



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:53 PM BST

PDB ID : 6CBL
Title : x-ray structure of NeoB from *Streptomyces fradiae* in complex with neamine as an external aldimine
Authors : Thoden, J.B.; Dow, G.T.; Holden, H.M.
Deposited on : 2018-02-03
Resolution : 1.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

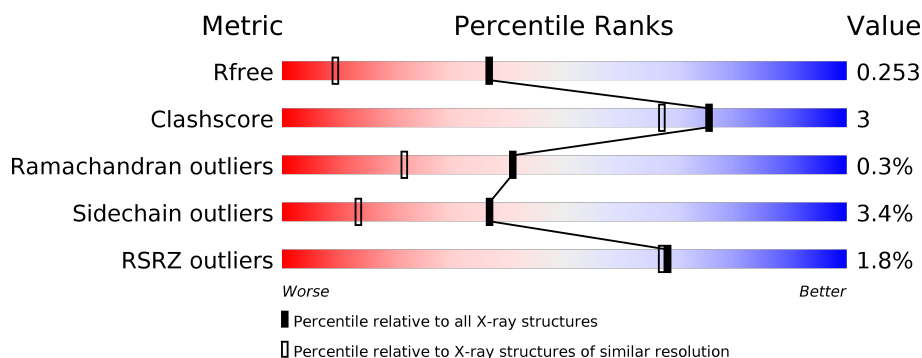
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	424	<div> <div>90%</div> <div>5% . .</div> </div>
1	B	424	<div> <div>3%</div> <div>88%</div> <div>7% .</div> </div>
1	C	424	<div> <div>%</div> <div>86%</div> <div>10% .</div> </div>
1	D	424	<div> <div>%</div> <div>86%</div> <div>10% .</div> </div>
1	E	424	<div> <div>2%</div> <div>85%</div> <div>10% . .</div> </div>
1	F	424	<div> <div>3%</div> <div>85%</div> <div>10% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	424	<div><div></div><div>86%</div><div>10% •</div></div>
1	H	424	<div><div>3%</div><div></div><div>90%</div><div>5% • •</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27720 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 Neamine transaminase NeoN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	9	0
			3157	1995	578	576	8			
1	B	409	Total	C	N	O	S	0	5	0
			3126	1976	566	576	8			
1	C	409	Total	C	N	O	S	0	4	0
			3115	1969	563	575	8			
1	D	409	Total	C	N	O	S	0	5	0
			3123	1974	566	575	8			
1	E	409	Total	C	N	O	S	0	1	0
			3100	1958	560	574	8			
1	F	409	Total	C	N	O	S	0	2	0
			3108	1963	563	574	8			
1	G	409	Total	C	N	O	S	0	1	0
			3104	1959	563	574	8			
1	H	409	Total	C	N	O	S	0	3	0
			3120	1969	569	574	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	-	expression tag	UNP Q53U08
A	418	GLU	-	expression tag	UNP Q53U08
A	419	HIS	-	expression tag	UNP Q53U08
A	420	HIS	-	expression tag	UNP Q53U08
A	421	HIS	-	expression tag	UNP Q53U08
A	422	HIS	-	expression tag	UNP Q53U08
A	423	HIS	-	expression tag	UNP Q53U08
A	424	HIS	-	expression tag	UNP Q53U08
B	417	LEU	-	expression tag	UNP Q53U08
B	418	GLU	-	expression tag	UNP Q53U08
B	419	HIS	-	expression tag	UNP Q53U08
B	420	HIS	-	expression tag	UNP Q53U08
B	421	HIS	-	expression tag	UNP Q53U08

Continued on next page...

Continued from previous page...

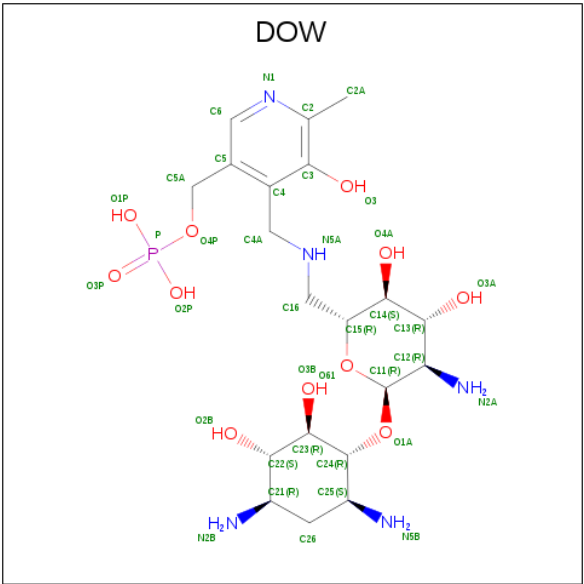
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	expression tag	UNP Q53U08
B	423	HIS	-	expression tag	UNP Q53U08
B	424	HIS	-	expression tag	UNP Q53U08
C	417	LEU	-	expression tag	UNP Q53U08
C	418	GLU	-	expression tag	UNP Q53U08
C	419	HIS	-	expression tag	UNP Q53U08
C	420	HIS	-	expression tag	UNP Q53U08
C	421	HIS	-	expression tag	UNP Q53U08
C	422	HIS	-	expression tag	UNP Q53U08
C	423	HIS	-	expression tag	UNP Q53U08
C	424	HIS	-	expression tag	UNP Q53U08
D	417	LEU	-	expression tag	UNP Q53U08
D	418	GLU	-	expression tag	UNP Q53U08
D	419	HIS	-	expression tag	UNP Q53U08
D	420	HIS	-	expression tag	UNP Q53U08
D	421	HIS	-	expression tag	UNP Q53U08
D	422	HIS	-	expression tag	UNP Q53U08
D	423	HIS	-	expression tag	UNP Q53U08
D	424	HIS	-	expression tag	UNP Q53U08
E	417	LEU	-	expression tag	UNP Q53U08
E	418	GLU	-	expression tag	UNP Q53U08
E	419	HIS	-	expression tag	UNP Q53U08
E	420	HIS	-	expression tag	UNP Q53U08
E	421	HIS	-	expression tag	UNP Q53U08
E	422	HIS	-	expression tag	UNP Q53U08
E	423	HIS	-	expression tag	UNP Q53U08
E	424	HIS	-	expression tag	UNP Q53U08
F	417	LEU	-	expression tag	UNP Q53U08
F	418	GLU	-	expression tag	UNP Q53U08
F	419	HIS	-	expression tag	UNP Q53U08
F	420	HIS	-	expression tag	UNP Q53U08
F	421	HIS	-	expression tag	UNP Q53U08
F	422	HIS	-	expression tag	UNP Q53U08
F	423	HIS	-	expression tag	UNP Q53U08
F	424	HIS	-	expression tag	UNP Q53U08
G	417	LEU	-	expression tag	UNP Q53U08
G	418	GLU	-	expression tag	UNP Q53U08
G	419	HIS	-	expression tag	UNP Q53U08
G	420	HIS	-	expression tag	UNP Q53U08
G	421	HIS	-	expression tag	UNP Q53U08
G	422	HIS	-	expression tag	UNP Q53U08
G	423	HIS	-	expression tag	UNP Q53U08

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	424	HIS	-	expression tag	UNP Q53U08
H	417	LEU	-	expression tag	UNP Q53U08
H	418	GLU	-	expression tag	UNP Q53U08
H	419	HIS	-	expression tag	UNP Q53U08
H	420	HIS	-	expression tag	UNP Q53U08
H	421	HIS	-	expression tag	UNP Q53U08
H	422	HIS	-	expression tag	UNP Q53U08
H	423	HIS	-	expression tag	UNP Q53U08
H	424	HIS	-	expression tag	UNP Q53U08

- Molecule 2 is (1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl 2-amino-2,6-dideoxy-6-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino]-alpha-D-glucopyranoside (three-letter code: DOW) (formula: C₂₀H₃₆N₅O₁₁P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	B	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	C	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	D	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	E	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	F	1	Total	C	N	O	P	0	0
			37	20	5	11	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			37	20	5	11	1		
2	H	1	Total	C	N	O	P	0	0
			37	20	5	11	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

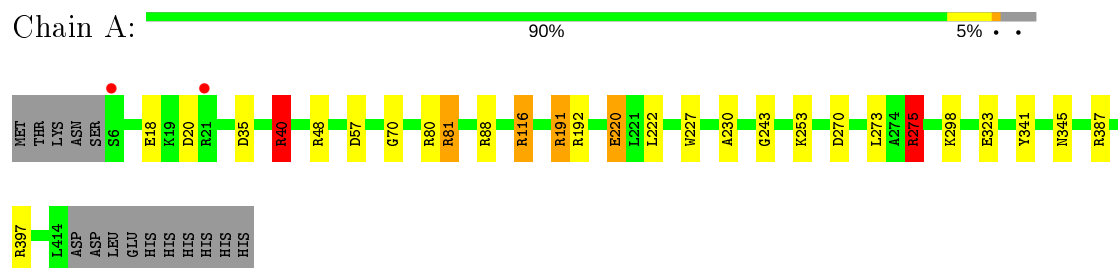
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total	O	0	0
			343	343		
4	B	277	Total	O	0	0
			277	277		
4	C	302	Total	O	0	0
			302	302		
4	D	331	Total	O	0	0
			331	331		
4	E	278	Total	O	0	0
			278	278		
4	F	298	Total	O	0	0
			298	298		
4	G	317	Total	O	0	0
			317	317		
4	H	324	Total	O	0	0
			324	324		

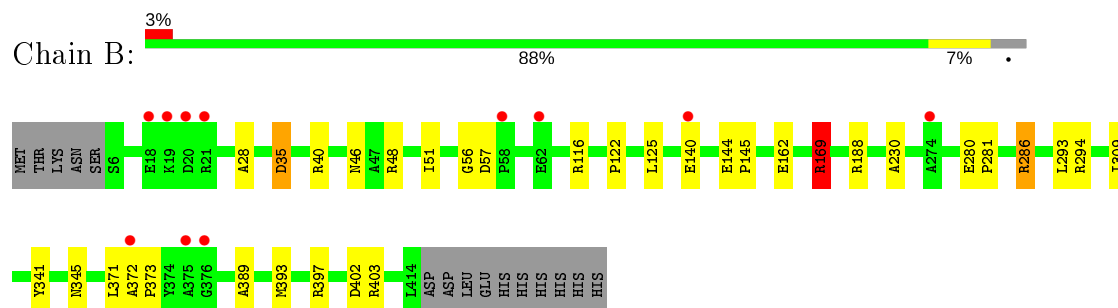
3 Residue-property plots

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.

