0.67
1:B:112:ASP:OD1	1:B:116:LYS:HE2	1.94	0.66
1:B:169:LEU:HD12	1:B:219:ALA:HA	1.76	0.66
1:D:326:ARG:NH2	4:D:701:HOH:O	2.28	0.66
1:F:48:LYS:NZ	1:F:420:GLY:O	2.30	0.64
1:A:232:ILE:O	1:A:235:LEU:O	2.15	0.63
1:G:481:VAL:CG2	4:G:969:HOH:O	2.47	0.62
1:G:481:VAL:HG23	4:G:969:HOH:O	2.00	0.62
1:D:326:ARG:HG3	1:D:326:ARG:NH2	2.03	0.60
1:H:541:TRP:CG	1:H:566:ARG:HH11	2.19	0.59
1:E:179:LYS:HD2	4:E:784:HOH:O	2.03	0.58
1:H:169:LEU:CD1	1:H:219:ALA:HA	2.33	0.58
1:F:318:LEU:C	1:F:318:LEU:HD12	2.28	0.58
1:C:481:VAL:O	1:C:481:VAL:HG22	2.03	0.58
1:E:326:ARG:HG3	1:E:356:PHE:CZ	2.39	0.58
1:B:481:VAL:HG22	1:B:481:VAL:O	2.04	0.57
1:F:541:TRP:CD2	1:F:566:ARG:HD2	2.40	0.57
1:H:541:TRP:CD2	1:H:566:ARG:HD2	2.39	0.57
1:D:326:ARG:HH21	1:D:326:ARG:CG	2.03	0.56
1:D:326:ARG:NH2	1:D:326:ARG:CG	2.67	0.56
1:B:361:PHE:CD2	1:B:493:GLY:HA3	2.41	0.56
1:H:235:LEU:HB3	1:H:237:LEU:HD13	1.88	0.56
1:B:48:LYS:NZ	1:B:420:GLY:O	2.39	0.54
1:B:477:PRO:HD2	1:B:482:THR:HG22	1.88	0.54
1:E:318:LEU:C	1:E:318:LEU:HD12	2.32	0.54
1:D:528:ILE:CD1	1:D:569:MET:SD	2.88	0.54
1:D:45:ASN:ND2	4:D:705:HOH:O	2.41	0.54
1:D:318:LEU:HD12	1:D:318:LEU:C	2.32	0.53
1:E:530:ARG:NH1	4:E:701:HOH:O	2.33	0.53
1:F:541:TRP:CG	1:F:566:ARG:HH11	2.27	0.53
1:E:190:LYS:HG3	1:E:191:ARG:HG2	1.90	0.53
1:F:155:VAL:HG23	1:F:163:LEU:HB2	1.91	0.52
1:C:241:THR:O	1:C:245:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:482[A]:THR:HG23	4:G:785:HOH:O	2.10	0.52
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.45	0.52
1:G:397:GLU:O	1:G:401:GLN:HG3	2.09	0.51
1:G:157:LYS:HE3	1:G:161:ASP:HB2	1.93	0.51
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.46	0.51
1:F:155:VAL:CG2	1:F:163:LEU:HB2	2.41	0.51
1:A:254:PHE:O	1:A:258:GLN:HG2	2.11	0.50
1:A:99:ILE:O	1:A:106:PHE:HA	2.11	0.50
1:D:169:LEU:CD1	1:D:219:ALA:HA	2.42	0.49
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.48	0.49
1:D:390:VAL:HG22	4:D:957:HOH:O	2.13	0.48
1:B:528:ILE:HG21	1:B:531:VAL:HG23	1.95	0.48
1:G:169:LEU:HD13	1:G:219:ALA:HA	1.95	0.48
1:H:397:GLU:O	1:H:401:GLN:HG3	2.13	0.48
1:C:390:VAL:HG22	4:C:904:HOH:O	2.14	0.47
1:B:231:LEU:HG	1:B:235:LEU:HD22	1.96	0.47
1:H:199:MET:CG	1:H:277:PRO:HB2	2.36	0.47
1:F:254:PHE:O	1:F:258:GLN:HG2	2.13	0.47
1:G:169:LEU:CD1	1:G:219:ALA:HA	2.44	0.47
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.51	0.46
1:D:83:GLU:HA	1:D:83:GLU:OE1	2.16	0.46
1:D:541:TRP:CE2	1:D:566:ARG:HD3	2.51	0.46
1:G:227:VAL:HB	1:G:232:ILE:HD11	1.99	0.45
1:H:412:GLU:HG2	1:H:536:PHE:CG	2.52	0.45
1:H:528:ILE:HG21	1:H:531:VAL:HG23	1.98	0.45
1:A:178:LYS:HG3	1:A:269:ALA:CB	2.47	0.45
1:D:235:LEU:HB3	1:D:237:LEU:HG	1.98	0.45
1:D:99:ILE:O	1:D:106:PHE:HA	2.17	0.44
1:E:254:PHE:O	1:E:258:GLN:HG2	2.18	0.44
1:G:229:ASP:O	1:G:233:GLN:HG2	2.18	0.44
1:H:95:ALA:O	1:H:98:GLN:HG2	2.18	0.44
1:G:407:ASN:N	1:G:408:PRO:HD2	2.33	0.44
1:D:230:ASP:OD2	1:D:234:LYS:HE3	2.17	0.43
1:G:199:MET:HG2	1:G:277:PRO:HB2	1.99	0.43
1:C:261:ARG:O	1:C:265:GLU:HG3	2.18	0.43
1:C:254:PHE:O	1:C:258:GLN:HG2	2.19	0.43
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.53	0.43
1:H:169:LEU:HD13	1:H:219:ALA:HA	1.99	0.43
1:F:313:ALA:HB1	1:F:316:ILE:HD12	2.00	0.42
1:F:541:TRP:CE2	1:F:566:ARG:CD	3.02	0.42
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LEU:O	1:D:295:GLN:HB2	2.19	0.42
1:H:99:ILE:O	1:H:106:PHE:HA	2.20	0.42
1:D:140:TYR:CZ	1:E:548:ASN:HB3	2.54	0.42
1:G:477:PRO:HD2	1:G:482[B]:THR:HG22	2.01	0.42
1:B:200:VAL:O	1:B:278:MET:HA	2.20	0.42
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.55	0.42
1:G:481:VAL:HG22	1:G:481:VAL:O	2.20	0.42
1:C:292:LEU:O	1:C:295:GLN:HB2	2.19	0.42
1:E:179:LYS:HB2	1:E:179:LYS:HE2	1.28	0.42
1:B:318:LEU:C	1:B:318:LEU:HD12	2.45	0.41
1:C:292:LEU:HB2	1:C:295:GLN:NE2	2.36	0.41
1:E:134:LYS:HD3	1:E:134:LYS:C	2.45	0.41
1:A:318:LEU:C	1:A:318:LEU:HD12	2.45	0.41
1:B:45:ASN:OD1	1:B:418:TYR:OH	2.39	0.41
1:E:191:ARG:HD3	1:E:191:ARG:HA	1.89	0.41
1:C:313:ALA:HB1	1:C:316:ILE:HD12	2.01	0.41
1:H:541:TRP:CE2	1:H:566:ARG:CD	3.04	0.41
1:C:134:LYS:HD3	1:C:134:LYS:C	2.46	0.41
1:F:40:PRO:HA	1:F:52:MET:O	2.21	0.41
1:F:99:ILE:O	1:F:106:PHE:HA	2.21	0.41
1:F:541:TRP:CE2	1:F:566:ARG:HD3	2.56	0.41
1:G:95:ALA:O	1:G:98:GLN:HG2	2.21	0.41
1:H:407:ASN:N	1:H:408:PRO:HD2	2.36	0.40
1:G:418:TYR:HD2	1:G:419:GLN:HE21	1.70	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	524/550 (95%)	501 (96%)	22 (4%)	1 (0%)	43 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/550 (95%)	499 (96%)	23 (4%)	0	100	100
1	C	523/550 (95%)	501 (96%)	21 (4%)	1 (0%)	43	22
1	D	531/550 (96%)	511 (96%)	19 (4%)	1 (0%)	43	22
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%)	43	22
1	H	524/550 (95%)	504 (96%)	20 (4%)	0	100	100
All	All	4215/4400 (96%)	4042 (96%)	169 (4%)	4 (0%)	48	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	491	ALA
1	A	491	ALA
1	G	491	ALA
1	D	491	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/461 (93%)	420 (98%)	7 (2%)	55	28
1	B	429/461 (93%)	421 (98%)	8 (2%)	50	22
1	C	425/461 (92%)	417 (98%)	8 (2%)	50	22
1	D	432/461 (94%)	424 (98%)	8 (2%)	50	22
1	E	427/461 (93%)	420 (98%)	7 (2%)	55	28
1	F	432/461 (94%)	425 (98%)	7 (2%)	55	28
1	G	434/461 (94%)	430 (99%)	4 (1%)	70	49
1	H	422/461 (92%)	414 (98%)	8 (2%)	50	22
All	All	3428/3688 (93%)	3371 (98%)	57 (2%)	55	26

