



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

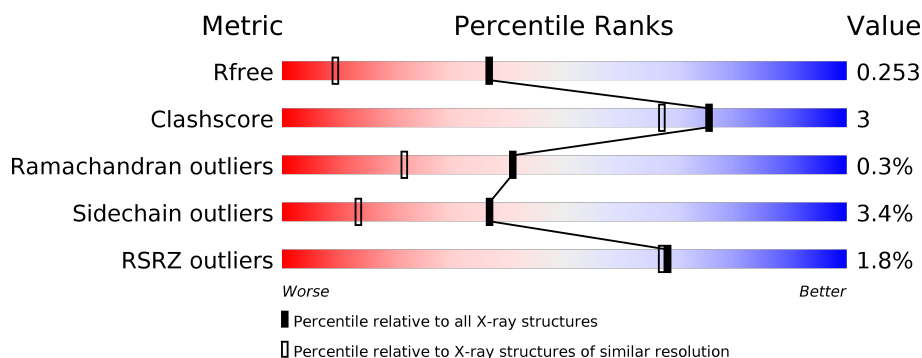
# 1 Overall quality at a glance

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  $\geq 3$ , 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>

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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

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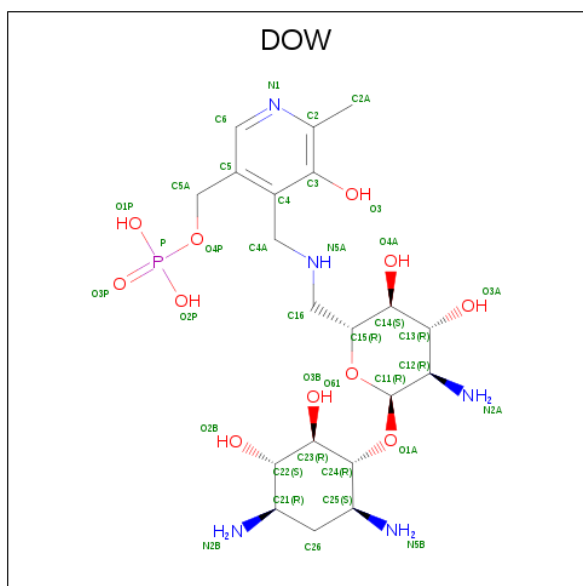
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	expression tag	UNP Q53U08
B	423	HIS	-	expression tag	UNP Q53U08
B	424	HIS	-	expression tag	UNP Q53U08
C	417	LEU	-	expression tag	UNP Q53U08
C	418	GLU	-	expression tag	UNP Q53U08
C	419	HIS	-	expression tag	UNP Q53U08
C	420	HIS	-	expression tag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

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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: C<sub>20</sub>H<sub>36</sub>N<sub>5</sub>O<sub>11</sub>P).



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		

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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		

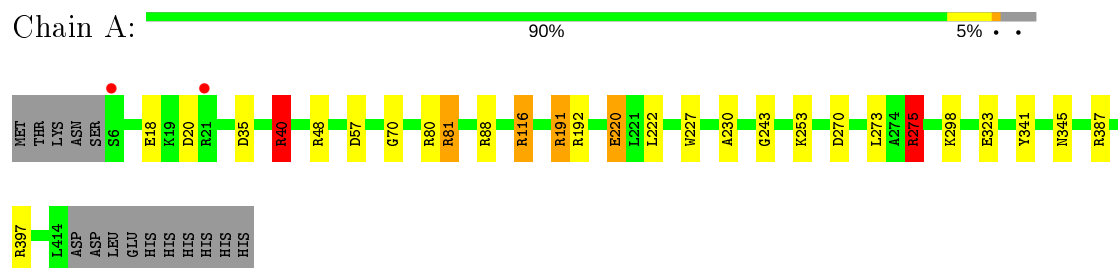
- Molecule 4 is water.

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		

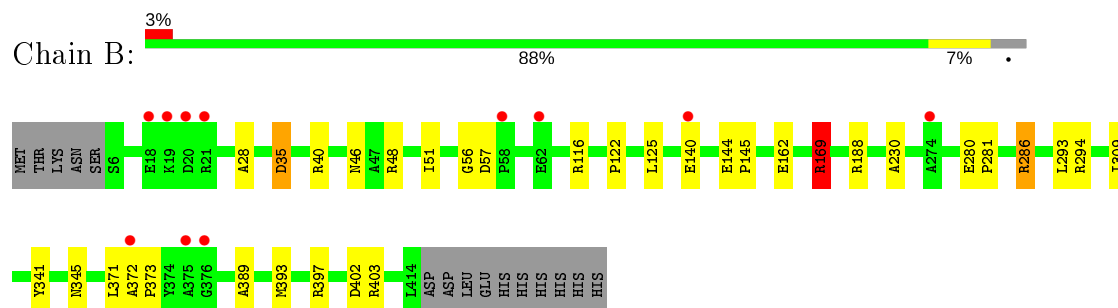
### 3 Residue-property plots [i](#)

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.

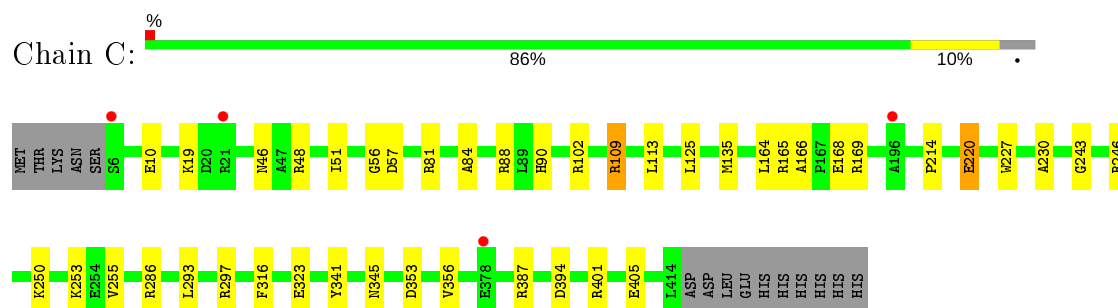
- Molecule 1: Neamine transaminase NeoN



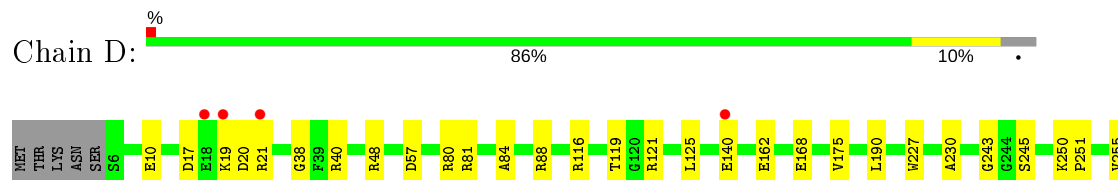
- Molecule 1: Neamine transaminase NeoN



- Molecule 1: Neamine transaminase NeoN



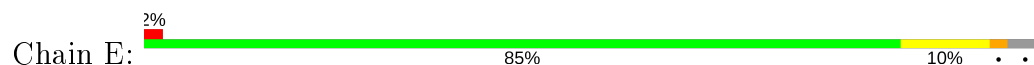
- Molecule 1: Neamine transaminase NeoN



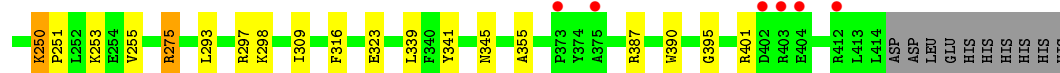
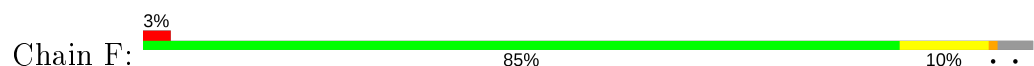




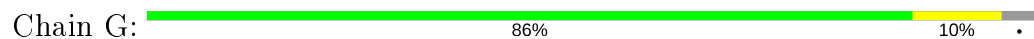
• Molecule 1: Neamine transaminase NeoN



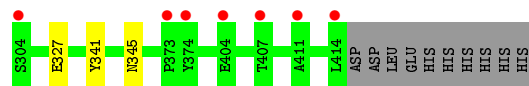
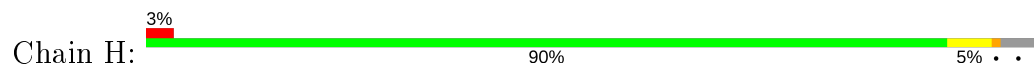
• Molecule 1: Neamine transaminase NeoN



• 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, $\alpha$ , $\beta$ , $\gamma$	70.36 Å 107.36 Å 217.53 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.92 (at 1.60 Å)	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 <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 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.