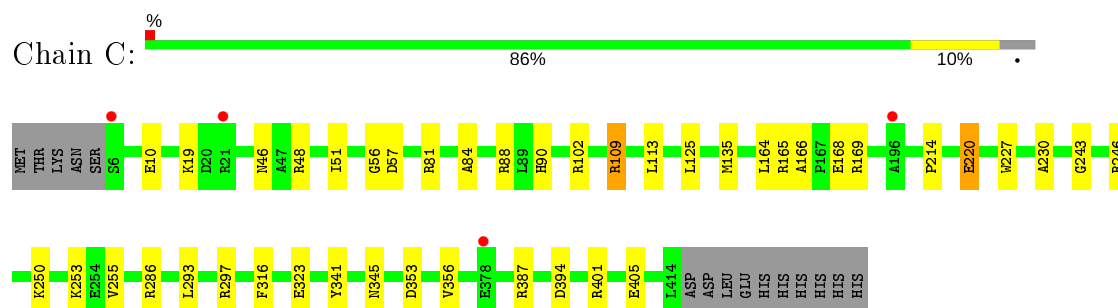
• Molecule 1: Neamine transaminase NeoN



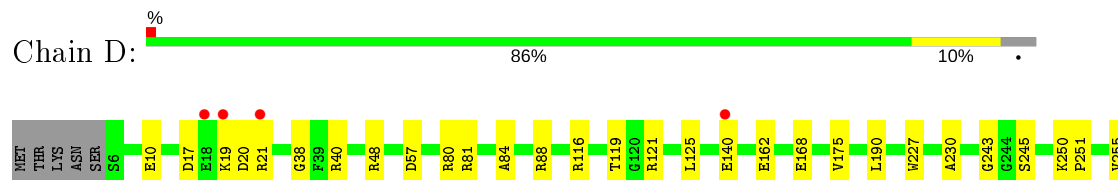
• Molecule 1: Neamine transaminase NeoN



• Molecule 1: Neamine transaminase NeoN

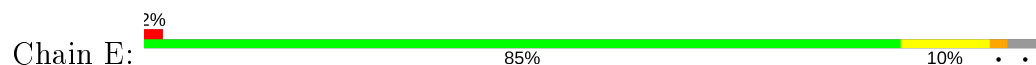


• Molecule 1: Neamine transaminase NeoN

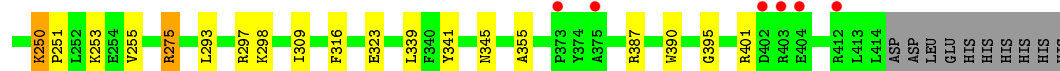
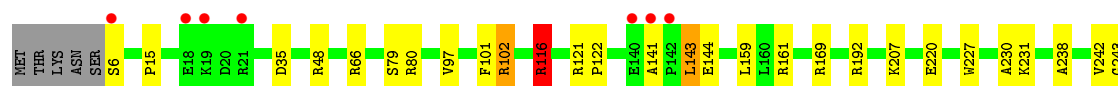
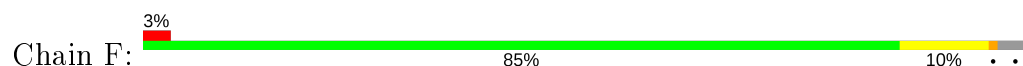




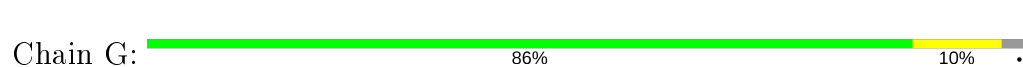
• Molecule 1: Neamine transaminase NeoN



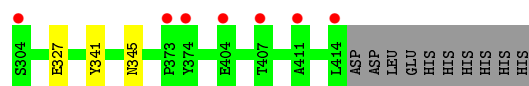
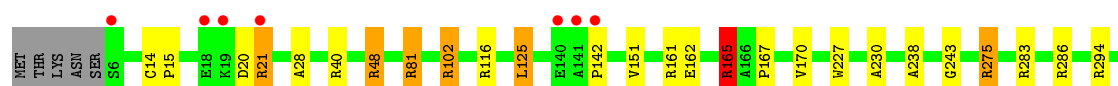
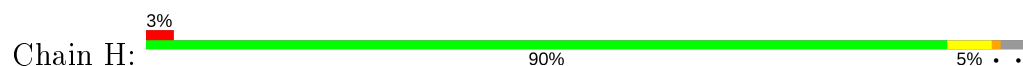
• Molecule 1: Neamine transaminase NeoN



• Molecule 1: Neamine transaminase NeoN



• Molecule 1: Neamine transaminase NeoN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.36Å 107.36Å 217.53Å 90.00° 98.24° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 29.57 – 1.60	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-1.60) 87.3 (29.57-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.92 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.196 , 0.243 0.209 , 0.253	Depositor DCC
R_{free} test set	18346 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27720	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2133e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/3253	1.08	16/4421 (0.4%)
1	B	0.60	0/3210	0.99	10/4366 (0.2%)
1	C	0.59	0/3196	0.94	7/4348 (0.2%)
1	D	0.57	0/3207	0.97	11/4362 (0.3%)
1	E	0.57	0/3172	0.97	9/4316 (0.2%)
1	F	0.58	0/3183	1.02	11/4330 (0.3%)
1	G	0.57	0/3176	1.00	9/4321 (0.2%)
1	H	0.59	0/3198	1.03	9/4349 (0.2%)
All	All	0.59	0/25595	1.00	82/34813 (0.2%)

There are no bond length outliers.

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	275	ARG	NE-CZ-NH1	-18.12	111.24	120.30
1	H	165	ARG	NE-CZ-NH1	17.08	128.84	120.30
1	F	275	ARG	NE-CZ-NH1	-14.15	113.22	120.30
1	E	275	ARG	NE-CZ-NH1	-13.50	113.55	120.30
1	F	275	ARG	NE-CZ-NH2	11.60	126.10	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	A	3157	0	3143	18	0
1	B	3126	0	3093	16	1
1	C	3115	0	3079	24	0
1	D	3123	0	3092	18	0
1	E	3100	0	3052	29	1
1	F	3108	0	3065	28	0
1	G	3104	0	3056	18	0
1	H	3120	0	3082	16	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
2	C	37	0	0	1	0
2	D	37	0	0	1	0
2	E	37	0	0	0	0
2	F	37	0	0	0	0
2	G	37	0	0	1	0
2	H	37	0	0	0	0
3	A	1	0	0	0	0
4	A	343	0	0	4	0
4	B	277	0	0	2	0
4	C	302	0	0	7	0
4	D	331	0	0	1	0
4	E	278	0	0	6	0
4	F	298	0	0	8	0
4	G	317	0	0	1	0
4	H	324	0	0	5	0
All	All	27720	0	24662	156	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 156 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:A:275[B]:ARG:HG2	1:A:275[B]:ARG:HH21	1.14	1.06
1:B:286[B]:ARG:HH11	1:B:286[B]:ARG:HG3	1.29	0.96
1:C:246:ARG:NH1	4:C:601:HOH:O	1.99	0.93
1:G:378:GLU:HG3	1:G:379:PRO:HD2	1.54	0.90
1:A:220:GLU:HG3	4:A:634:HOH:O	1.73	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:NH2	1:E:404:GLU:OE1[1_455]	2.16	0.04

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	416/424 (98%)	405 (97%)	10 (2%)	1 (0%)	47	26
1	B	412/424 (97%)	402 (98%)	8 (2%)	2 (0%)	29	11
1	C	411/424 (97%)	399 (97%)	10 (2%)	2 (0%)	29	11
1	D	412/424 (97%)	405 (98%)	6 (2%)	1 (0%)	47	26
1	E	408/424 (96%)	398 (98%)	9 (2%)	1 (0%)	47	26
1	F	409/424 (96%)	400 (98%)	8 (2%)	1 (0%)	47	26
1	G	408/424 (96%)	400 (98%)	7 (2%)	1 (0%)	47	26
1	H	410/424 (97%)	398 (97%)	11 (3%)	1 (0%)	47	26
All	All	3286/3392 (97%)	3207 (98%)	69 (2%)	10 (0%)	41	21