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	220	GLN
1	A	232	ILE
1	A	235	LEU
1	A	389	LYS
1	A	390	VAL
1	A	537	GLU
1	B	82	MET
1	B	136	ASN
1	B	173	THR
1	B	235	LEU
1	B	245	VAL
1	B	292	LEU
1	B	389	LYS
1	B	421	GLN
1	C	136	ASN
1	C	158	GLU
1	C	217	PRO
1	C	237	LEU
1	C	245	VAL
1	C	292	LEU
1	C	326	ARG
1	C	537	GLU
1	D	41	GLU
1	D	76	LYS
1	D	136	ASN
1	D	245	VAL
1	D	326	ARG
1	D	419	GLN
1	D	429	LEU
1	D	537	GLU
1	E	45	ASN
1	E	82	MET
1	E	83	GLU
1	E	136	ASN
1	E	179	LYS
1	E	183	GLU
1	E	537	GLU
1	F	136	ASN
1	F	268	VAL
1	F	292	LEU
1	F	429	LEU

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Mol	Chain	Res	Type
1	F	449	GLU
1	F	537	GLU
1	F	573	SER
1	G	82	MET
1	G	136	ASN
1	G	453	LYS
1	G	537	GLU
1	H	136	ASN
1	H	173	THR
1	H	194[A]	ASP
1	H	194[B]	ASP
1	H	199	MET
1	H	326	ARG
1	H	366	LYS
1	H	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	B	236	GLN
1	B	315	ASN
1	B	419	GLN
1	C	45	ASN
1	C	64	GLN
1	C	172	ASN
1	C	315	ASN
1	C	354	GLN
1	C	451	HIS
1	D	45	ASN
1	F	315	ASN
1	G	275	ASN
1	G	419	GLN
1	H	64	GLN
1	H	275	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	N0W	B	602	-	13,13,35	1.29	1 (7%)	10,17,49	1.23	1 (10%)
3	N0W	A	604	-	21,21,35	1.76	2 (9%)	21,28,49	3.00	3 (14%)
3	N0W	E	605	-	15,15,35	1.79	5 (33%)	13,19,49	1.04	1 (7%)
3	N0W	G	604	-	15,15,35	1.24	2 (13%)	13,19,49	1.27	1 (7%)
3	N0W	F	605	-	21,21,35	1.76	3 (14%)	21,28,49	1.72	3 (14%)
3	N0W	C	604	-	12,12,35	1.70	1 (8%)	11,16,49	0.77	1 (9%)
3	N0W	D	606	-	21,21,35	2.01	4 (19%)	21,28,49	1.56	4 (19%)
3	N0W	H	605	-	15,15,35	1.05	1 (6%)	13,19,49	1.15	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	B	602	-	-	2/5/22/40	0/1/1/3
3	N0W	A	604	-	-	4/13/30/40	0/1/1/3
3	N0W	E	605	-	-	2/7/24/40	0/1/1/3
3	N0W	G	604	-	-	4/7/24/40	0/1/1/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N0W	F	605	-	-	3/13/30/40	0/1/1/3
3	N0W	C	604	-	-	2/4/21/40	0/1/1/3
3	N0W	D	606	-	-	3/13/30/40	0/1/1/3
3	N0W	H	605	-	-	3/7/24/40	0/1/1/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	N0W	C6-S3	-6.93	1.59	1.75
3	F	605	N0W	C6-S3	-6.20	1.61	1.75
3	D	606	N0W	C6-S3	-5.81	1.62	1.75
3	C	604	N0W	CAI-CAJ	4.22	1.56	1.52
3	E	605	N0W	CAD-CAC	-4.21	1.48	1.53
3	D	606	N0W	CAI-CAJ	4.16	1.56	1.52
3	D	606	N0W	CAD-CAC	-3.52	1.49	1.53
3	G	604	N0W	CAI-CAJ	3.34	1.55	1.52
3	F	605	N0W	CAI-CAJ	3.27	1.55	1.52
3	D	606	N0W	CAI-NAB	2.99	1.51	1.47
3	E	605	N0W	CAJ-CAC	2.94	1.57	1.52
3	E	605	N0W	CAL-CAA	2.53	1.58	1.52
3	G	604	N0W	CAA-NAB	2.52	1.51	1.47
3	F	605	N0W	CAD-CAC	2.42	1.55	1.53
3	B	602	N0W	CAA-NAB	2.41	1.51	1.47
3	E	605	N0W	CAI-CAJ	2.38	1.54	1.52
3	E	605	N0W	CAI-NAB	2.26	1.50	1.47
3	A	604	N0W	CAI-CAJ	2.22	1.54	1.52
3	H	605	N0W	CAI-NAB	2.12	1.50	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	N0W	O5-S3-O4	-9.63	105.96	118.87
3	A	604	N0W	C6-S3-N2	8.83	113.59	107.82
3	F	605	N0W	CAI-CAJ-CAC	5.25	116.66	110.25
3	D	606	N0W	O5-S3-N2	-4.04	101.71	107.33
3	D	606	N0W	O5-S3-O4	-3.60	114.05	118.87
3	F	605	N0W	O5-S3-O4	-3.34	114.39	118.87
3	H	605	N0W	OAE-CAC-CAD	2.96	115.97	109.94
3	D	606	N0W	O5-S3-C6	2.91	112.87	108.26
3	G	604	N0W	OAF-CAJ-CAI	2.59	114.66	109.65
3	A	604	N0W	O4-S3-N2	2.56	110.90	107.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	605	N0W	OAE-CAC-CAD	2.49	115.02	109.94
3	D	606	N0W	OAF-CAJ-CAI	-2.45	104.91	109.65
3	F	605	N0W	O5-S3-C6	2.29	111.88	108.26
3	C	604	N0W	OAK-CAH-CAD	2.08	116.14	111.22
3	B	602	N0W	OAF-CAJ-CAC	2.01	114.31	110.15

There are no chirality outliers.