All (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
1	H	165	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	G	275	ARG	NE-CZ-NH2	10.91	125.76	120.30
1	B	116	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	H	275	ARG	NE-CZ-NH1	-10.41	115.09	120.30
1	A	192	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	B	116	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	A	116	ARG	NE-CZ-NH1	-8.83	115.88	120.30
1	A	116	ARG	NE-CZ-NH2	8.71	124.65	120.30
1	A	275[A]	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	A	275[B]	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	E	275	ARG	NE-CZ-NH2	8.38	124.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	A	40	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	H	116	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	G	102	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	D	275[A]	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	D	275[B]	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	A	81	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	81	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	F	192	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	116	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	B	402	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	169	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	G	116	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	E	188	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	H	102	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	275[A]	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	A	275[B]	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	C	286	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	191[A]	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	191[B]	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	169	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	F	102	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	F	192	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	401	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	C	102	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	G	275	ARG	CG-CD-NE	-6.41	98.33	111.80
1	A	270	ASP	CB-CG-OD2	6.28	123.95	118.30
1	D	385	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	81	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	G	116	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	F	297	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	275	ARG	CG-CD-NE	-6.00	99.20	111.80
1	E	275	ARG	CG-CD-NE	-5.99	99.21	111.80
1	H	40	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	35	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	102	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	F	116	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	B	397	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	G	290	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	401	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	F	102	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	275[A]	ARG	NE-CZ-NH2	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	275[B]	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	135	MET	CG-SD-CE	5.56	109.10	100.20
1	H	161	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	17	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	165	ARG	CD-NE-CZ	5.44	131.21	123.60
1	B	48	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	D	362	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	E	102	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	H	81	ARG	CG-CD-NE	5.27	122.86	111.80
1	A	35	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	401	ARG	CB-CA-C	-5.21	99.97	110.40
1	B	188	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	F	401	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	G	297	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	G	211	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	F	297	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	109	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	E	412	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	116	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	E	211	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	D	394	ASP	CB-CG-OD1	5.01	122.81	118.30
1	E	161	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	397	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	48	ARG	CG-CD-NE	-5.00	101.30	111.80

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:191[B]:ARG:NH2	4:A:601:HOH:O	1.97	0.83
1:C:169:ARG:CD	1:F:355:ALA:HB2	2.11	0.80
1:A:191[A]:ARG:NE	1:A:222:LEU:O	2.16	0.79
1:B:286[B]:ARG:HH11	1:B:286[B]:ARG:CG	1.96	0.78
1:A:275[B]:ARG:CG	1:A:275[B]:ARG:HH21	1.95	0.78
1:E:117:GLU:OE2	4:E:601:HOH:O	2.01	0.76
1:G:62:GLU:OE2	4:G:601:HOH:O	2.04	0.76
1:D:57:ASP:OD2	1:D:275[A]:ARG:NH1	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:OE2	4:E:602:HOH:O	2.07	0.73
1:A:275[B]:ARG:HG2	1:A:275[B]:ARG:NH2	1.96	0.72
1:C:169:ARG:HD3	1:F:355:ALA:HB2	1.72	0.70
1:C:169:ARG:HD2	1:F:355:ALA:HB2	1.73	0.69
1:G:161:ARG:NH2	1:G:189:GLU:OE1	2.25	0.69
1:H:286[A]:ARG:HD3	4:H:677:HOH:O	1.94	0.68
1:F:161:ARG:NH1	4:F:602:HOH:O	2.23	0.67
1:D:389:ALA:O	1:D:393:MET:HG2	1.94	0.66
1:C:10:GLU:HG2	1:D:255:VAL:HB	1.79	0.64
1:F:66[B]:ARG:NH2	4:F:604:HOH:O	2.31	0.64
1:E:403:ARG:NH1	4:E:606:HOH:O	2.25	0.63
1:H:294[B]:ARG:HD3	4:H:663:HOH:O	1.98	0.63
1:D:162:GLU:OE2	1:D:403:ARG:NH1	2.31	0.63
1:A:220:GLU:HB2	4:A:820:HOH:O	1.99	0.62
1:H:283:ARG:NH1	4:H:602:HOH:O	2.32	0.61
1:C:84:ALA:O	1:C:88:ARG:HG3	2.01	0.60
1:E:323:GLU:OE2	4:E:603:HOH:O	2.16	0.60
1:A:40:ARG:NH2	4:A:605:HOH:O	2.33	0.60
1:C:297:ARG:NH1	4:C:605:HOH:O	2.34	0.60
1:C:169:ARG:HD3	1:F:355:ALA:CB	2.32	0.60
1:A:57:ASP:OD2	1:A:275[A]:ARG:NH1	2.30	0.59
1:E:291:ARG:NH2	1:E:354:GLU:OE2	2.35	0.59
1:H:21[B]:ARG:HA	1:H:21[B]:ARG:NE	2.18	0.58
1:E:253:LYS:CD	4:F:748:HOH:O	2.52	0.58
1:B:162[A]:GLU:OE2	1:B:403:ARG:NH1	2.22	0.57
1:F:116:ARG:HG3	1:F:121:ARG:O	2.05	0.57
1:C:90:HIS:HD2	4:C:663:HOH:O	1.88	0.57
1:F:141:ALA:HB3	1:F:144:GLU:CG	2.35	0.57
1:A:323:GLU:HG2	1:A:387:ARG:CZ	2.36	0.56
1:E:191:ARG:HD3	1:E:191:ARG:O	2.05	0.56
1:G:389:ALA:O	1:G:393:MET:HG2	2.04	0.56
1:F:141:ALA:HB3	1:F:144:GLU:HG3	1.87	0.56
1:F:323:GLU:HG2	1:F:387:ARG:CZ	2.37	0.55
1:A:40:ARG:HH21	1:A:40:ARG:CB	2.19	0.55
1:E:66:ARG:NH2	4:E:609:HOH:O	2.34	0.55
1:A:88[B]:ARG:HG2	1:A:273:LEU:HB3	1.89	0.54
1:F:161:ARG:NH2	4:F:607:HOH:O	2.39	0.54
1:D:81:ARG:HD3	1:D:267:ALA:HA	1.89	0.54
1:C:220:GLU:HG3	4:C:777:HOH:O	2.08	0.53
1:E:10:GLU:HG2	1:F:255:VAL:HB	1.91	0.53
1:B:46:ASN:HB3	1:B:51:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:TRP:CZ2	1:F:243:GLY:HA3	2.44	0.52
1:G:323:GLU:HG2	1:G:387:ARG:CZ	2.39	0.52
1:H:48:ARG:HG2	4:H:865:HOH:O	2.10	0.52
1:D:175:VAL:HG21	1:D:190:LEU:HD21	1.91	0.52
1:E:108:VAL:HG11	1:E:130:HIS:HB3	1.93	0.51
1:H:227:TRP:CZ2	1:H:243:GLY:HA3	2.45	0.51
1:E:115:VAL:HG11	1:E:172:ALA:HB2	1.92	0.51
1:E:253:LYS:HD3	4:F:748:HOH:O	2.08	0.51
1:G:108:VAL:HG11	1:G:130:HIS:HB3	1.92	0.51
1:E:39:PHE:HE2	1:E:337:GLY:HA3	1.75	0.51
1:A:253:LYS:HD2	4:B:624:HOH:O	2.10	0.51
1:H:125:LEU:HD22	1:H:170:VAL:HG11	1.93	0.51
1:H:162:GLU:HA	1:H:165:ARG:HD2	1.93	0.50
1:B:293:LEU:CD2	1:B:309:ILE:HG21	2.41	0.50
1:H:125:LEU:HD12	1:H:151:VAL:HB	1.94	0.50
1:B:286[B]:ARG:NH1	1:B:286[B]:ARG:CG	2.64	0.49
1:G:293:LEU:HD21	1:G:316:PHE:CG	2.47	0.49
1:G:378:GLU:HG3	1:G:379:PRO:CD	2.36	0.49
1:B:294:ARG:NE	4:B:604:HOH:O	2.36	0.49
1:D:291:ARG:NH2	1:D:354:GLU:OE2	2.43	0.49
1:G:213:ALA:HB1	1:G:214:PRO:HD2	1.94	0.49
1:E:372:ALA:N	1:E:373:PRO:CD	2.76	0.48
1:H:14:CYS:HB2	1:H:15:PRO:HD2	1.96	0.48
1:E:238:ALA:HB1	1:F:102:ARG:HD2	1.95	0.47
1:D:227:TRP:CZ2	1:D:243:GLY:HA3	2.49	0.47
2:A:501:DOW:O3	2:A:501:DOW:N5A	2.48	0.47
1:F:116:ARG:HD2	1:F:122:PRO:O	2.14	0.47
1:E:191:ARG:HD3	1:E:191:ARG:C	2.35	0.47
1:B:372:ALA:N	1:B:373:PRO:CD	2.78	0.47
1:F:169:ARG:HD3	4:F:711:HOH:O	2.13	0.47
1:C:46:ASN:HB3	1:C:51:ILE:HB	1.95	0.47
1:A:80[B]:ARG:HA	1:A:80[B]:ARG:HD3	1.70	0.47
1:C:56:GLY:O	1:C:57:ASP:C	2.54	0.46
1:F:227:TRP:CE2	1:F:243:GLY:HA3	2.49	0.46
1:C:164:LEU:C	1:C:166:ALA:H	2.19	0.46
1:E:295:HIS:CG	1:E:361:GLU:HG2	2.51	0.45
1:F:143:LEU:HD11	1:F:159:LEU:HD22	1.97	0.45
1:F:207:LYS:HA	1:F:231:LYS:HD2	1.97	0.45
1:E:293:LEU:HD21	1:E:316:PHE:CG	2.51	0.45
1:H:162:GLU:OE2	1:H:165:ARG:HD3	2.17	0.45
1:C:227:TRP:CZ2	1:C:243:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:CZ	1:C:113:LEU:HD11	2.47	0.44
1:E:253:LYS:HD2	4:F:748:HOH:O	2.17	0.44
1:C:405:GLU:OE2	4:C:602:HOH:O	2.21	0.44
1:D:119:THR:HB	1:D:121:ARG:HD3	2.00	0.44
1:E:403:ARG:HD3	1:E:403:ARG:HA	1.82	0.44
1:A:40:ARG:HH21	1:A:40:ARG:CG	2.31	0.44
1:D:121:ARG:NH2	4:D:2514:HOH:O	2.51	0.44
1:C:88:ARG:NH2	1:C:88:ARG:HG2	2.33	0.44
1:D:84:ALA:O	1:D:88:ARG:HG3	2.18	0.43
1:C:293:LEU:HD21	1:C:316:PHE:CG	2.54	0.43
1:F:293:LEU:HD21	1:F:316:PHE:CG	2.53	0.43
1:B:56:GLY:O	1:B:57:ASP:C	2.56	0.43
2:B:501:DOW:O3	2:B:501:DOW:N5A	2.51	0.43
1:E:48:ARG:HG3	1:E:341:TYR:CE2	2.53	0.43
1:C:323:GLU:HG2	1:C:387:ARG:CZ	2.49	0.43
1:G:115:VAL:HG11	1:G:172:ALA:HB2	2.00	0.43
1:G:15:PRO:HB3	1:G:339:LEU:HD11	1.99	0.43
1:F:390:TRP:CZ3	1:F:395:GLY:HA2	2.54	0.43
1:G:291:ARG:NH2	1:G:354:GLU:OE2	2.48	0.43
1:G:394:ASP:OD2	2:G:501:DOW:O3B	2.37	0.43
1:G:102:ARG:HD2	1:H:238:ALA:HB1	2.01	0.43
1:B:280:GLU:N	1:B:281:PRO:HD2	2.34	0.42
1:G:21:ARG:NE	1:G:21:ARG:HA	2.34	0.42
1:D:291:ARG:HD3	1:D:357:LEU:HD13	2.01	0.42
1:E:9:ALA:HB2	1:F:97:VAL:HB	2.00	0.42
1:B:389:ALA:O	1:B:393:MET:HG2	2.20	0.42
1:C:255:VAL:HB	1:D:10:GLU:HG2	2.02	0.42
1:E:402:ASP:OD2	4:E:604:HOH:O	2.22	0.42
1:E:323:GLU:HG3	1:E:387:ARG:CZ	2.50	0.42
1:F:35:ASP:OD2	4:F:601:HOH:O	2.22	0.42
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.93	0.42
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.33	0.42
1:F:101:PHE:HE2	1:F:242[A]:VAL:HG22	1.84	0.42
1:G:74:THR:HB	1:H:28:ALA:HB2	2.02	0.42
1:B:280:GLU:N	1:B:281:PRO:CD	2.83	0.42
1:C:394:ASP:OD2	2:C:501:DOW:O3B	2.38	0.42
1:B:371:LEU:C	1:B:373:PRO:HD2	2.41	0.41
1:D:293:LEU:HD21	1:D:316:PHE:CG	2.55	0.41
1:G:238:ALA:HB1	1:H:102:ARG:HD2	2.02	0.41
1:D:80:ARG:HA	1:D:80:ARG:HD3	1.88	0.41
1:E:227:TRP:CZ2	1:E:243:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:NZ	4:C:609:HOH:O	2.45	0.41
1:C:220:GLU:CG	4:C:681:HOH:O	2.68	0.41
1:D:121:ARG:HG2	1:D:168:GLU:O	2.21	0.41
1:E:372:ALA:N	1:E:373:PRO:HD2	2.35	0.41
1:E:102:ARG:HD2	1:F:238:ALA:HB1	2.01	0.41
1:F:293:LEU:CD2	1:F:309:ILE:HG21	2.50	0.41
1:H:227:TRP:CE2	1:H:243:GLY:HA3	2.55	0.41
1:E:222:LEU:O	1:E:223:ALA:C	2.59	0.41
1:A:40:ARG:NH1	4:H:608:HOH:O	2.53	0.41
1:E:250:LYS:N	1:E:251:PRO:CD	2.84	0.41
1:A:70:GLY:HA3	1:B:28:ALA:O	2.21	0.41
1:C:353:ASP:OD2	1:C:356:VAL:HG23	2.21	0.40
1:A:227:TRP:CZ2	1:A:243:GLY:HA3	2.56	0.40
1:F:250:LYS:N	1:F:251:PRO:CD	2.85	0.40
1:F:15:PRO:HB3	1:F:339:LEU:HD11	2.03	0.40
1:H:21[B]:ARG:HA	1:H:21[B]:ARG:HE	1.86	0.40
1:D:38:GLY:O	1:D:40:ARG:NH2	2.54	0.40
1:D:250:LYS:N	1:D:251:PRO:CD	2.85	0.40
2:D:501:DOW:O3	2:D:501:DOW:N5A	2.54	0.40
1:G:64:VAL:HG13	1:G:264:THR:HB	2.03	0.40