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ARG
1	F	230	ALA
1	C	230	ALA
1	G	230	ALA
1	H	230	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/318 (98%)	300 (96%)	12 (4%)	33	10
1	B	308/318 (97%)	300 (97%)	8 (3%)	46	21
1	C	307/318 (96%)	298 (97%)	9 (3%)	42	18
1	D	308/318 (97%)	297 (96%)	11 (4%)	35	12
1	E	304/318 (96%)	293 (96%)	11 (4%)	35	12
1	F	305/318 (96%)	292 (96%)	13 (4%)	29	9
1	G	304/318 (96%)	294 (97%)	10 (3%)	38	14
1	H	306/318 (96%)	293 (96%)	13 (4%)	30	9
All	All	2454/2544 (96%)	2367 (96%)	87 (4%)	37	13

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	345	ASN
1	E	341	TYR
1	H	142	PRO
1	E	20	ASP
1	E	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	HIS
1	G	90	HIS
1	E	334	ASN
1	B	295	HIS
1	C	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is 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
2	DOW	G	501	-	39,39,39	1.77	5 (12%)	53,58,58	1.55	9 (16%)
2	DOW	C	501	-	39,39,39	1.78	4 (10%)	53,58,58	1.61	10 (18%)
2	DOW	E	501	-	39,39,39	1.72	4 (10%)	53,58,58	1.33	6 (11%)
2	DOW	A	501	-	39,39,39	1.51	4 (10%)	53,58,58	1.33	6 (11%)
2	DOW	H	501	-	39,39,39	1.57	4 (10%)	53,58,58	1.53	10 (18%)
2	DOW	D	501	-	39,39,39	1.85	6 (15%)	53,58,58	1.43	9 (16%)
2	DOW	F	501	-	39,39,39	1.58	4 (10%)	53,58,58	1.54	10 (18%)
2	DOW	B	501	-	39,39,39	1.70	4 (10%)	53,58,58	1.56	7 (13%)

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
2	DOW	G	501	-	-	3/16/56/56	0/3/3/3
2	DOW	C	501	-	-	3/16/56/56	0/3/3/3
2	DOW	E	501	-	-	3/16/56/56	0/3/3/3
2	DOW	A	501	-	-	3/16/56/56	0/3/3/3
2	DOW	H	501	-	-	3/16/56/56	0/3/3/3
2	DOW	D	501	-	-	4/16/56/56	0/3/3/3
2	DOW	F	501	-	-	3/16/56/56	0/3/3/3
2	DOW	B	501	-	-	3/16/56/56	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	DOW	C3-C2	7.64	1.48	1.40
2	C	501	DOW	C3-C2	7.35	1.48	1.40
2	E	501	DOW	C3-C2	6.77	1.47	1.40
2	B	501	DOW	C3-C2	6.57	1.47	1.40
2	G	501	DOW	C5-C4	6.47	1.49	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	DOW	C4A-C4-C3	5.26	125.68	120.04
2	G	501	DOW	C23-C22-C21	-5.21	102.58	111.37
2	B	501	DOW	C4-C4A-N5A	4.95	120.83	111.58
2	B	501	DOW	C26-C21-C22	4.72	117.17	110.04
2	C	501	DOW	C26-C21-C22	4.49	116.82	110.04

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	501	DOW	C5-C4-C4A-N5A
2	G	501	DOW	C15-C16-N5A-C4A
2	C	501	DOW	C5-C4-C4A-N5A
2	C	501	DOW	C15-C16-N5A-C4A
2	E	501	DOW	C5-C4-C4A-N5A

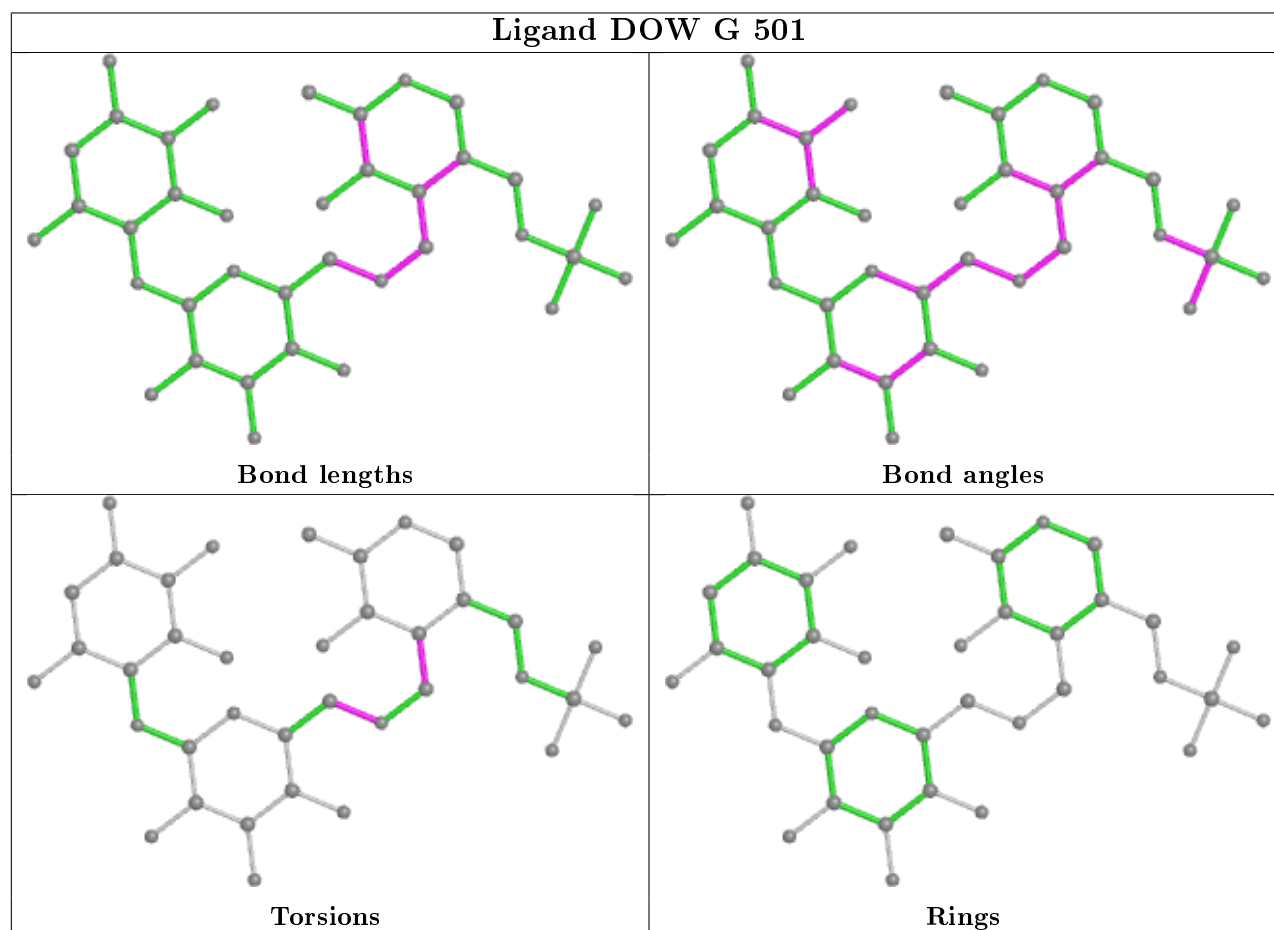
There are no ring outliers.

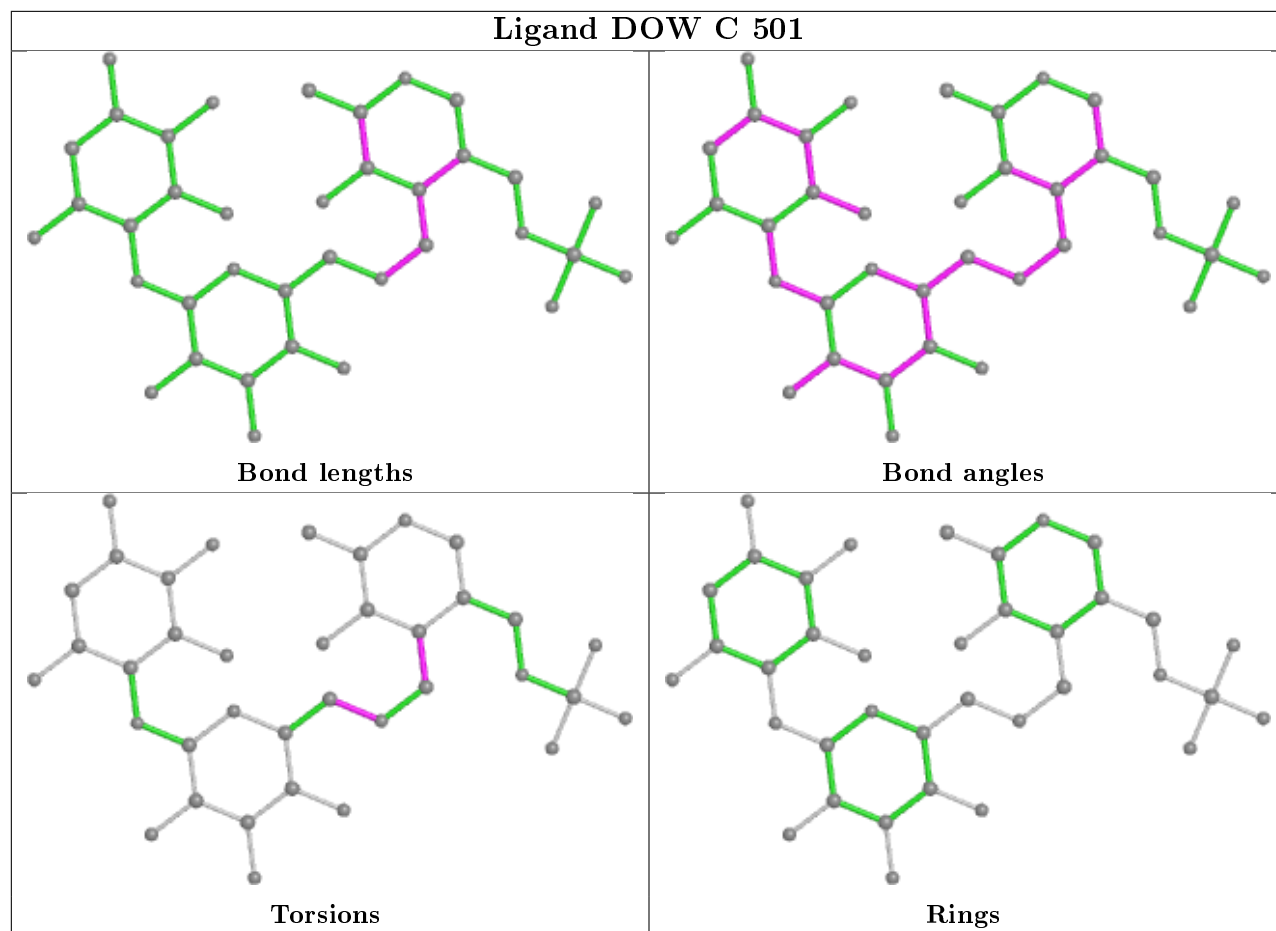
5 monomers are involved in 5 short contacts:

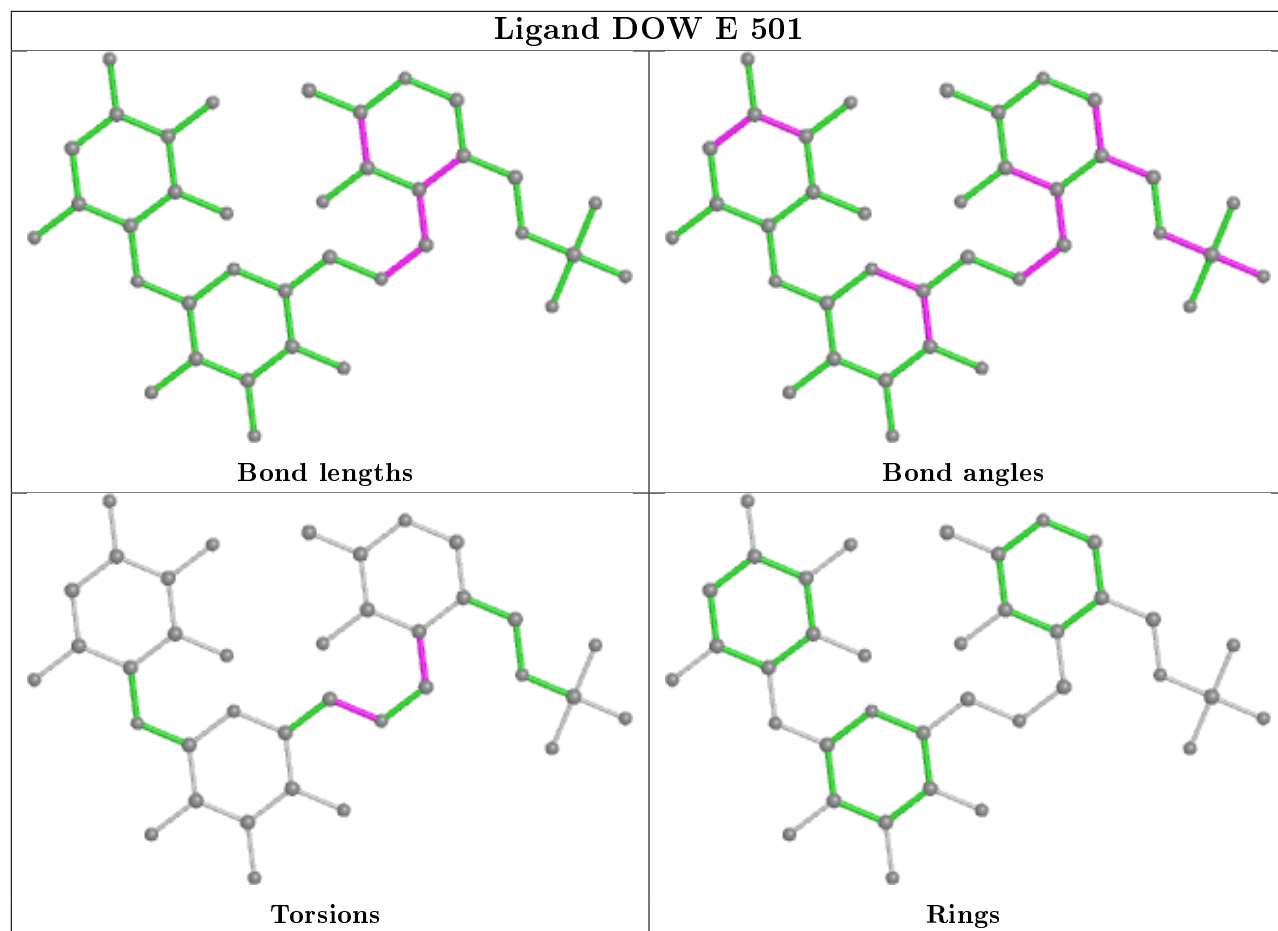
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	DOW	1	0
2	C	501	DOW	1	0
2	A	501	DOW	1	0
2	D	501	DOW	1	0
2	B	501	DOW	1	0

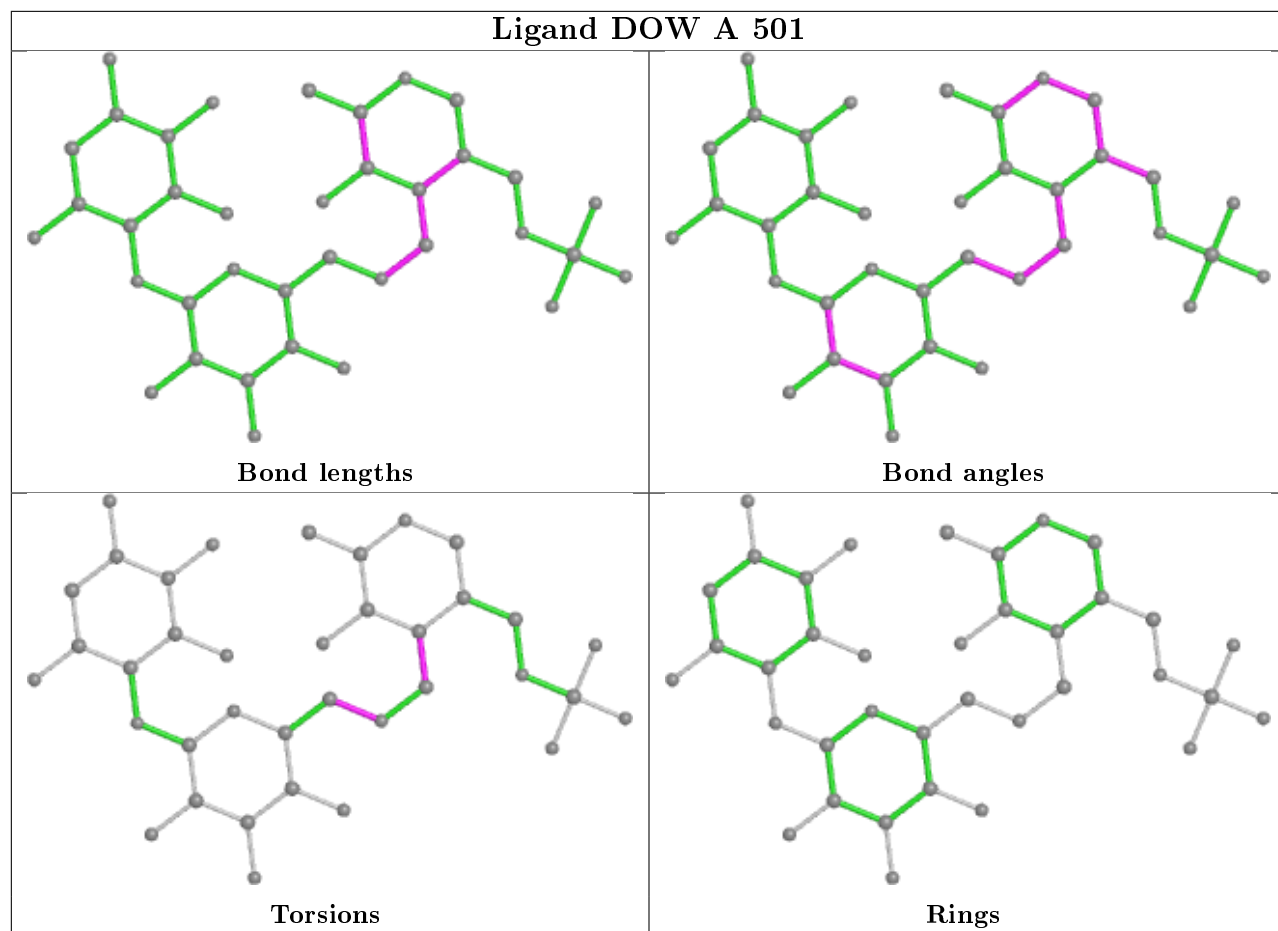
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