All (23) torsion outliers are listed below:

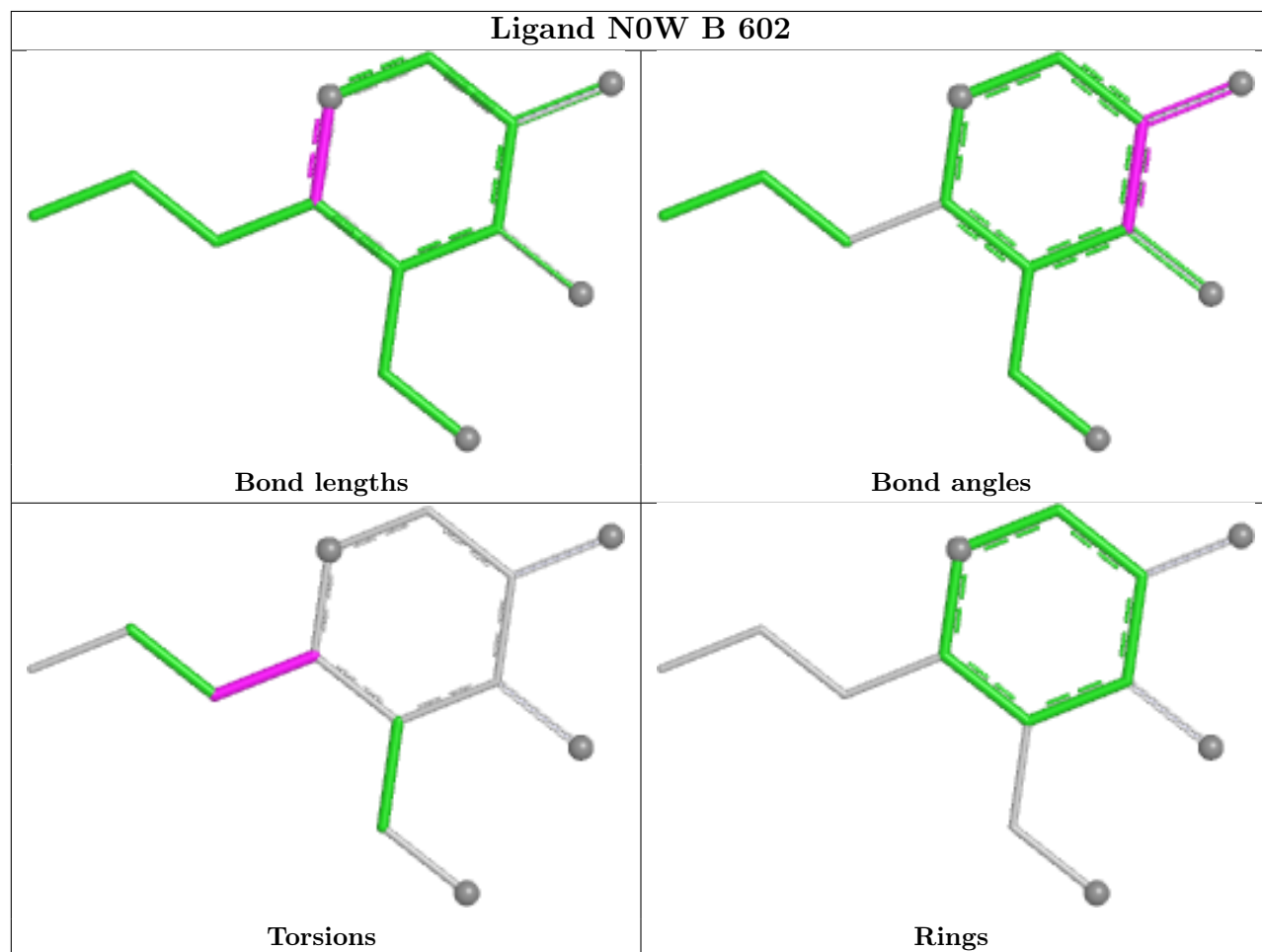
Mol	Chain	Res	Type	Atoms
3	A	604	N0W	C1-N2-S3-O5
3	A	604	N0W	NAB-CAA-CAL-CAM
3	A	604	N0W	CAD-CAA-CAL-CAM
3	B	602	N0W	NAB-CAA-CAL-CAM
3	B	602	N0W	CAD-CAA-CAL-CAM
3	C	604	N0W	NAB-CAA-CAL-CAM
3	D	606	N0W	C1-N2-S3-C6
3	D	606	N0W	NAB-CAA-CAL-CAM
3	D	606	N0W	CAD-CAA-CAL-CAM
3	E	605	N0W	NAB-CAA-CAL-CAM
3	E	605	N0W	CAD-CAA-CAL-CAM
3	F	605	N0W	NAB-CAA-CAL-CAM
3	F	605	N0W	CAD-CAA-CAL-CAM
3	G	604	N0W	NAB-CAA-CAL-CAM
3	H	605	N0W	NAB-CAA-CAL-CAM
3	H	605	N0W	CAD-CAA-CAL-CAM
3	C	604	N0W	CAD-CAA-CAL-CAM
3	A	604	N0W	N2-C1-CAP-CAO
3	G	604	N0W	CAA-CAL-CAM-CAN
3	G	604	N0W	CAM-CAN-CAO-CAP
3	G	604	N0W	CAD-CAA-CAL-CAM
3	F	605	N0W	CAN-CAO-CAP-C1
3	H	605	N0W	CAM-CAN-CAO-CAP