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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	A	230	ALA
1	B	230	ALA
1	D	230	ALA
1	E	230	ALA
1	B	122	PRO

### 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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	20	ASP
1	A	40	ARG
1	A	48	ARG
1	A	81	ARG
1	A	116	ARG
1	A	220	GLU
1	A	275[A]	ARG
1	A	275[B]	ARG
1	A	298	LYS
1	A	341	TYR
1	A	345	ASN
1	B	35	ASP
1	B	125	LEU
1	B	140	GLU
1	B	169	ARG
1	B	286[A]	ARG
1	B	286[B]	ARG
1	B	341	TYR
1	B	345	ASN
1	C	48	ARG
1	C	125	LEU
1	C	168	GLU
1	C	214	PRO
1	C	220	GLU
1	C	250	LYS
1	C	253	LYS
1	C	341	TYR
1	C	345	ASN
1	D	19	LYS
1	D	20	ASP
1	D	21	ARG
1	D	48	ARG

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Mol	Chain	Res	Type
1	D	125	LEU
1	D	140	GLU
1	D	245	SER
1	D	275[A]	ARG
1	D	275[B]	ARG
1	D	341	TYR
1	D	345	ASN
1	E	20	ASP
1	E	48	ARG
1	E	125	LEU
1	E	144	GLU
1	E	168	GLU
1	E	191	ARG
1	E	275	ARG
1	E	291	ARG
1	E	341	TYR
1	E	345	ASN
1	E	403	ARG
1	F	6	SER
1	F	48	ARG
1	F	79	SER
1	F	80	ARG
1	F	116	ARG
1	F	143	LEU
1	F	220	GLU
1	F	250	LYS
1	F	253	LYS
1	F	275	ARG
1	F	298	LYS
1	F	341	TYR
1	F	345	ASN
1	G	18	GLU
1	G	48	ARG
1	G	125	LEU
1	G	168	GLU
1	G	191	ARG
1	G	220	GLU
1	G	253	LYS
1	G	275	ARG
1	G	341	TYR
1	G	345	ASN
1	H	20	ASP

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Mol	Chain	Res	Type
1	H	21[A]	ARG
1	H	21[B]	ARG
1	H	48	ARG
1	H	81	ARG
1	H	125	LEU
1	H	142	PRO
1	H	165	ARG
1	H	167	PRO
1	H	275	ARG
1	H	327	GLU
1	H	341	TYR
1	H	345	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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

### 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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
2	D	501	DOW	C5-C4	6.23	1.49	1.40
2	G	501	DOW	C3-C2	6.21	1.47	1.40
2	B	501	DOW	C5-C4	6.10	1.49	1.40
2	E	501	DOW	C5-C4	6.09	1.49	1.40
2	A	501	DOW	C3-C2	6.05	1.47	1.40
2	H	501	DOW	C3-C2	6.02	1.46	1.40
2	F	501	DOW	C3-C2	5.93	1.46	1.40
2	F	501	DOW	C5-C4	5.55	1.48	1.40
2	C	501	DOW	C5-C4	5.39	1.48	1.40
2	H	501	DOW	C5-C4	5.30	1.47	1.40
2	A	501	DOW	C5-C4	3.93	1.46	1.40
2	G	501	DOW	C4A-C4	-3.56	1.47	1.51
2	C	501	DOW	C4A-C4	-3.31	1.47	1.51
2	D	501	DOW	C4A-N5A	-3.31	1.30	1.46
2	H	501	DOW	C4A-C4	-3.18	1.47	1.51
2	A	501	DOW	C4A-N5A	-3.05	1.31	1.46
2	F	501	DOW	C4A-C4	-2.98	1.48	1.51
2	C	501	DOW	C4A-N5A	-2.88	1.32	1.46
2	F	501	DOW	C4A-N5A	-2.82	1.32	1.46
2	B	501	DOW	C4A-N5A	-2.81	1.32	1.46
2	B	501	DOW	C4A-C4	-2.80	1.48	1.51
2	E	501	DOW	C4A-C4	-2.75	1.48	1.51
2	H	501	DOW	C4A-N5A	-2.65	1.33	1.46
2	D	501	DOW	C4A-C4	-2.56	1.48	1.51
2	G	501	DOW	C4A-N5A	-2.56	1.34	1.46
2	E	501	DOW	C4A-N5A	-2.53	1.34	1.46
2	G	501	DOW	C16-N5A	-2.38	1.43	1.47
2	A	501	DOW	C4A-C4	-2.38	1.48	1.51
2	D	501	DOW	C12-N2A	-2.16	1.44	1.47
2	D	501	DOW	C16-N5A	-2.15	1.43	1.47