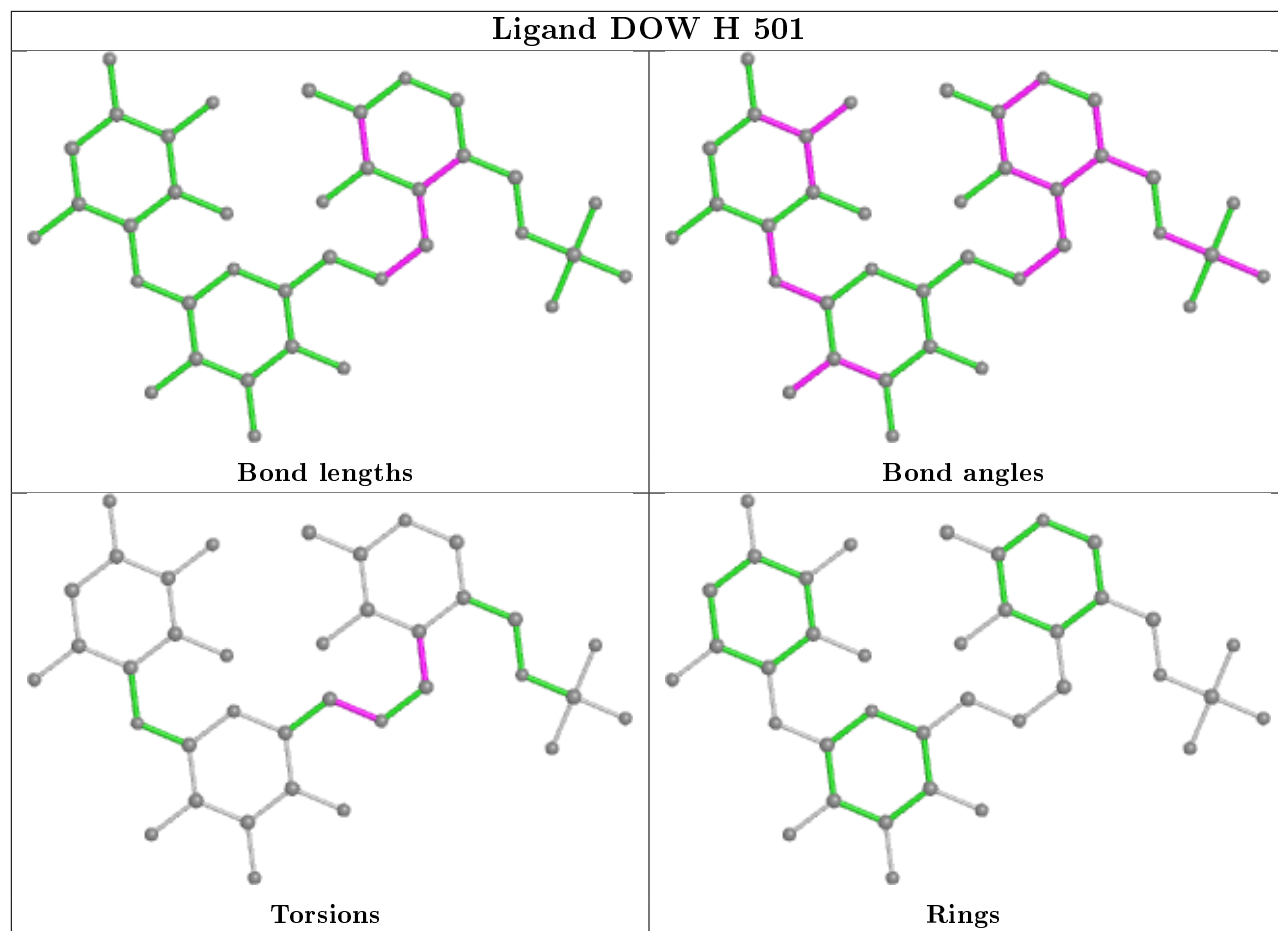
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