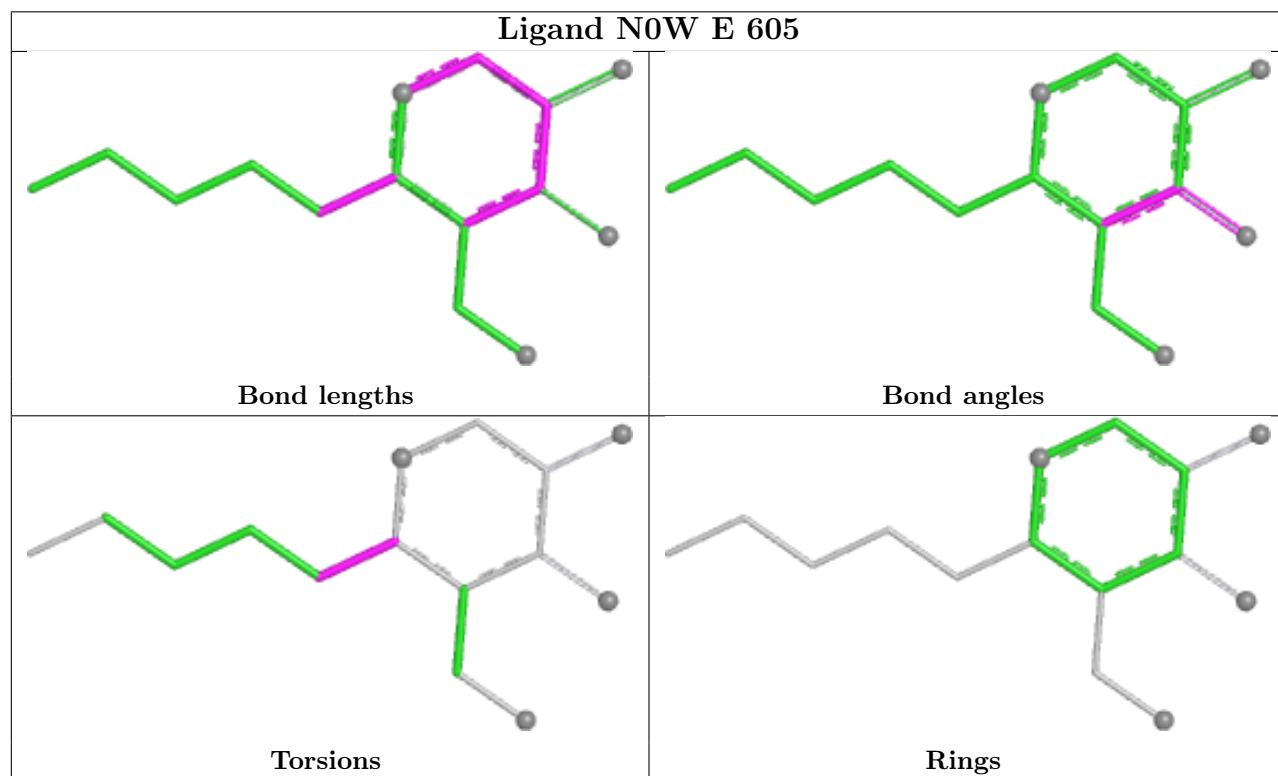
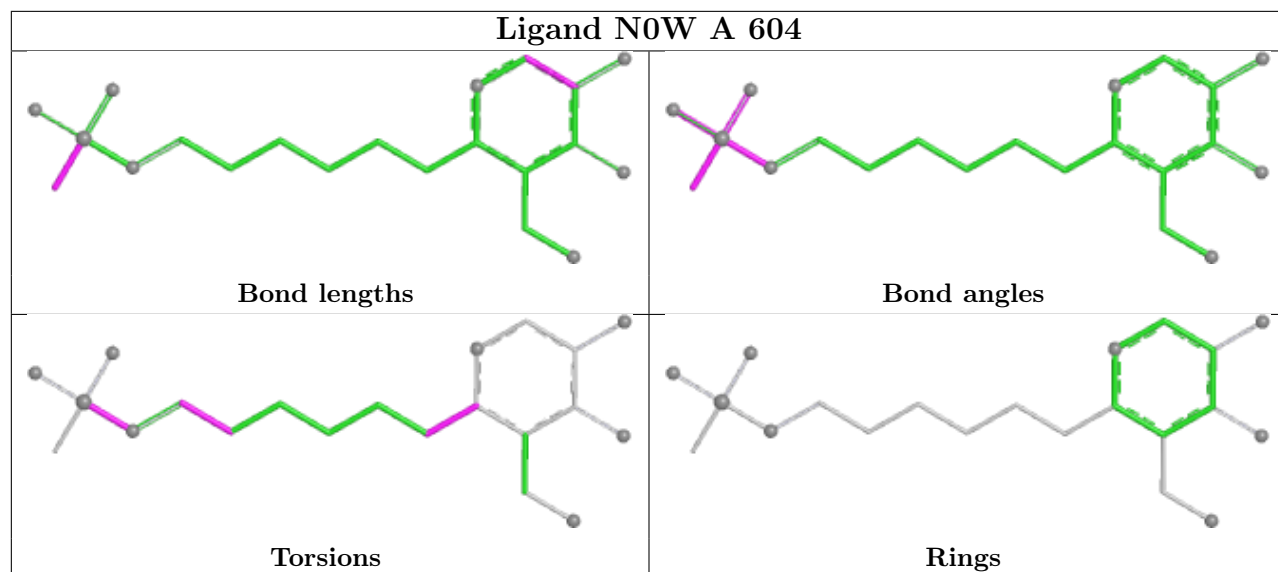
There are no ring outliers.

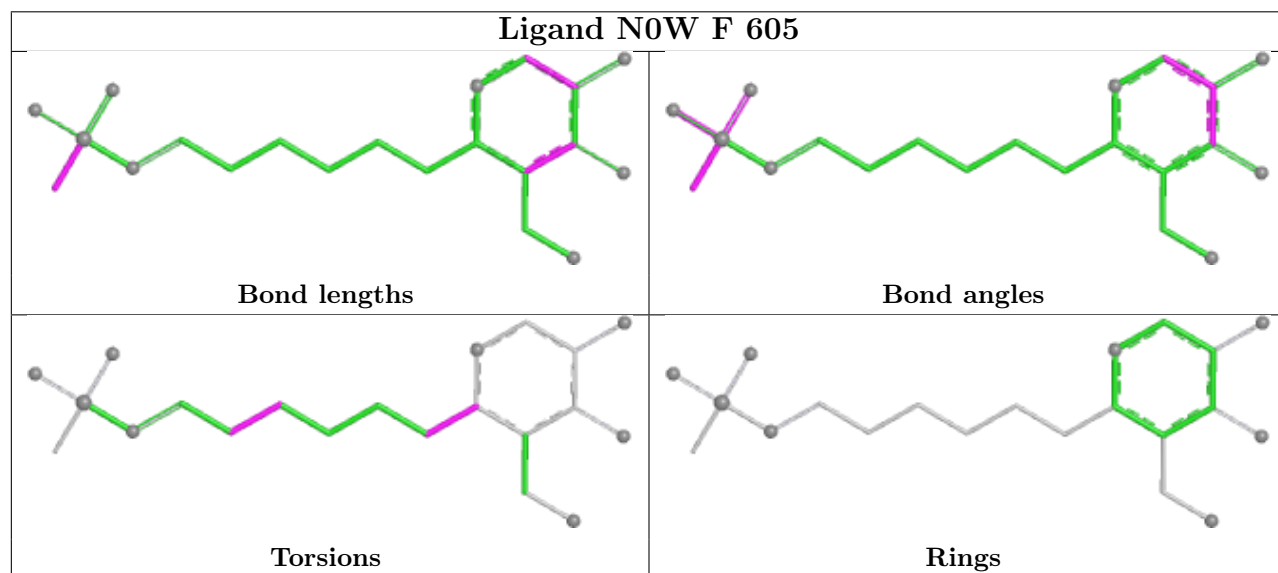
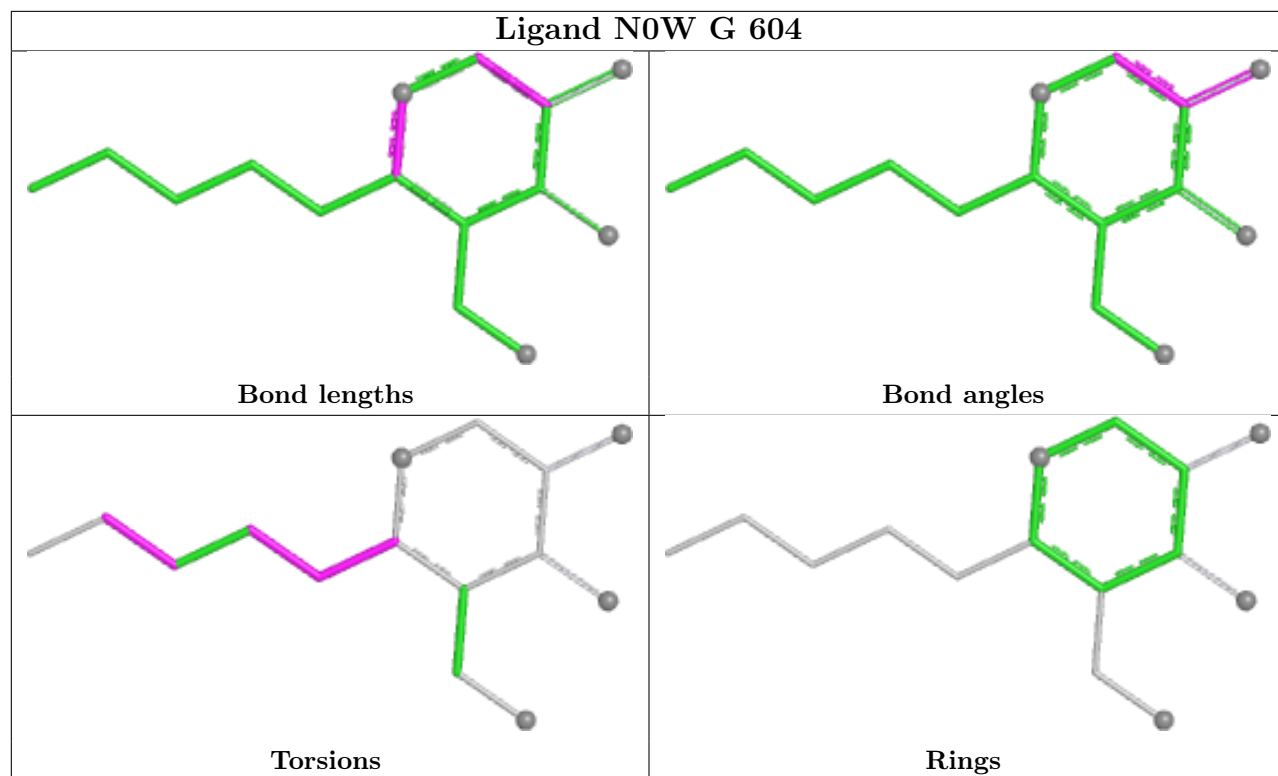
No monomer is involved in short contacts.