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	DOW	C26-C21-C22	4.49	116.82	110.04
2	G	501	DOW	C4A-C4-C3	3.88	124.19	120.04
2	F	501	DOW	C4-C4A-N5A	3.65	118.40	111.58
2	E	501	DOW	C26-C21-C22	3.54	115.38	110.04
2	C	501	DOW	C4-C4A-N5A	3.54	118.19	111.58
2	C	501	DOW	C11-O1A-C24	-3.46	109.40	117.96
2	D	501	DOW	C4-C4A-N5A	3.41	117.95	111.58
2	F	501	DOW	C21-C26-C25	3.32	118.00	111.18
2	H	501	DOW	C4-C4A-N5A	3.32	117.78	111.58
2	G	501	DOW	O61-C15-C16	3.28	112.08	105.96
2	C	501	DOW	O61-C15-C16	3.24	112.00	105.96
2	A	501	DOW	C4-C4A-N5A	3.14	117.44	111.58
2	H	501	DOW	O2B-C22-C21	3.12	115.53	109.81
2	F	501	DOW	C4A-C4-C3	3.11	123.38	120.04
2	G	501	DOW	C4-C4A-N5A	3.10	117.38	111.58
2	F	501	DOW	C14-C13-C12	-2.93	106.03	111.07
2	D	501	DOW	C11-O1A-C24	-2.92	110.74	117.96
2	E	501	DOW	C5A-C5-C6	2.86	124.08	119.37
2	D	501	DOW	C4-C3-C2	-2.84	115.70	120.06
2	E	501	DOW	C4-C4A-N5A	2.80	116.80	111.58
2	C	501	DOW	C4A-C4-C3	2.78	123.02	120.04
2	H	501	DOW	C11-O1A-C24	-2.71	111.27	117.96
2	D	501	DOW	O3-C3-C2	2.69	123.36	117.49
2	B	501	DOW	C6-C5-C4	2.68	120.02	118.12
2	D	501	DOW	C4A-N5A-C16	2.68	123.98	113.60
2	D	501	DOW	C6-N1-C2	2.66	124.10	119.17
2	D	501	DOW	O3A-C13-C12	-2.63	105.50	110.22
2	H	501	DOW	C5A-C5-C6	2.57	123.61	119.37
2	C	501	DOW	C6-C5-C4	2.57	119.94	118.12
2	F	501	DOW	C26-C21-C22	2.54	113.88	110.04
2	H	501	DOW	O4P-P-O3P	2.51	113.51	106.47
2	E	501	DOW	C4A-C4-C3	2.49	122.71	120.04
2	H	501	DOW	C4A-C4-C5	-2.44	117.00	119.71
2	G	501	DOW	C3-C4-C5	-2.43	116.39	118.72
2	C	501	DOW	C13-C12-N2A	-2.41	106.11	111.05
2	F	501	DOW	C26-C25-C24	2.40	115.60	109.53
2	A	501	DOW	C6-N1-C2	2.40	123.61	119.17
2	B	501	DOW	O3B-C23-C24	2.36	116.20	109.94
2	A	501	DOW	C5A-C5-C6	2.35	123.25	119.37
2	E	501	DOW	O61-C15-C14	-2.31	105.50	109.69
2	B	501	DOW	O3A-C13-C12	-2.30	106.09	110.22
2	C	501	DOW	C13-C14-C15	2.24	114.24	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	DOW	O4P-P-O3P	2.24	112.76	106.47
2	G	501	DOW	C4A-N5A-C16	2.24	122.27	113.60
2	D	501	DOW	C14-C13-C12	-2.22	107.25	111.07
2	C	501	DOW	O3B-C23-C22	2.22	115.47	110.35
2	A	501	DOW	C5-C6-N1	-2.18	120.19	123.82
2	B	501	DOW	C4A-C4-C5	2.16	122.11	119.71
2	H	501	DOW	C3-C2-N1	-2.16	117.98	120.77
2	H	501	DOW	C23-C22-C21	-2.15	107.73	111.37
2	F	501	DOW	O1P-P-O2P	2.15	115.83	107.64
2	F	501	DOW	C22-C21-N2B	-2.14	106.73	110.97
2	G	501	DOW	O2B-C22-C21	2.13	113.72	109.81
2	C	501	DOW	C4A-N5A-C16	2.12	121.83	113.60
2	F	501	DOW	O61-C15-C14	-2.11	105.86	109.69
2	G	501	DOW	C14-C13-C12	-2.09	107.47	111.07
2	F	501	DOW	C13-C12-N2A	-2.09	106.78	111.05
2	A	501	DOW	C4A-N5A-C16	2.08	121.67	113.60
2	D	501	DOW	O61-C15-C16	2.07	109.82	105.96
2	A	501	DOW	C11-C12-C13	2.06	115.61	110.21
2	B	501	DOW	O2B-C22-C23	-2.03	105.65	110.35
2	H	501	DOW	C13-C12-N2A	-2.02	106.91	111.05
2	G	501	DOW	O2P-P-O4P	2.02	112.11	106.73

There are no chirality outliers.

All (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
2	E	501	DOW	C15-C16-N5A-C4A
2	A	501	DOW	C5-C4-C4A-N5A
2	A	501	DOW	C15-C16-N5A-C4A
2	H	501	DOW	C5-C4-C4A-N5A
2	H	501	DOW	C15-C16-N5A-C4A
2	D	501	DOW	C5-C4-C4A-N5A
2	D	501	DOW	C15-C16-N5A-C4A
2	F	501	DOW	C5-C4-C4A-N5A
2	F	501	DOW	C15-C16-N5A-C4A
2	B	501	DOW	C5-C4-C4A-N5A
2	B	501	DOW	C15-C16-N5A-C4A

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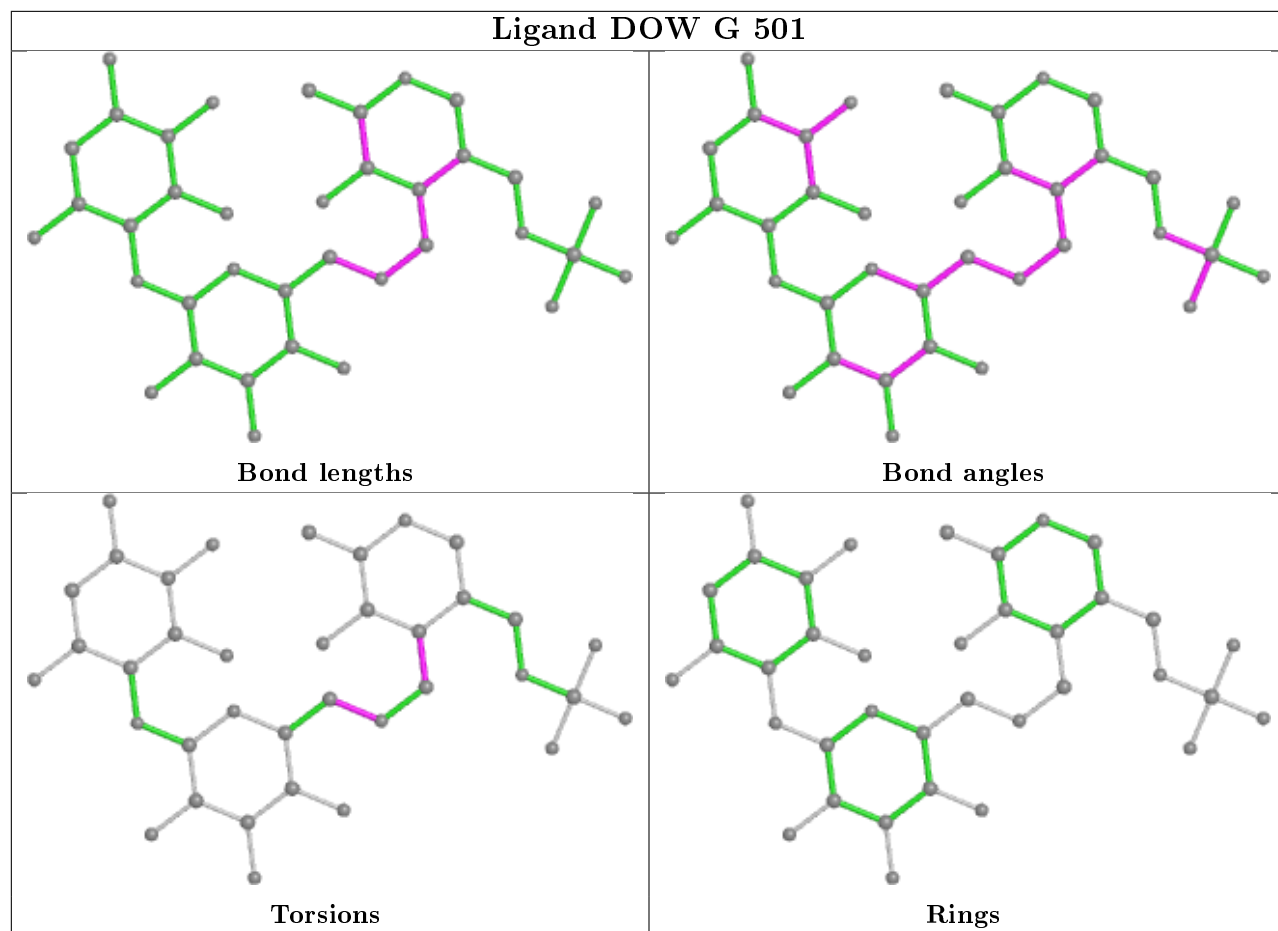
Mol	Chain	Res	Type	Atoms
2	D	501	DOW	C5A-O4P-P-O3P
2	G	501	DOW	C3-C4-C4A-N5A
2	C	501	DOW	C3-C4-C4A-N5A
2	E	501	DOW	C3-C4-C4A-N5A
2	A	501	DOW	C3-C4-C4A-N5A
2	H	501	DOW	C3-C4-C4A-N5A
2	D	501	DOW	C3-C4-C4A-N5A
2	F	501	DOW	C3-C4-C4A-N5A
2	B	501	DOW	C3-C4-C4A-N5A