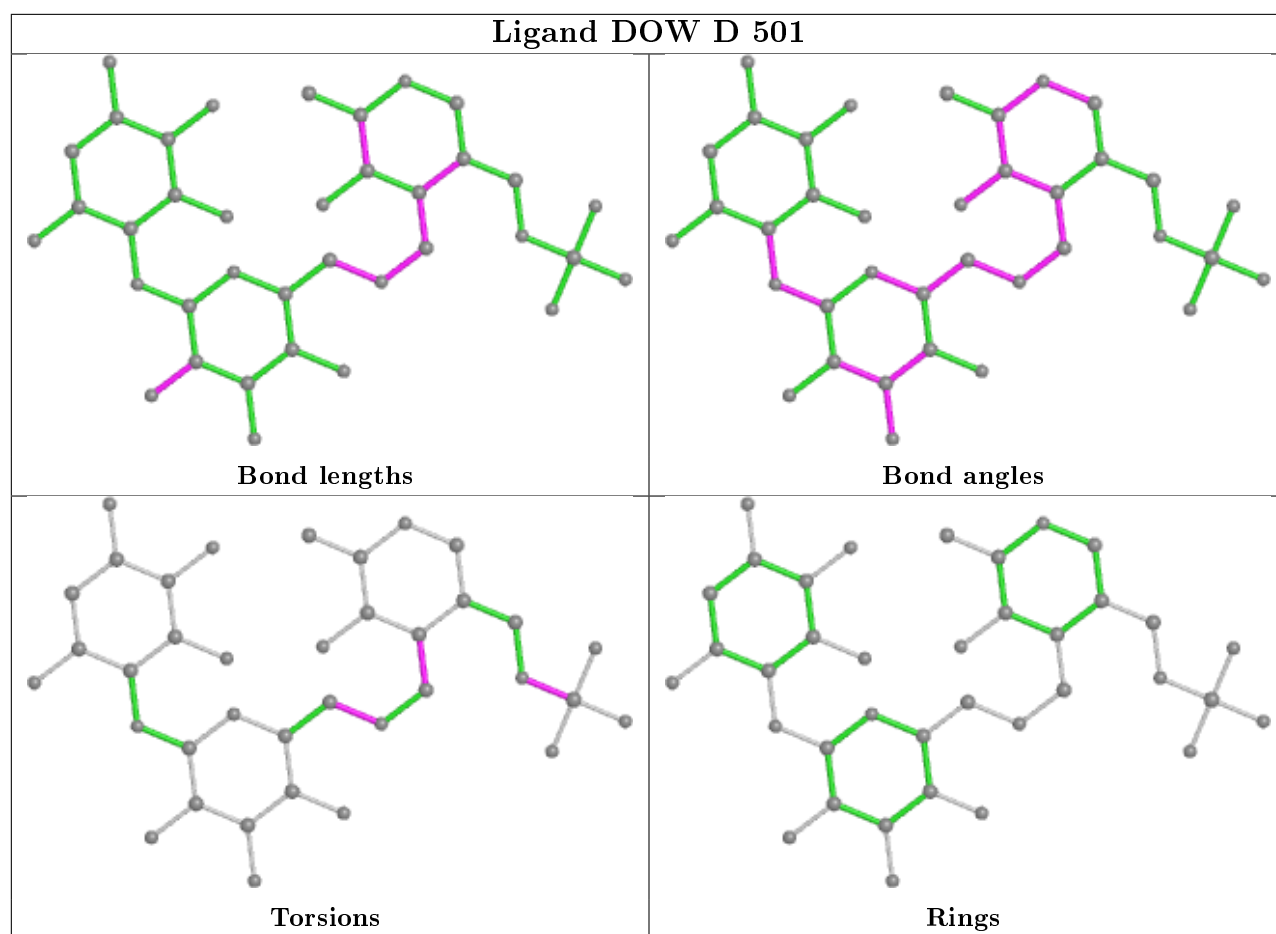


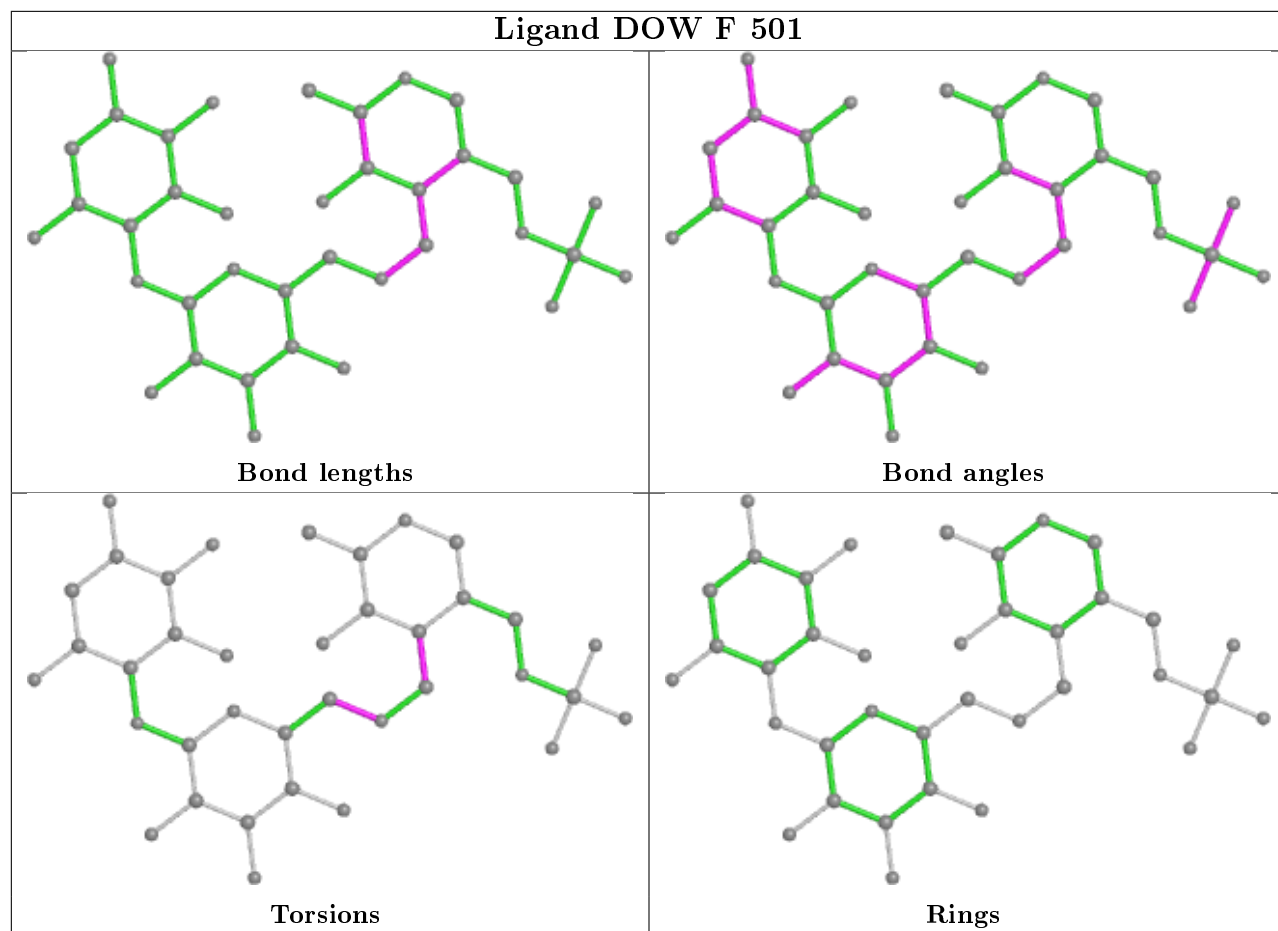


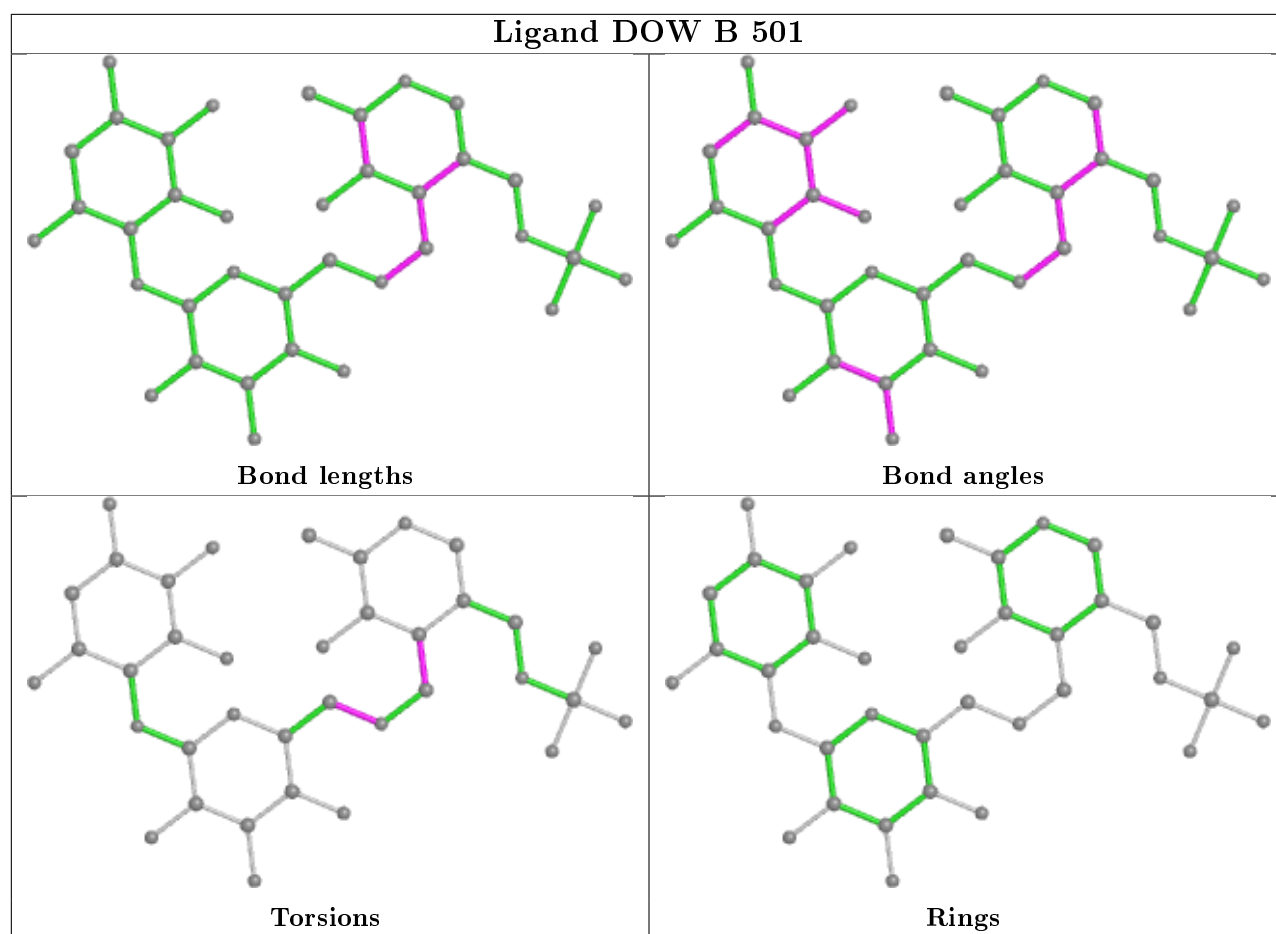












5.7 Other polymers [i](#)

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 ⓘ

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, 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	409/424 (96%)	-0.10	2 (0%) 91 90	11, 19, 34, 62	0
1	B	409/424 (96%)	0.16	11 (2%) 54 52	10, 23, 40, 59	0
1	C	409/424 (96%)	-0.07	4 (0%) 82 82	12, 21, 37, 56	0
1	D	409/424 (96%)	-0.05	6 (1%) 73 73	11, 21, 35, 57	0
1	E	409/424 (96%)	0.04	8 (1%) 65 64	13, 23, 38, 77	0
1	F	409/424 (96%)	0.19	13 (3%) 47 44	12, 22, 40, 75	0
1	G	409/424 (96%)	-0.00	2 (0%) 91 90	14, 22, 37, 52	0
1	H	409/424 (96%)	0.09	14 (3%) 45 42	12, 21, 38, 63	0
All	All	3272/3392 (96%)	0.03	60 (1%) 68 67	10, 22, 38, 77	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	141	ALA	6.6
1	F	142	PRO	6.3
1	F	21	ARG	4.9
1	B	19	LYS	4.1
1	E	19	LYS	4.1

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

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

6.3 Carbohydrates ⓘ

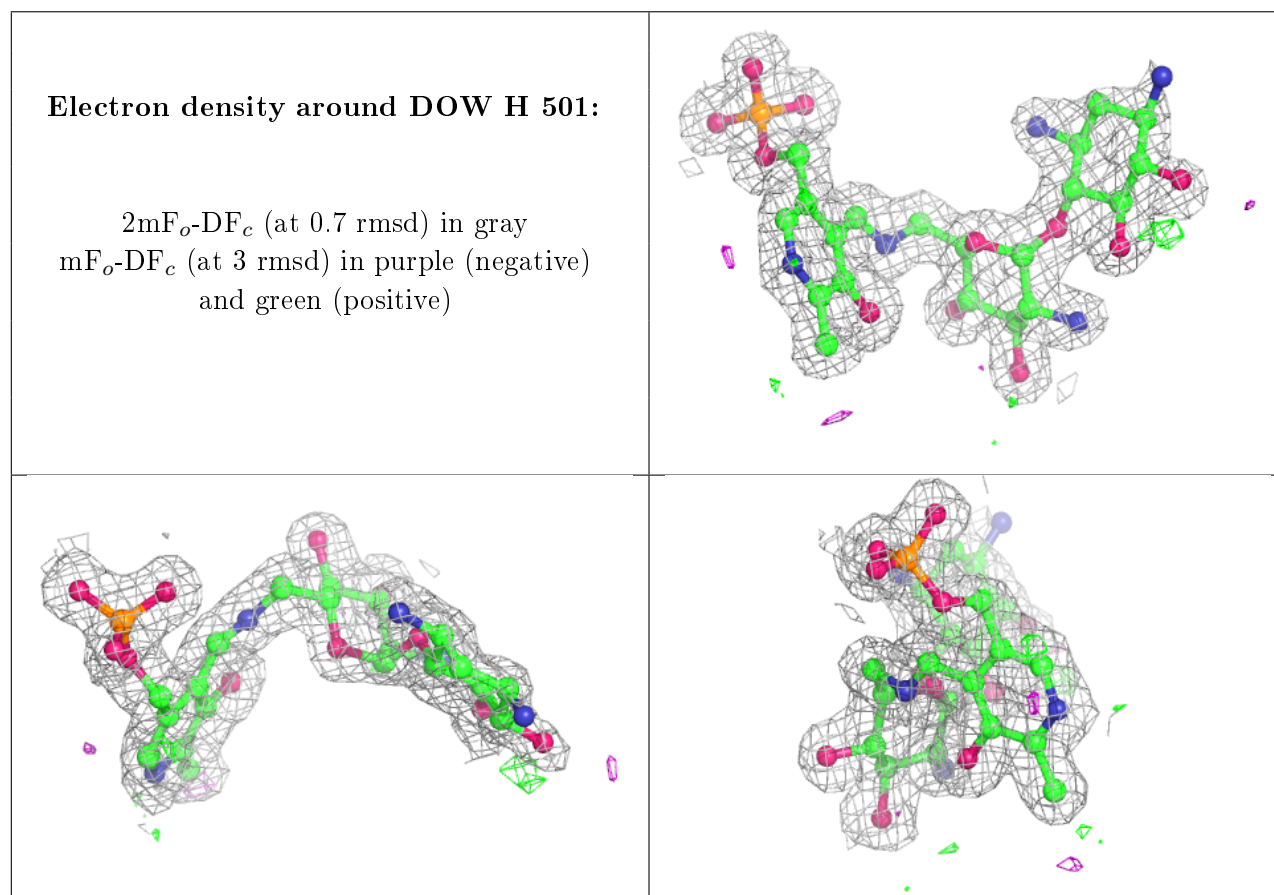
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