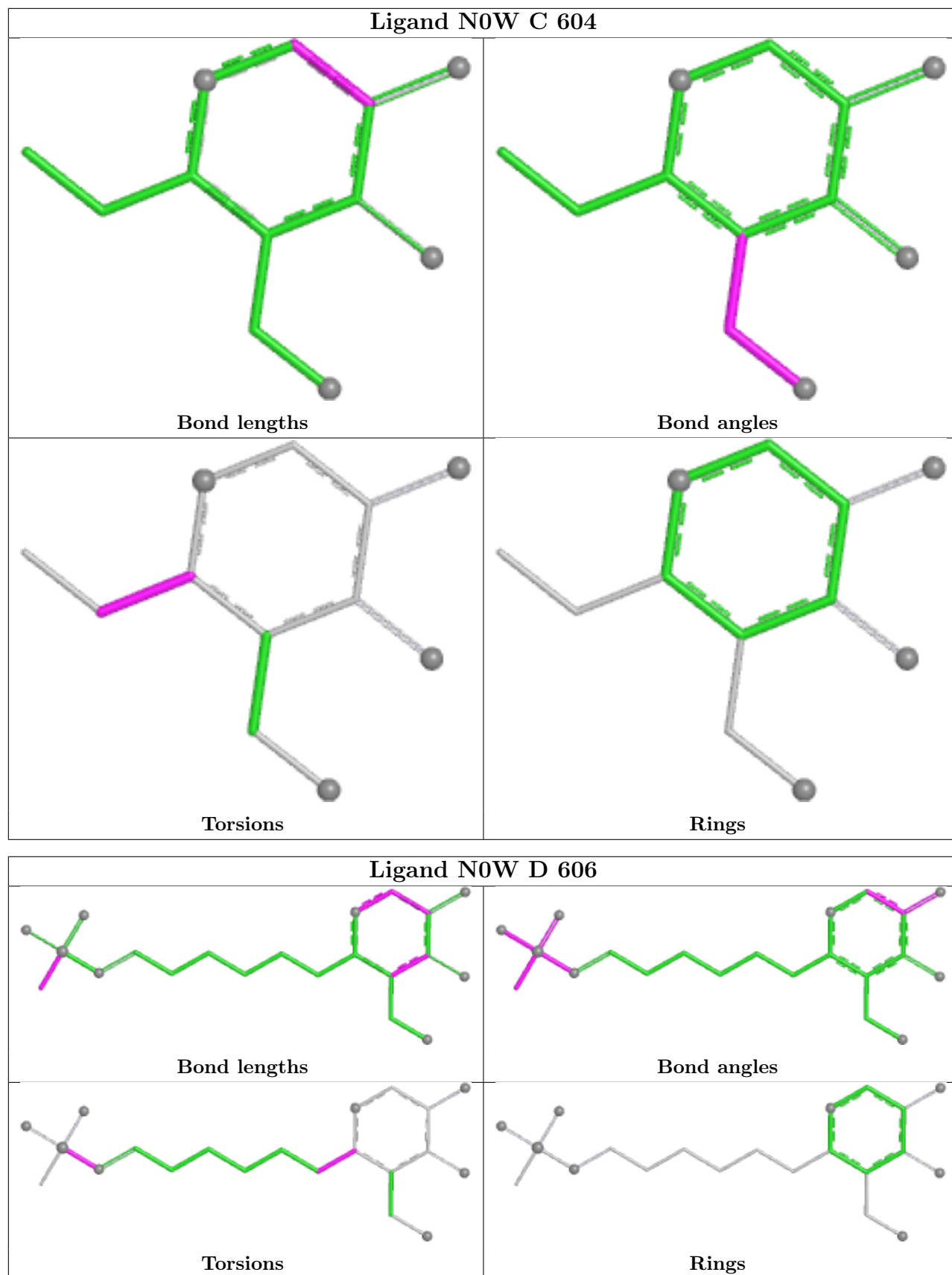
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