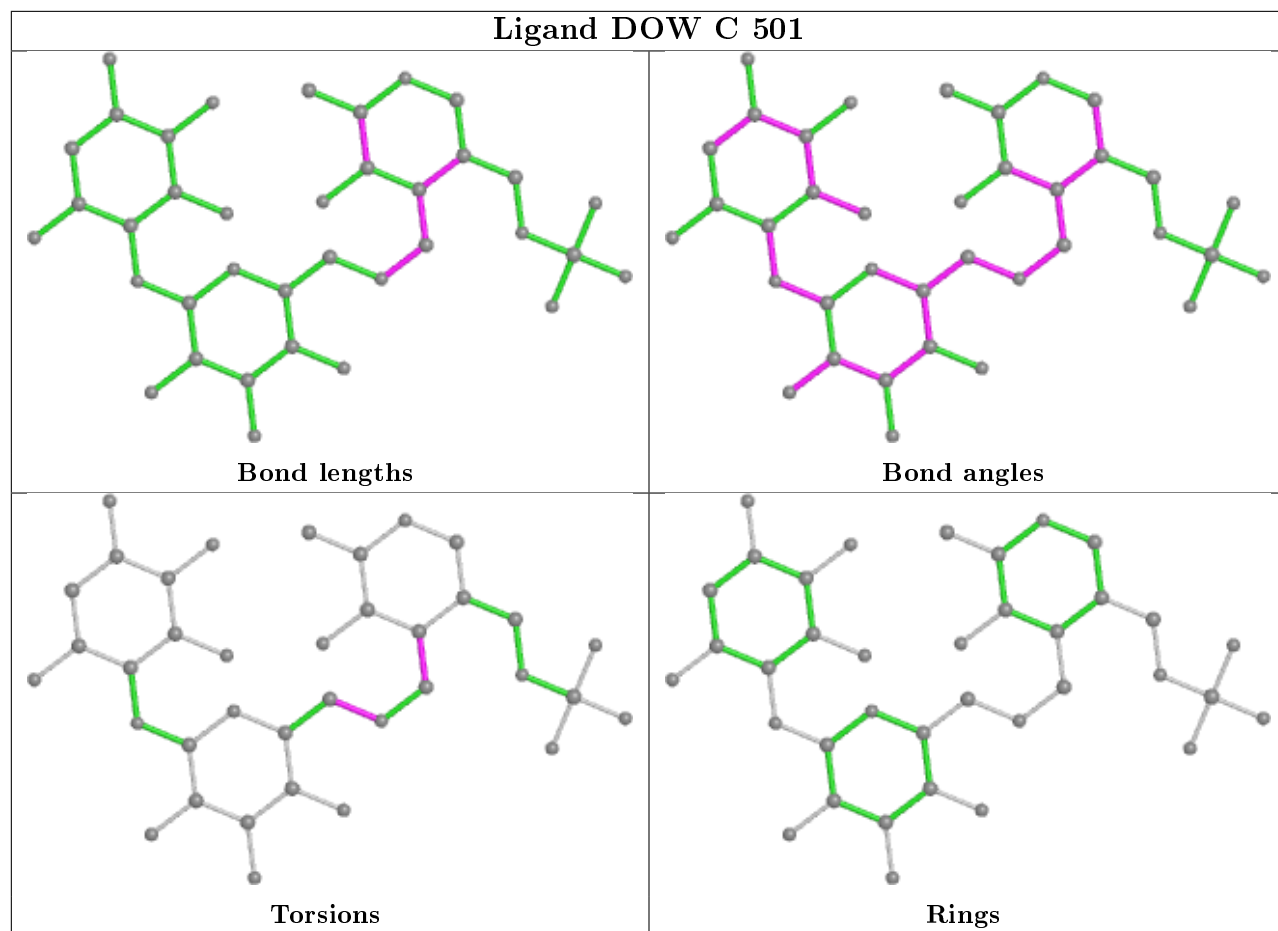
There are no ring outliers.

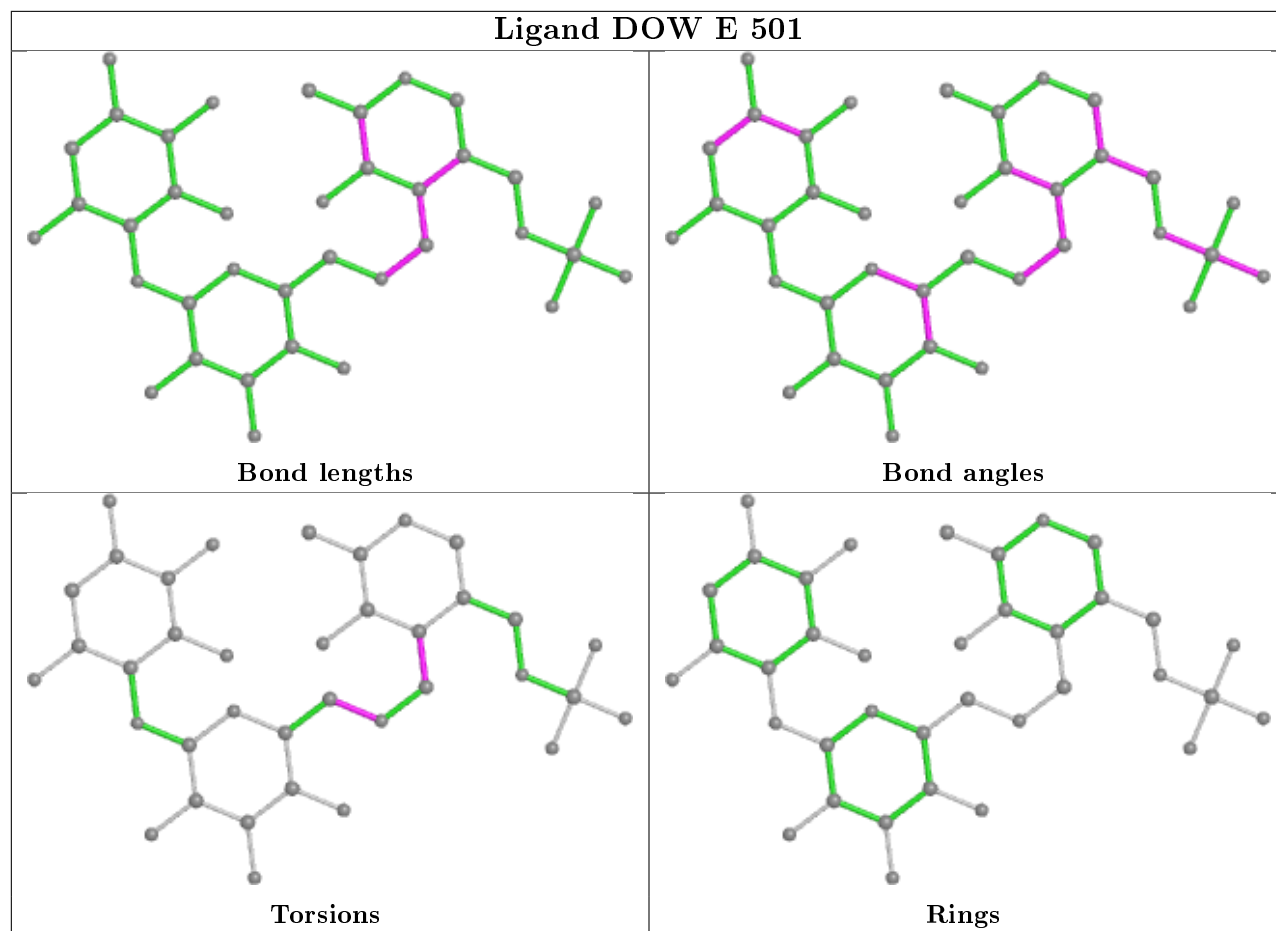
5 monomers are involved in 5 short contacts:

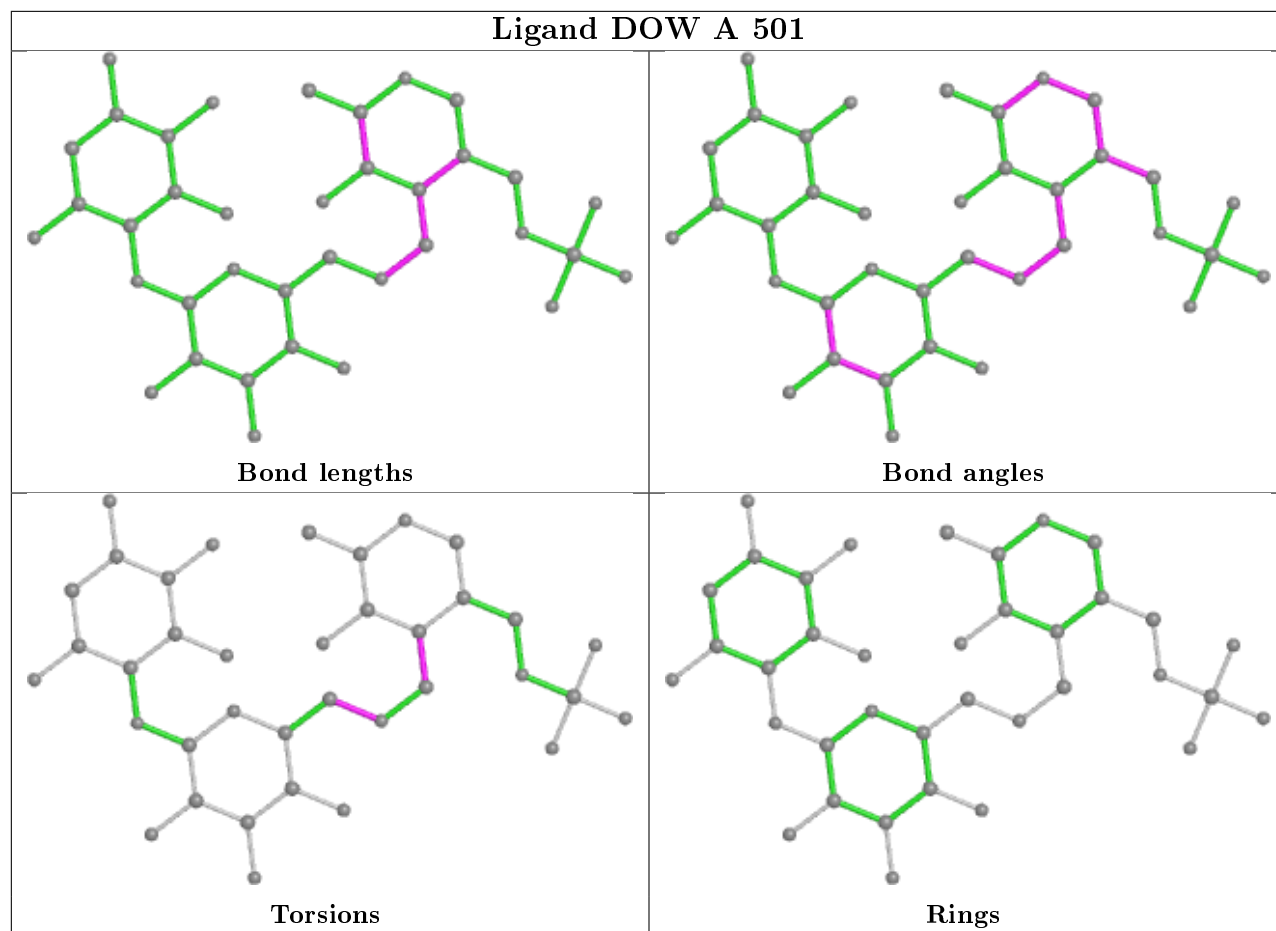
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	DOW	1	0
2	C	501	DOW	1	0
2	A	501	DOW	1	0
2	D	501	DOW	1	0
2	B	501	DOW	1	0