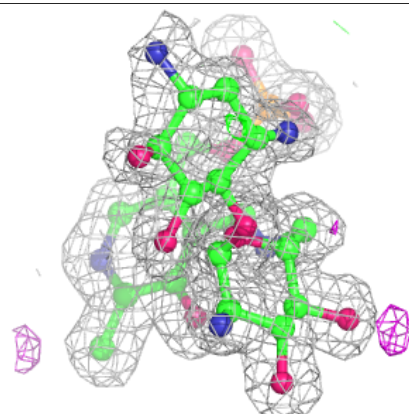
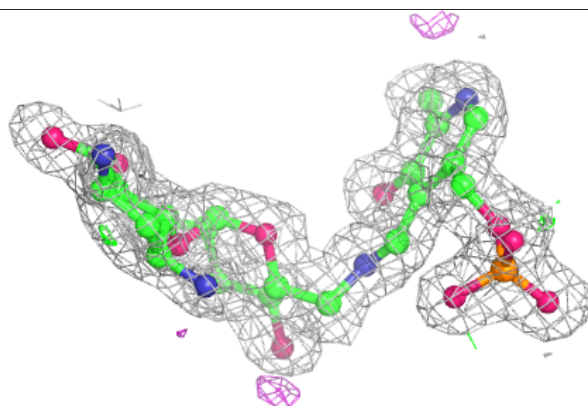
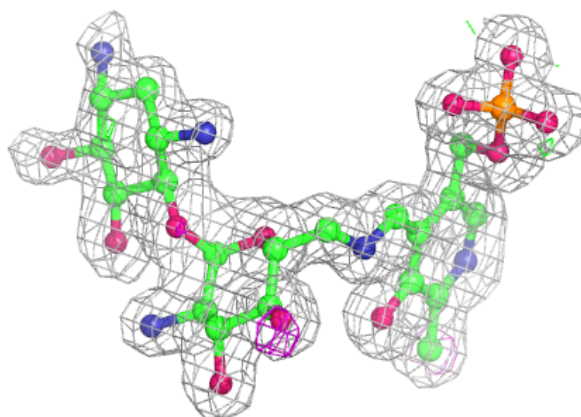
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOW	H	501	37/37	0.96	0.09	12,24,43,52	0
2	DOW	C	501	37/37	0.97	0.08	11,22,43,46	0
2	DOW	E	501	37/37	0.97	0.09	11,22,42,49	0
2	DOW	A	501	37/37	0.97	0.09	10,21,36,40	0
2	DOW	G	501	37/37	0.97	0.10	12,22,46,53	0
2	DOW	D	501	37/37	0.97	0.09	10,20,35,43	0
2	DOW	F	501	37/37	0.97	0.09	12,23,40,48	0
2	DOW	B	501	37/37	0.97	0.08	10,20,37,38	0
3	CL	A	502	1/1	0.99	0.04	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.

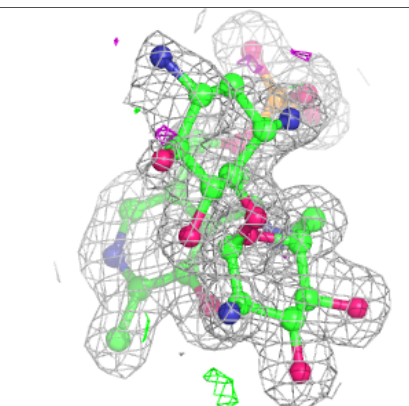
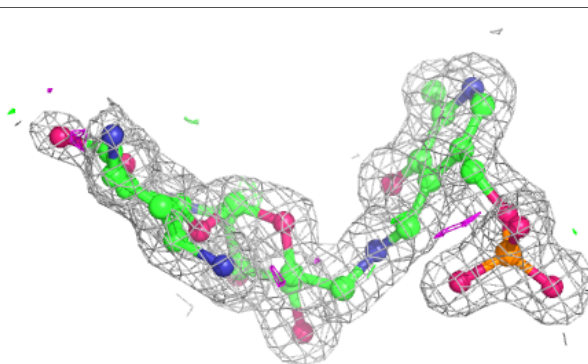
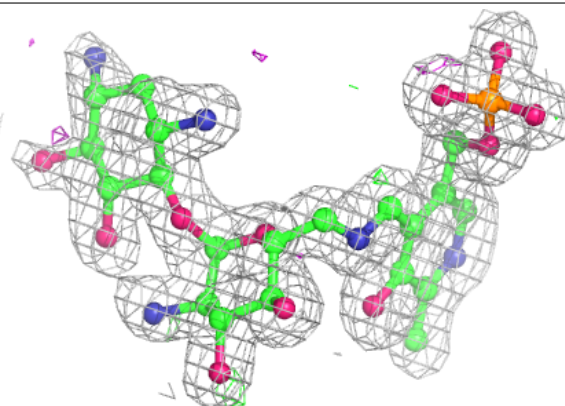


Electron density around DOW C 501:

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

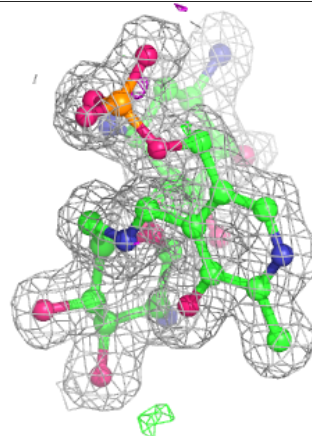
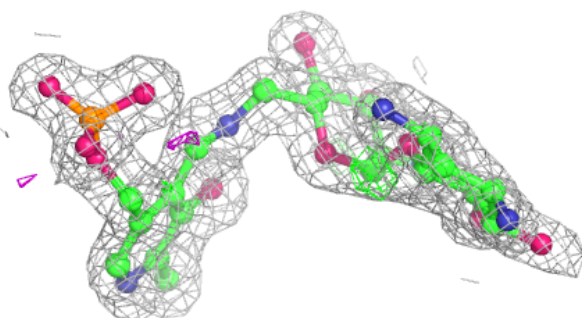
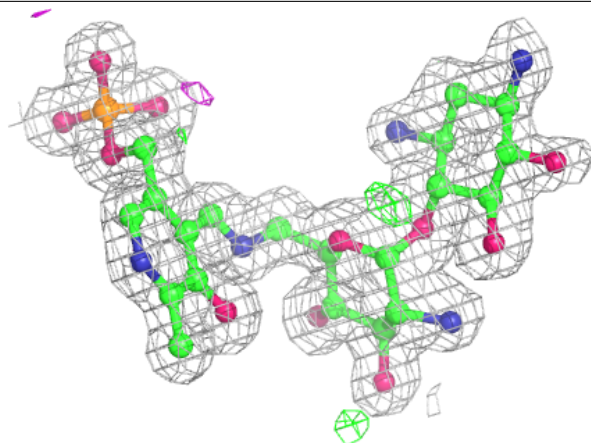
**Electron density around DOW E 501:**