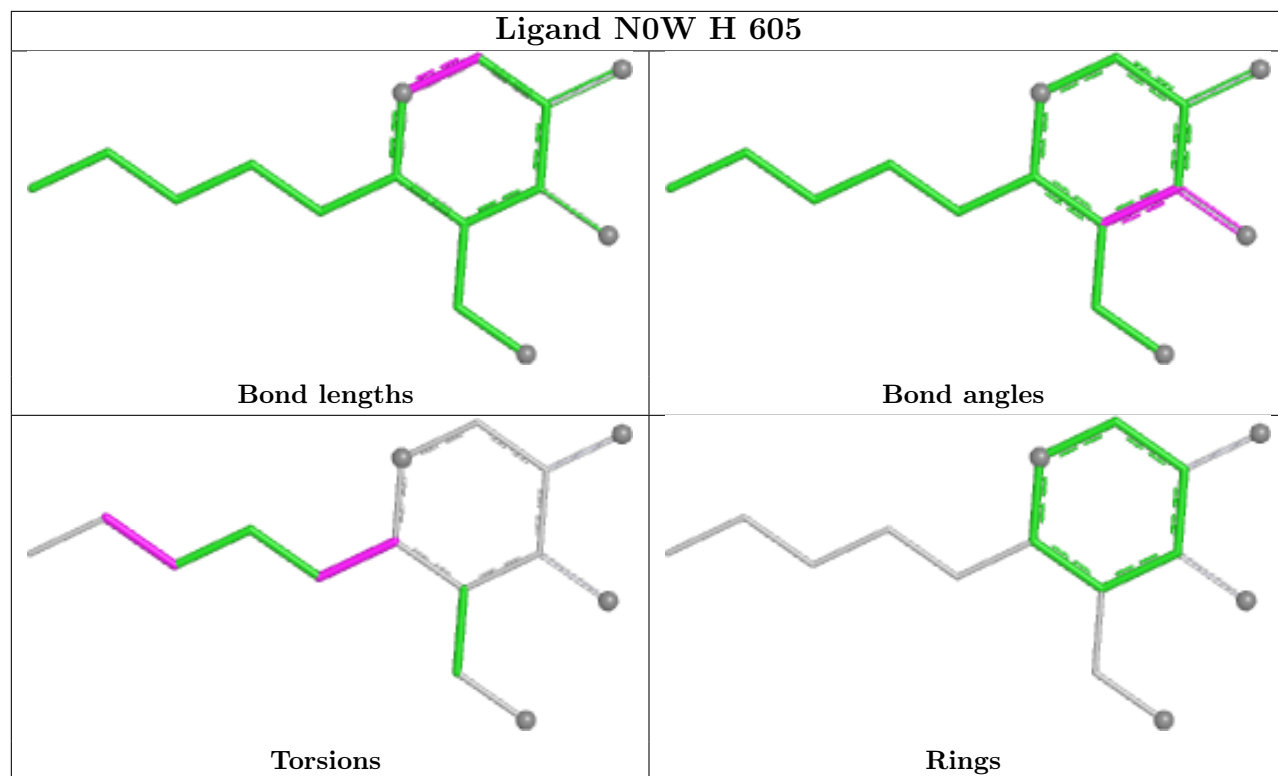
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/550 (95%)	-0.99	0 100 100	12, 22, 37, 53	6 (1%)
1	B	524/550 (95%)	-1.08	0 100 100	11, 21, 31, 45	8 (1%)
1	C	526/550 (95%)	-1.02	3 (0%) 85 88	11, 21, 31, 45	8 (1%)
1	D	531/550 (96%)	-1.13	0 100 100	9, 19, 33, 52	6 (1%)
1	E	532/550 (96%)	-1.10	1 (0%) 91 92	10, 20, 33, 44	4 (0%)
1	F	531/550 (96%)	-1.08	0 100 100	9, 20, 35, 43	5 (0%)
1	G	532/550 (96%)	-1.11	1 (0%) 91 92	10, 19, 34, 47	9 (1%)
1	H	523/550 (95%)	-0.99	0 100 100	10, 22, 34, 49	9 (1%)
All	All	4224/4400 (96%)	-1.06	5 (0%) 92 92	9, 20, 34, 53	55 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	GLU	3.9
1	C	521	LEU	3.7
1	G	36	ALA	3.6
1	E	445	PRO	2.8
1	C	519	GLN	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

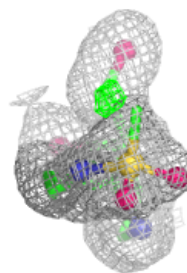
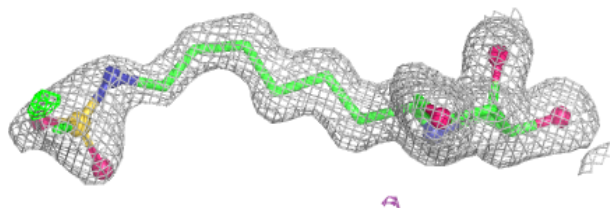
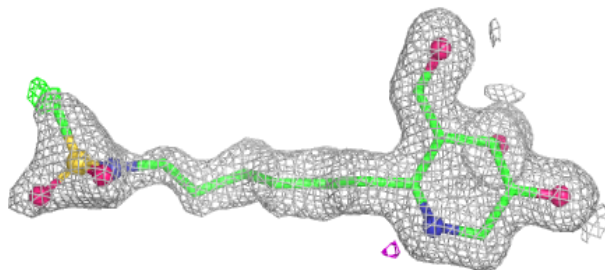
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	602	1/1	0.99	0.05	27,27,27,27	0
2	NA	A	603	1/1	0.99	0.04	28,28,28,28	0
2	NA	F	603	1/1	0.99	0.04	27,27,27,27	0
2	NA	F	604	1/1	0.99	0.03	28,28,28,28	0
2	NA	H	604	1/1	0.99	0.04	29,29,29,29	0
3	N0W	A	604	21/33	0.99	0.05	18,20,30,33	7
3	N0W	B	602	13/33	0.99	0.03	17,18,20,25	0
3	N0W	C	604	12/33	0.99	0.03	17,18,21,22	0
3	N0W	D	606	21/33	0.99	0.04	16,19,32,45	5
3	N0W	E	605	15/33	0.99	0.03	15,16,21,23	3
3	N0W	F	605	21/33	0.99	0.04	17,19,29,34	7
3	N0W	G	604	15/33	0.99	0.03	14,17,20,25	3
3	N0W	H	605	15/33	0.99	0.04	16,18,20,24	3
2	NA	E	602	1/1	1.00	0.01	23,23,23,23	0
2	NA	E	603	1/1	1.00	0.03	28,28,28,28	0
2	NA	E	604	1/1	1.00	0.03	25,25,25,25	0
2	NA	F	601	1/1	1.00	0.02	21,21,21,21	0
2	NA	F	602	1/1	1.00	0.02	26,26,26,26	0
2	NA	A	601	1/1	1.00	0.02	30,30,30,30	0
2	NA	B	601	1/1	1.00	0.02	28,28,28,28	0
2	NA	G	601	1/1	1.00	0.02	20,20,20,20	0
2	NA	G	602	1/1	1.00	0.03	28,28,28,28	0
2	NA	G	603	1/1	1.00	0.02	27,27,27,27	0
2	NA	H	601	1/1	1.00	0.02	25,25,25,25	0
2	NA	H	602	1/1	1.00	0.02	29,29,29,29	0
2	NA	H	603	1/1	1.00	0.03	32,32,32,32	0
2	NA	C	601	1/1	1.00	0.04	26,26,26,26	0
2	NA	C	602	1/1	1.00	0.04	29,29,29,29	0
2	NA	C	603	1/1	1.00	0.02	31,31,31,31	0
2	NA	D	601	1/1	1.00	0.02	22,22,22,22	0
2	NA	D	602	1/1	1.00	0.01	20,20,20,20	0
2	NA	D	603	1/1	1.00	0.03	24,24,24,24	0
2	NA	D	604	1/1	1.00	0.02	26,26,26,26	0
2	NA	D	605	1/1	1.00	0.06	28,28,28,28	0
2	NA	E	601	1/1	1.00	0.01	21,21,21,21	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.