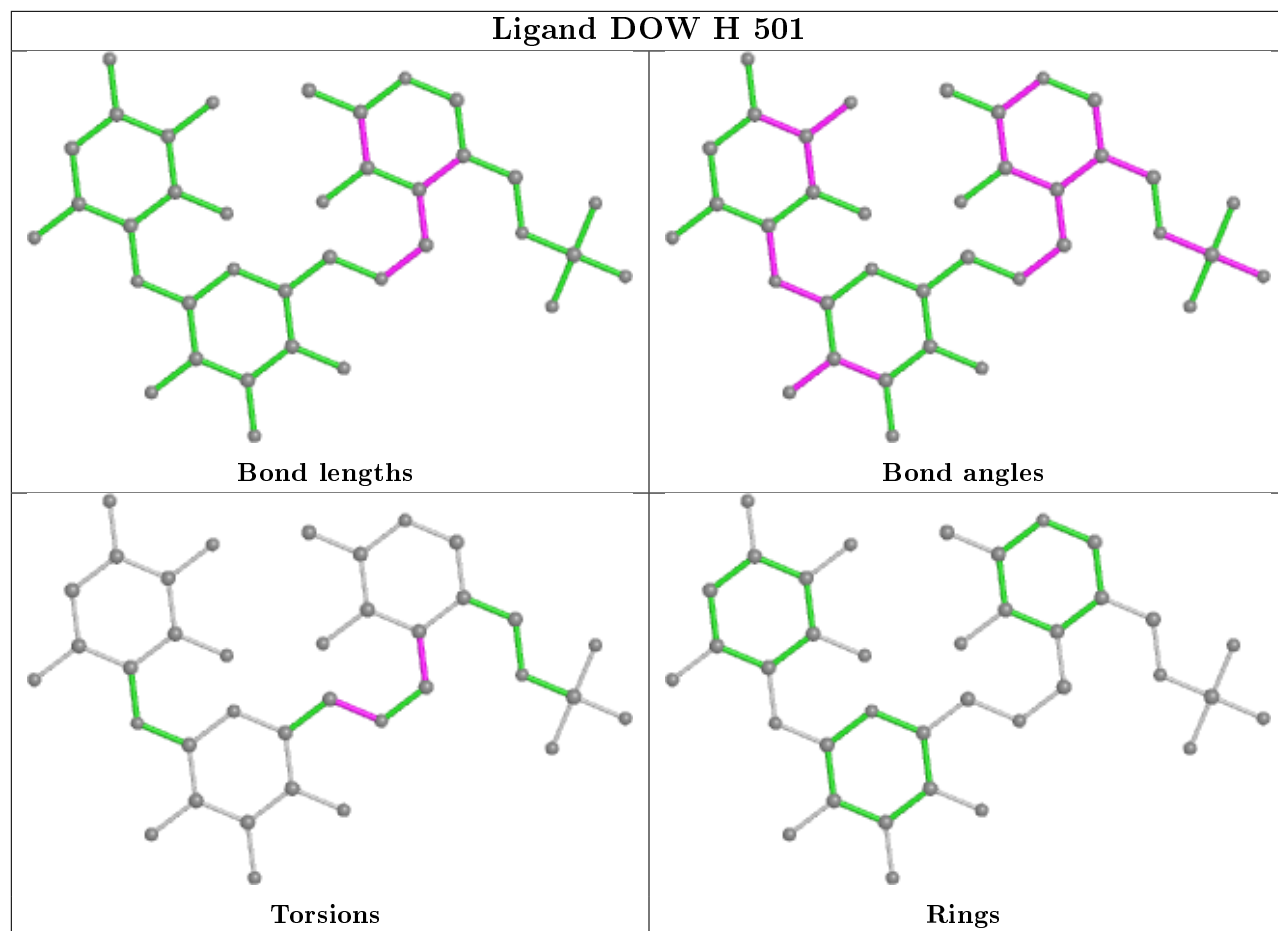
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