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



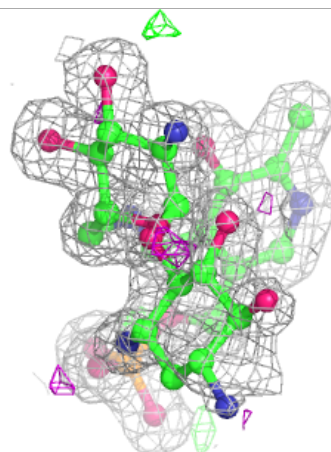
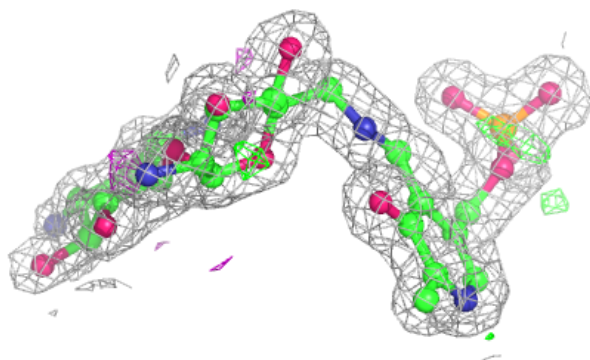
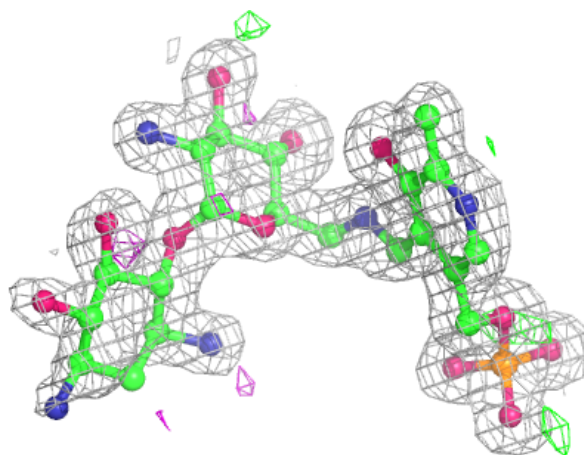
Electron density around DOW A 501:

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



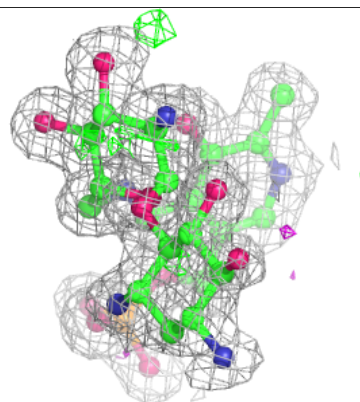
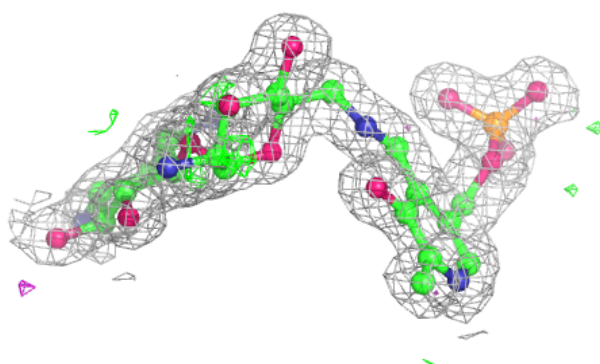
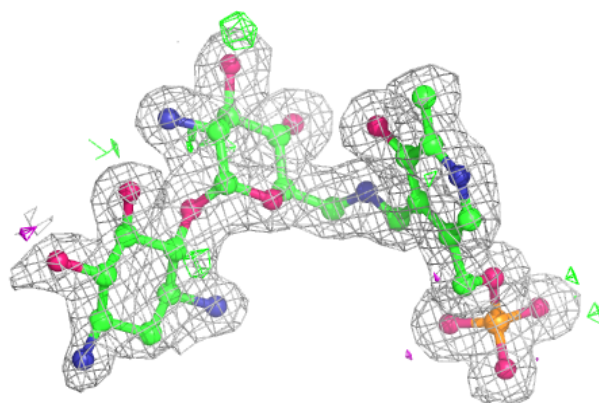
Electron density around DOW G 501:

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

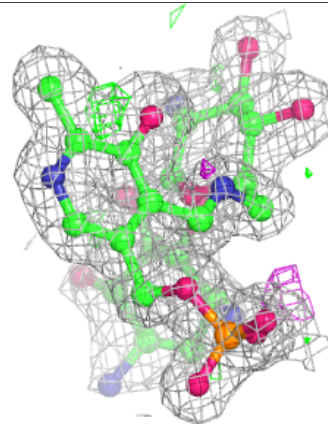
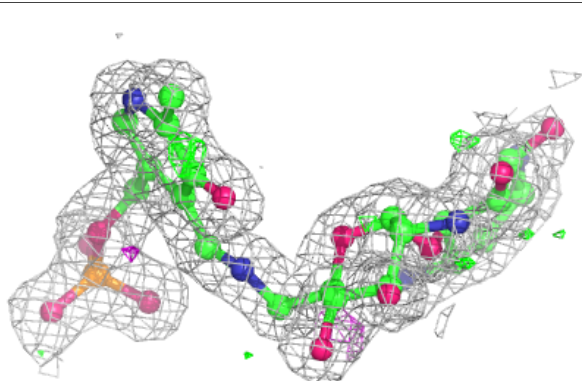
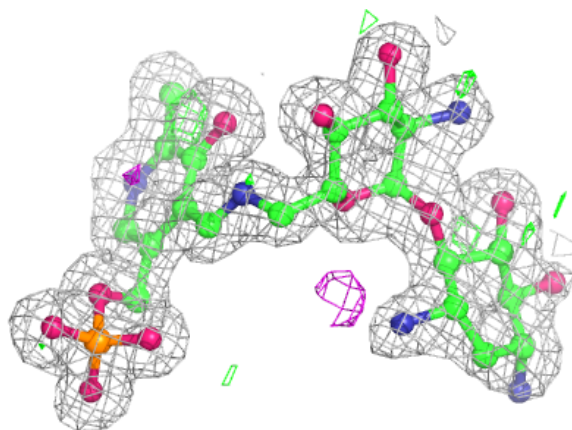


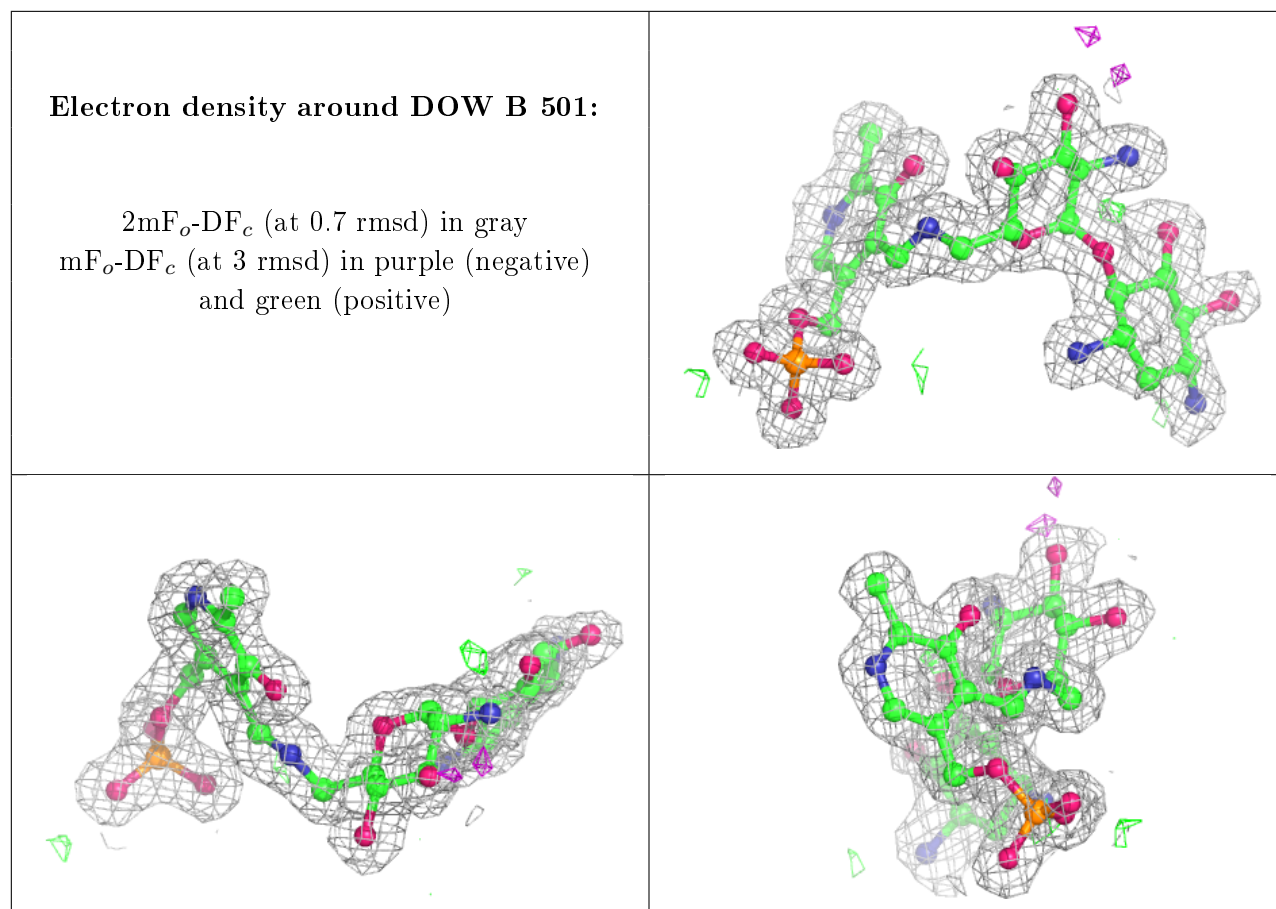
Electron density around DOW D 501:

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

**Electron density around DOW F 501:**

$2mF_o-DF_c$ (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.