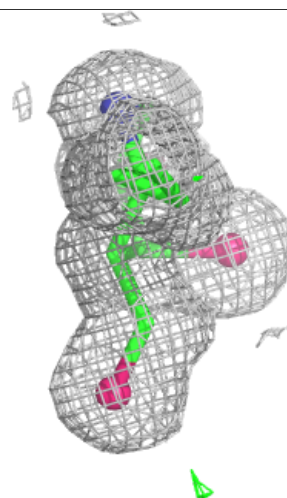
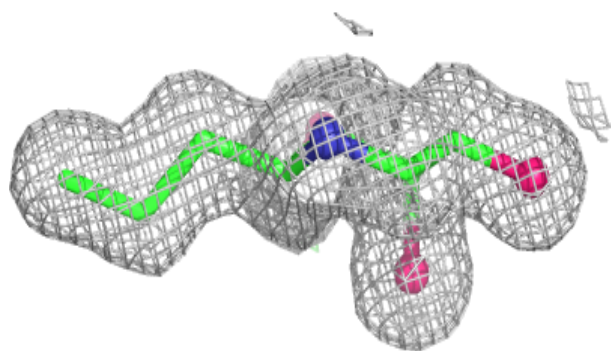
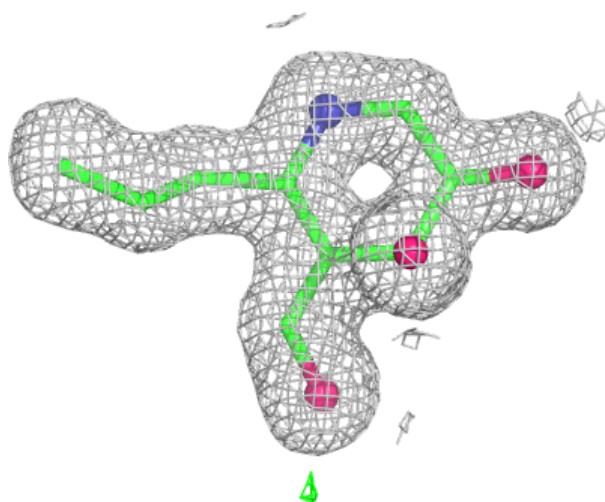
Electron density around NOW A 604:

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



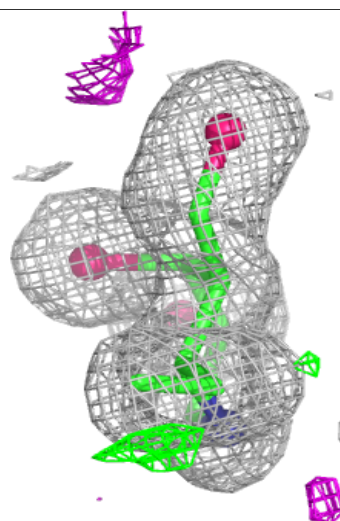
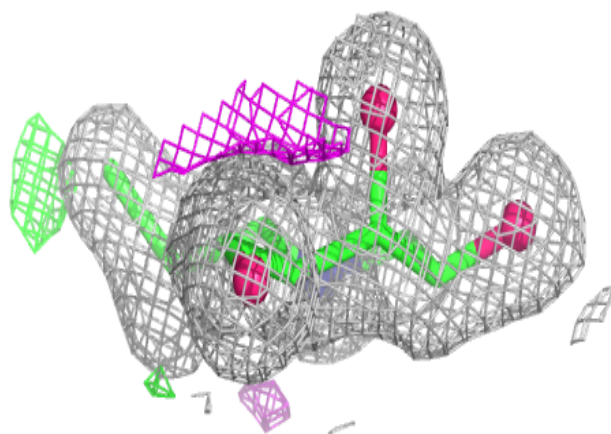
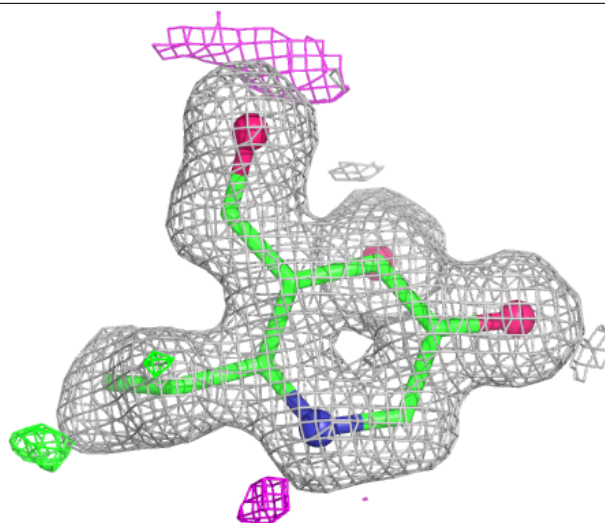
Electron density around N0W B 602:

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



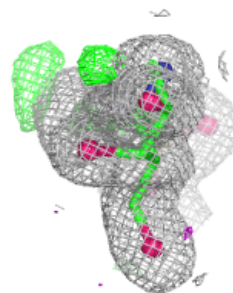
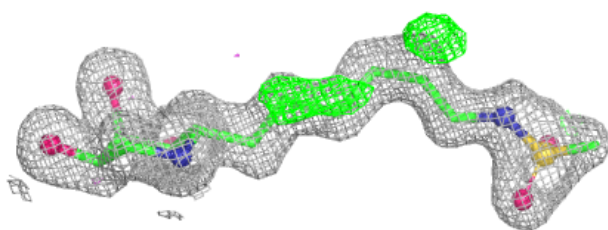
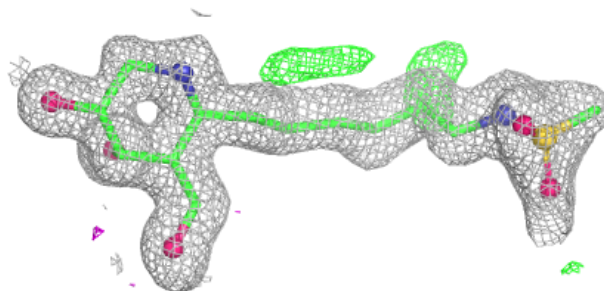
Electron density around N0W C 604:

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

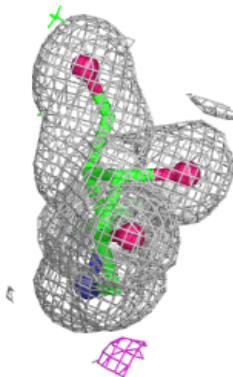
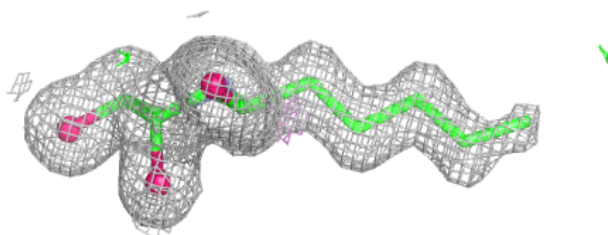
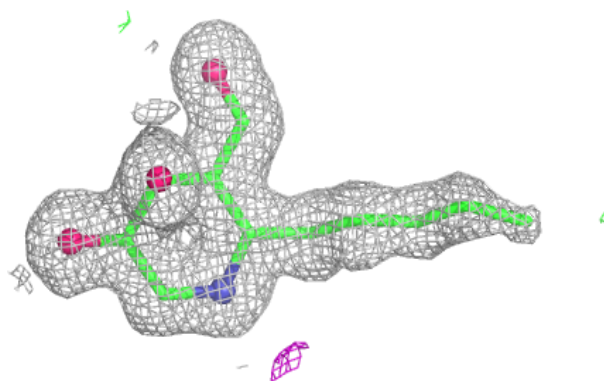