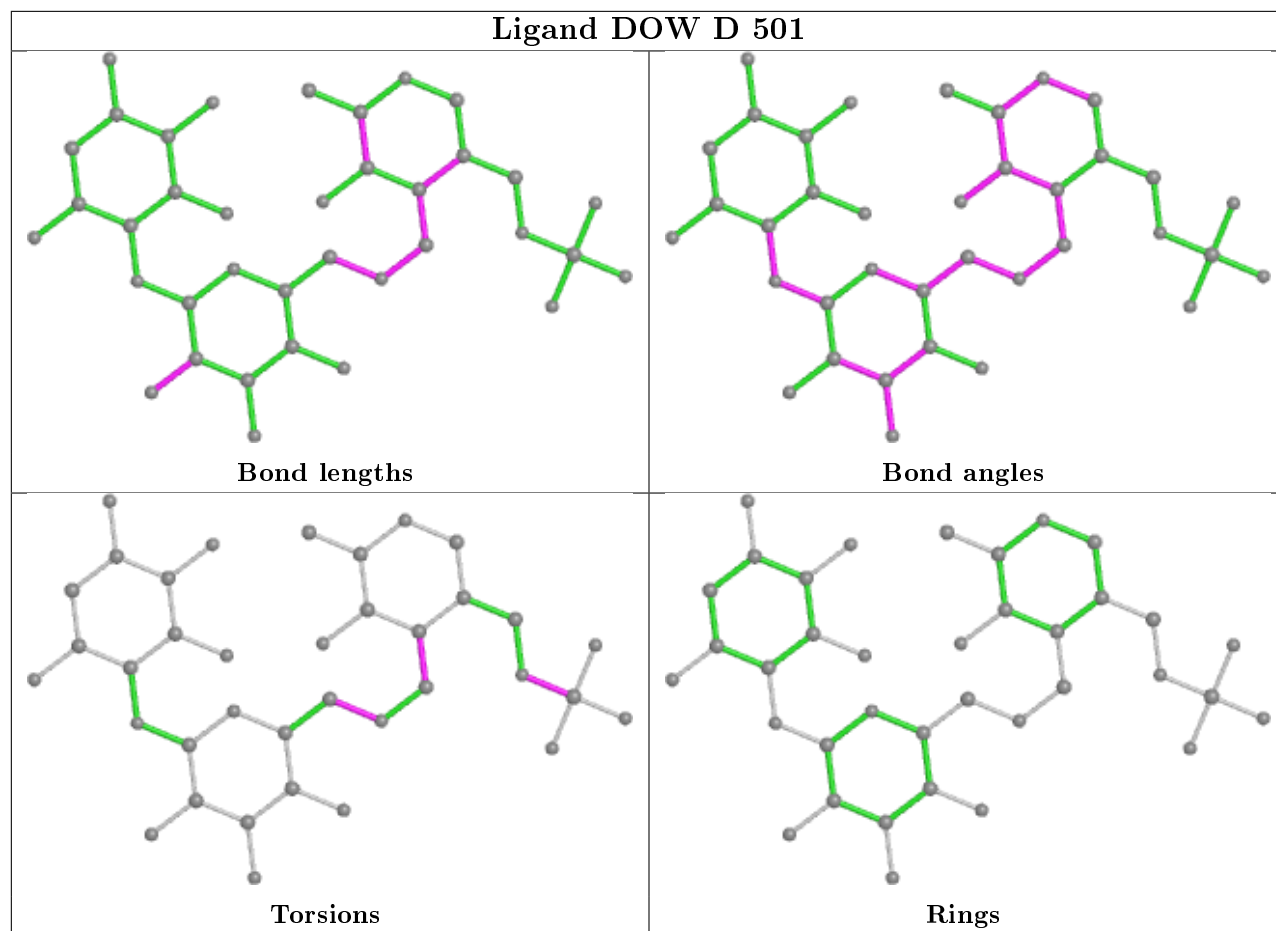


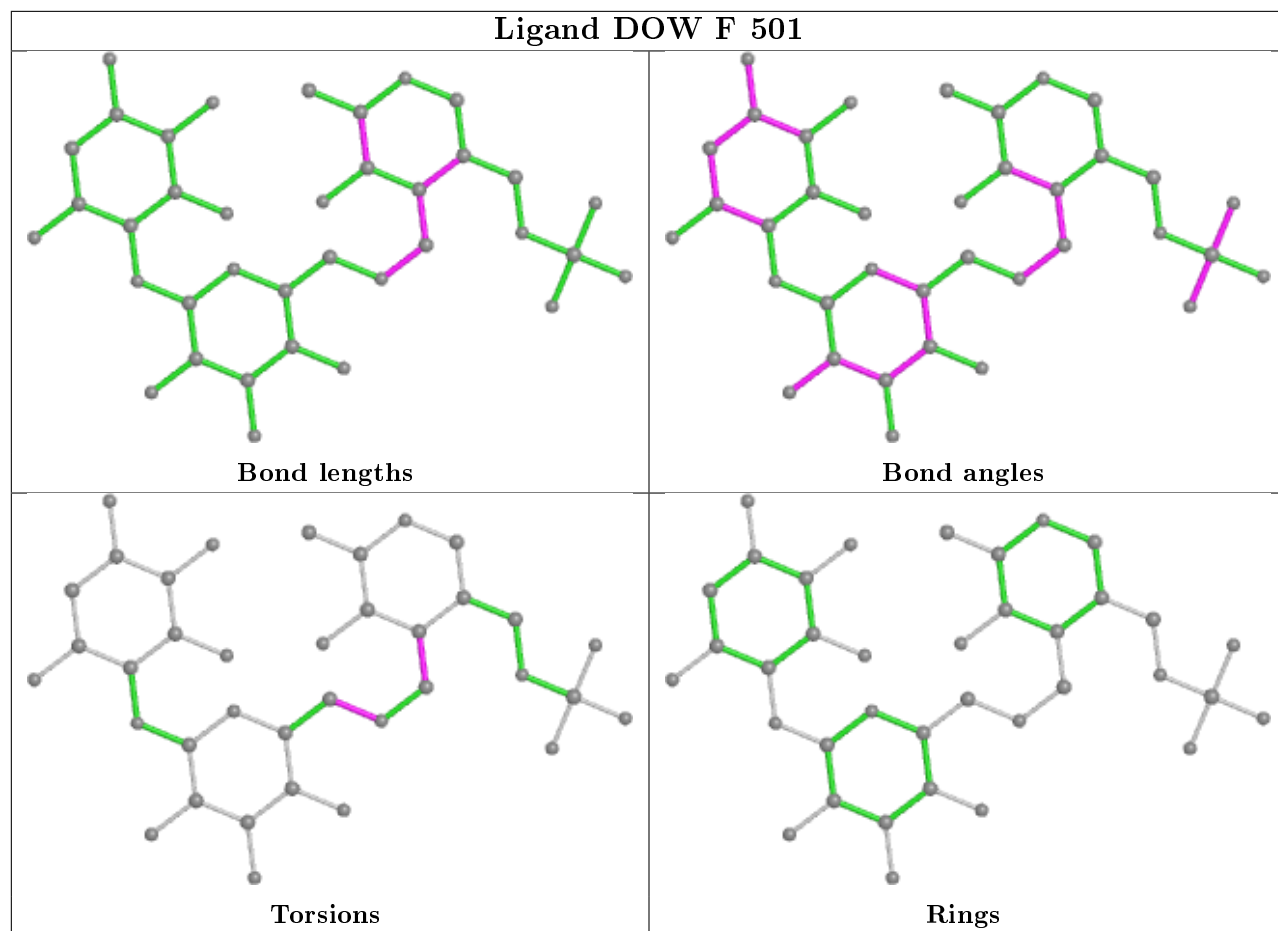


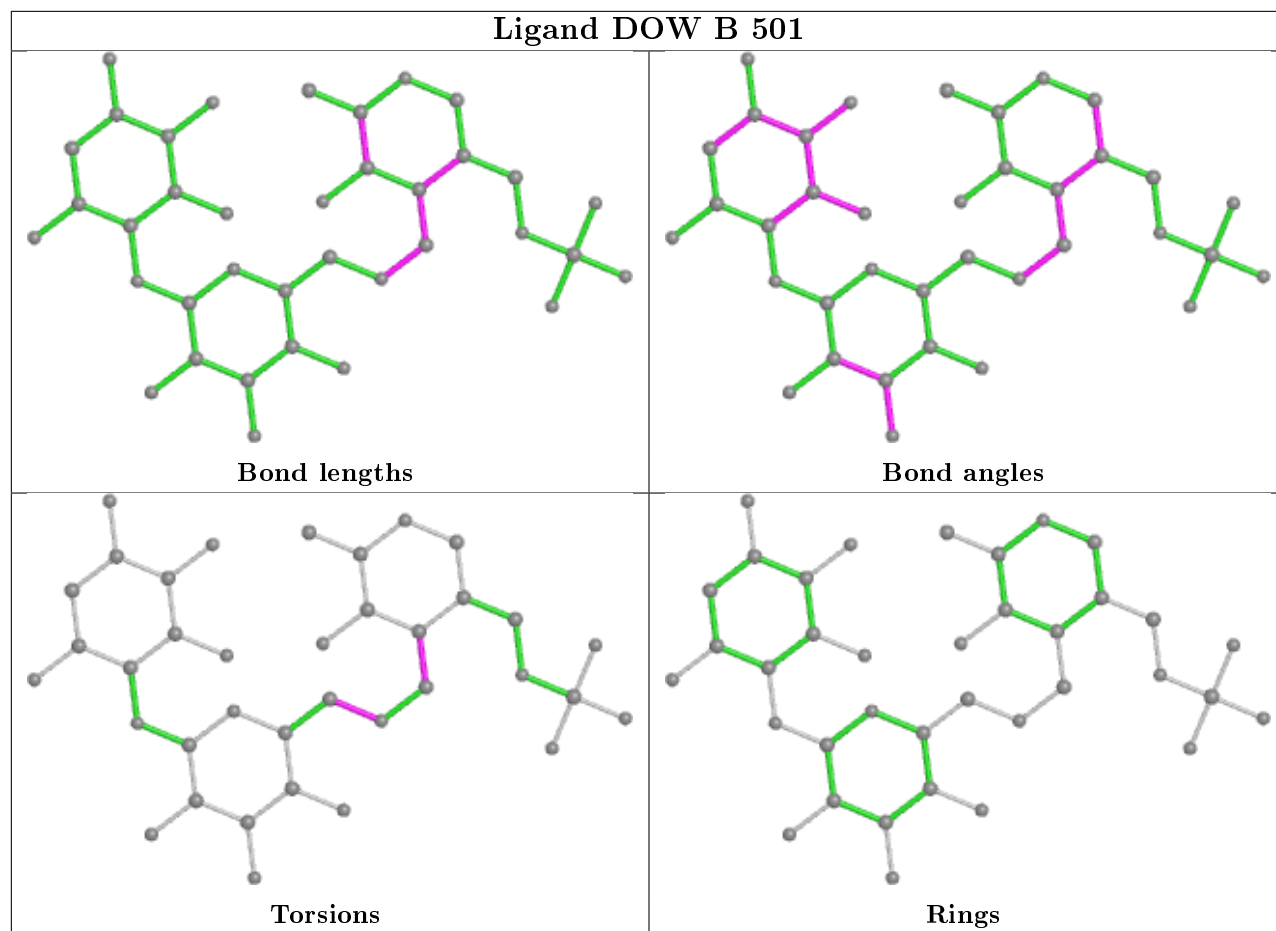












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	H	140	GLU	4.0
1	B	18	GLU	3.8
1	D	19	LYS	3.6
1	C	6	SER	3.6
1	F	19	LYS	3.6
1	H	19	LYS	3.6
1	F	140	GLU	3.6
1	F	402	ASP	3.6
1	H	21[A]	ARG	3.6
1	E	6	SER	3.5
1	E	165	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	375	ALA	3.3
1	B	372	ALA	3.3
1	F	6	SER	3.3
1	D	18	GLU	3.3
1	C	196	ALA	3.2
1	E	18	GLU	3.2
1	F	404	GLU	3.2
1	H	304	SER	3.1
1	F	373	PRO	3.1
1	H	373	PRO	3.1
1	H	6	SER	3.0
1	D	140	GLU	3.0
1	A	21	ARG	3.0
1	H	18	GLU	3.0
1	H	141	ALA	2.9
1	B	140	GLU	2.9
1	G	140	GLU	2.7
1	B	21	ARG	2.7
1	E	411	ALA	2.6
1	B	58	PRO	2.6
1	F	18	GLU	2.6
1	E	198	GLY	2.5
1	H	407	THR	2.5
1	D	21	ARG	2.5
1	A	6	SER	2.5
1	F	412	ARG	2.4
1	E	37	SER	2.4
1	F	403	ARG	2.3
1	H	414	LEU	2.3
1	G	120	GLY	2.3
1	H	142	PRO	2.2
1	B	375	ALA	2.2
1	B	20	ASP	2.2
1	D	274	ALA	2.2
1	C	21	ARG	2.2
1	H	374	TYR	2.2
1	B	376	GLY	2.2
1	B	274	ALA	2.2
1	C	378	GLU	2.1
1	H	404	GLU	2.1
1	D	372	ALA	2.1
1	B	62	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	376	GLY	2.0
1	H	411	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

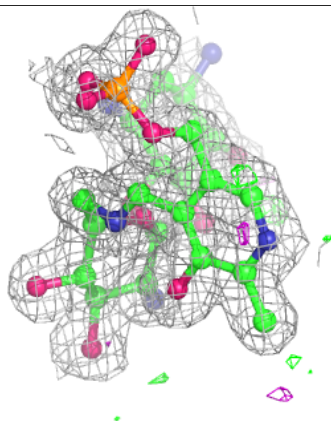
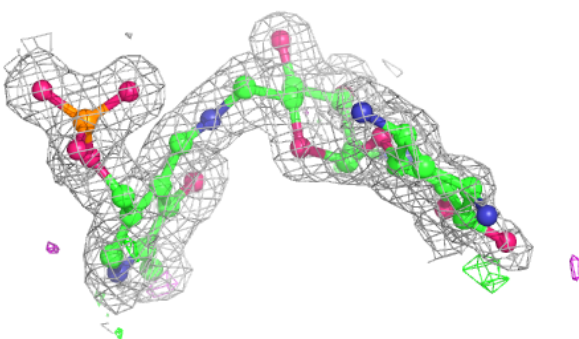
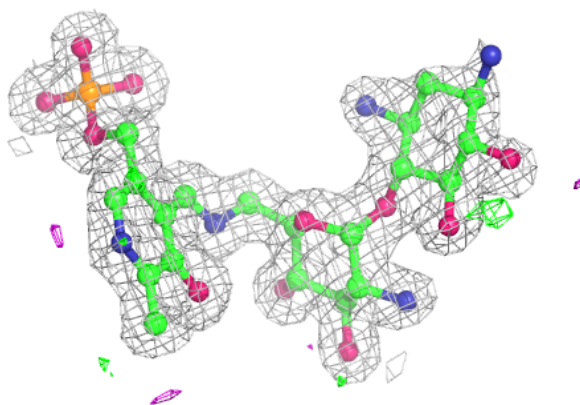
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	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