Electron density around NOW D 606:

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

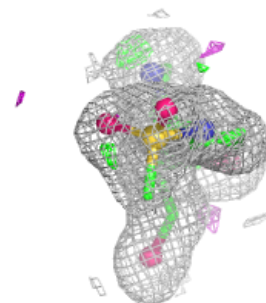
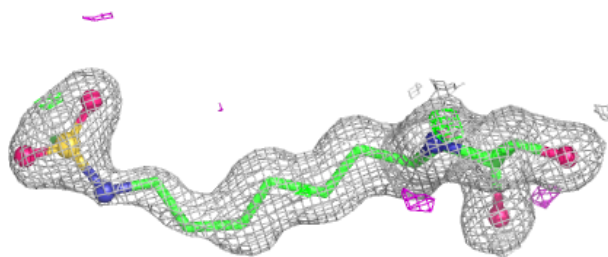
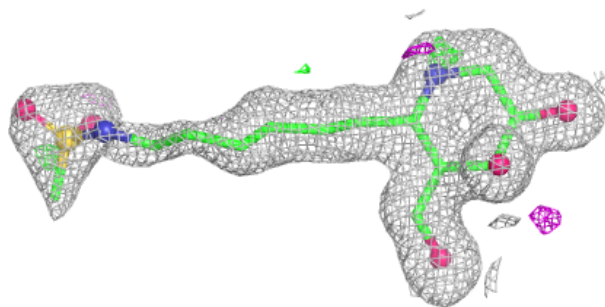
**Electron density around NOW E 605:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

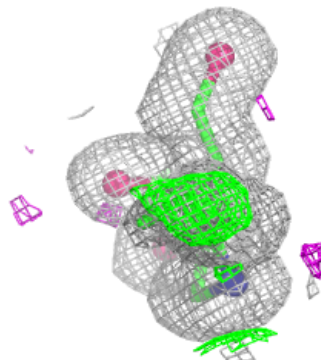
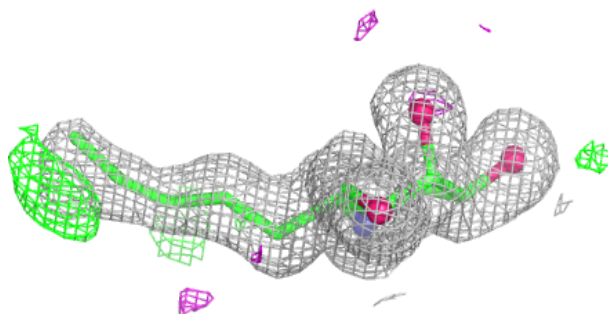
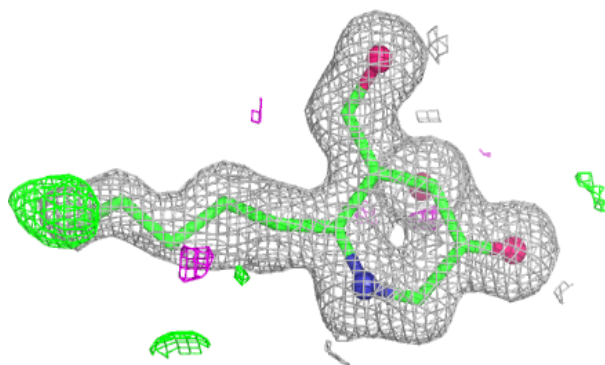


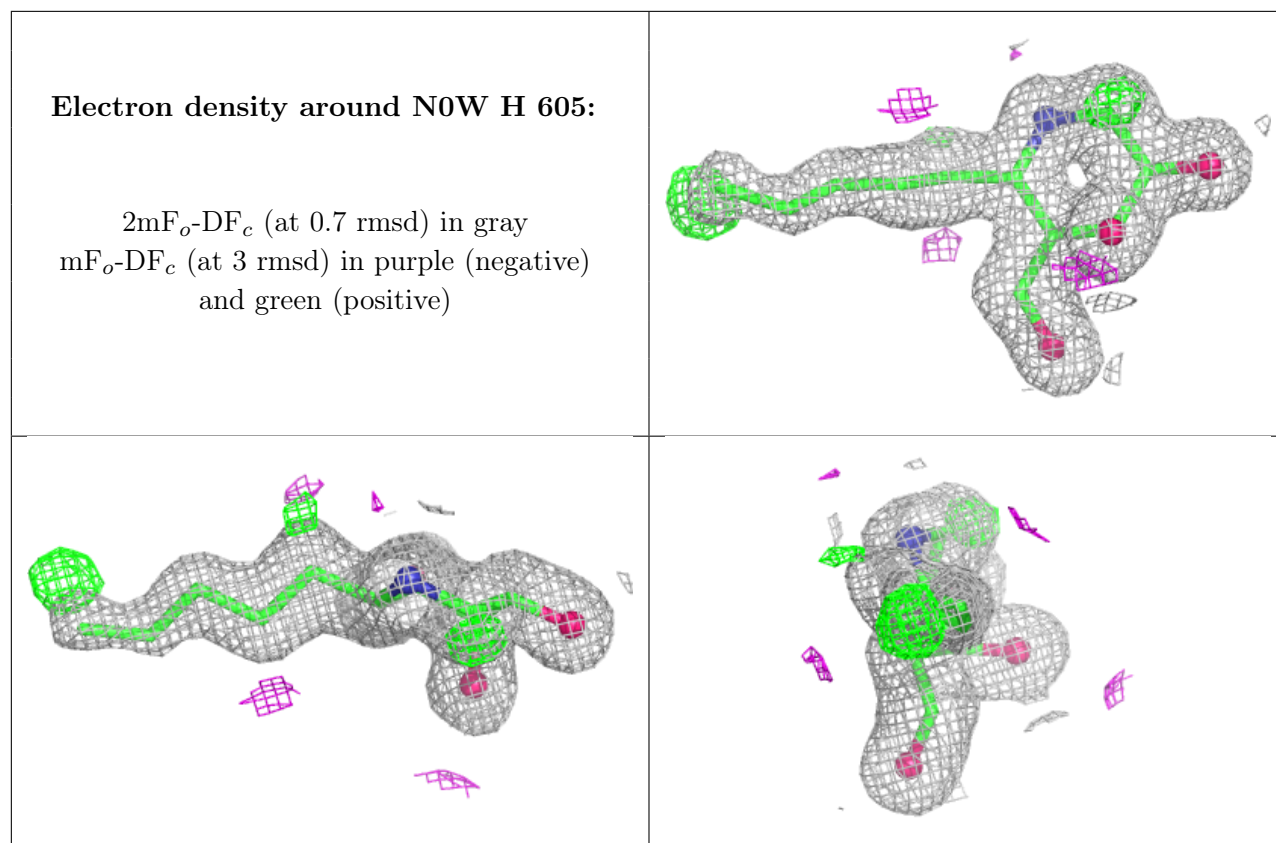
Electron density around N0W F 605:

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

**Electron density around N0W 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 ⓘ

There are no such residues in this entry.