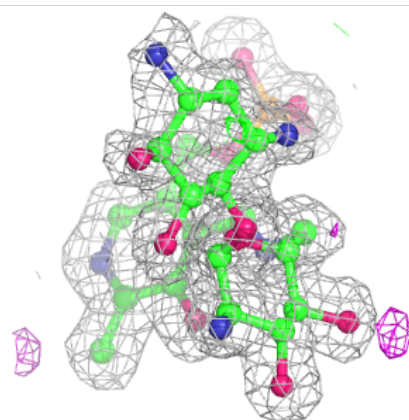
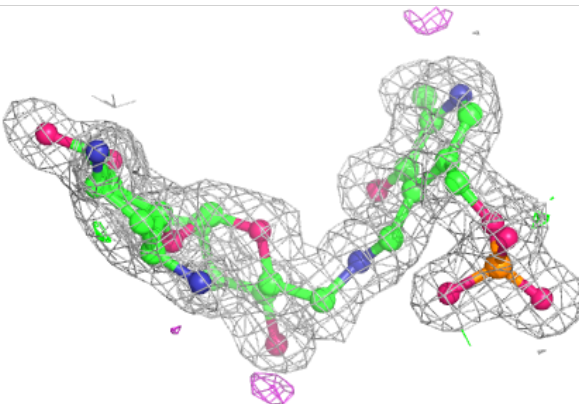
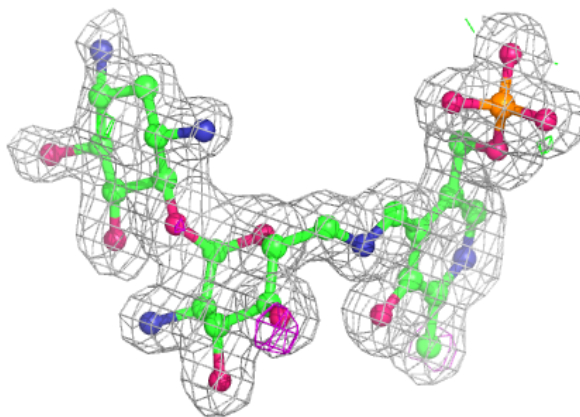
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DOW H 501:**

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

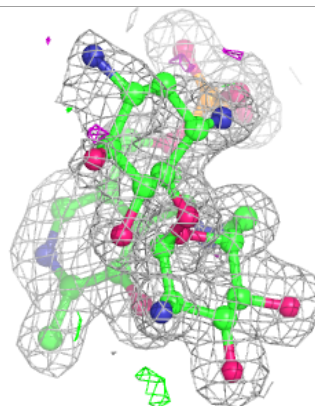
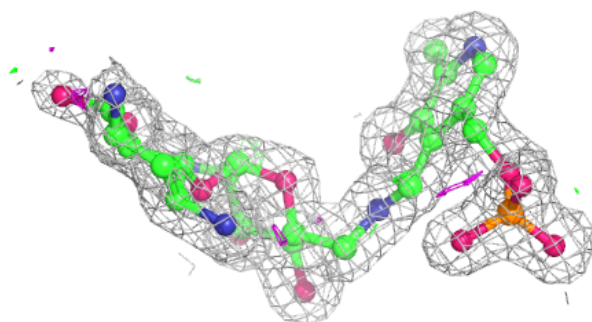
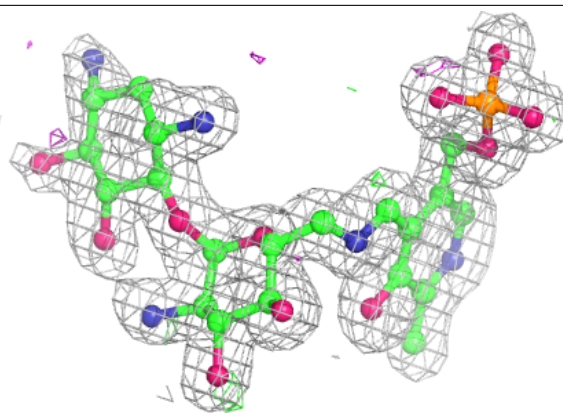
**Electron density around DOW C 501:**

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

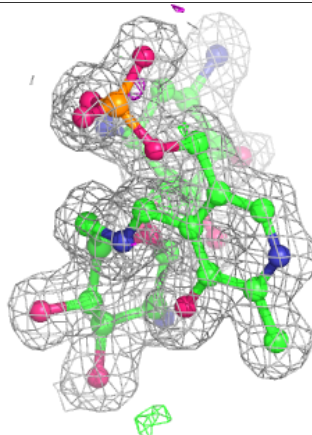
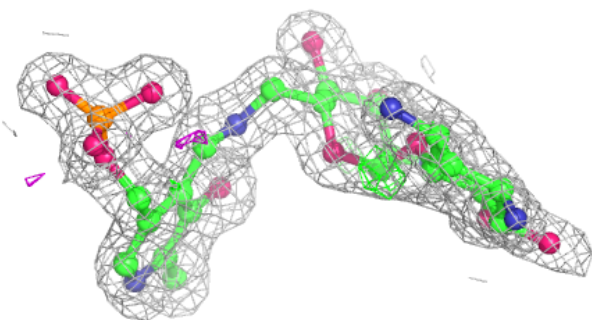
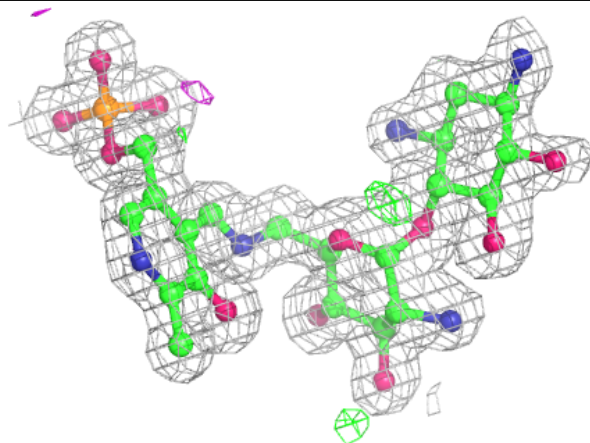


**Electron density around DOW E 501:**

$2mF_o-DF_c$  (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:**

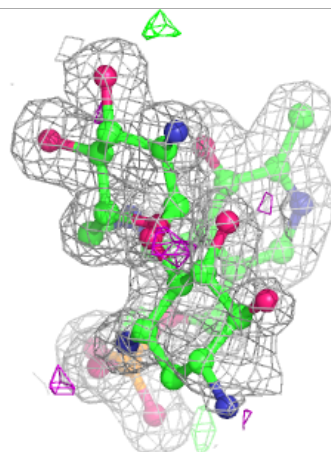
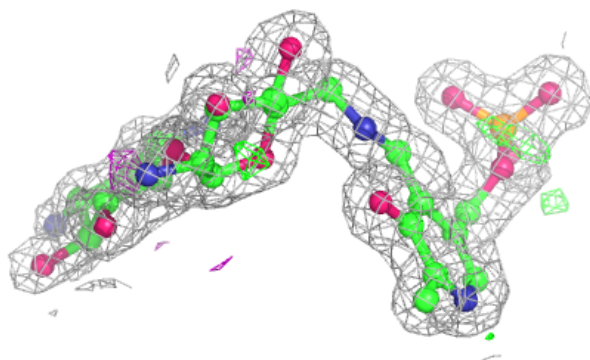
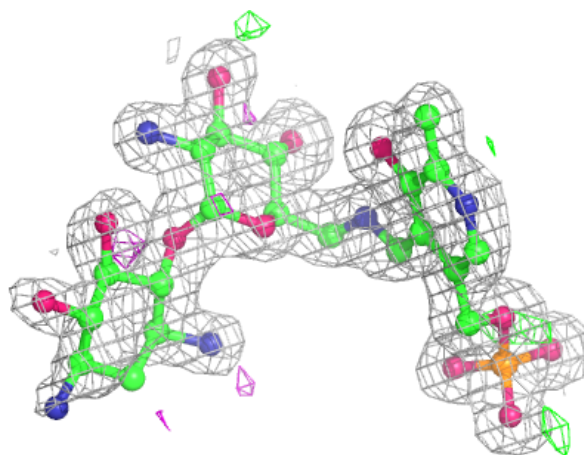
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





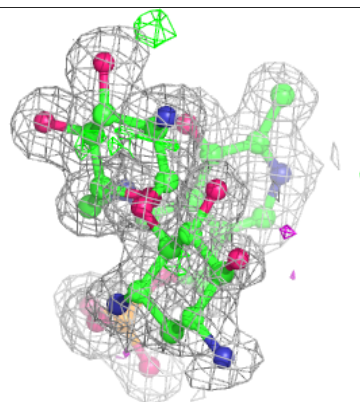
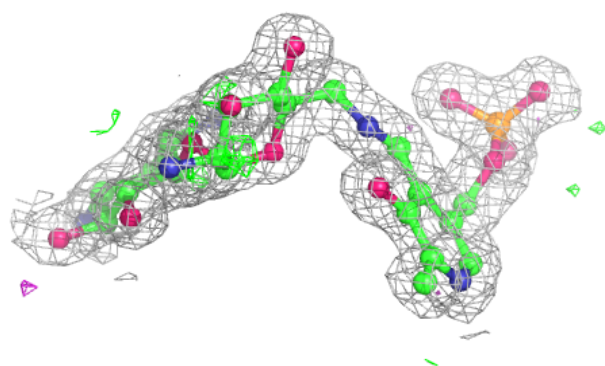
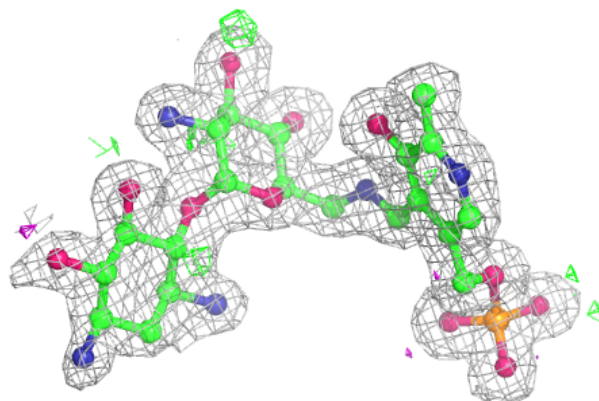
**Electron density around DOW G 501:**

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

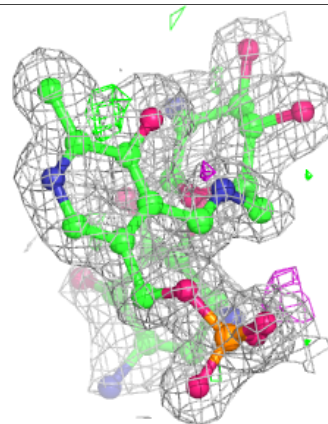
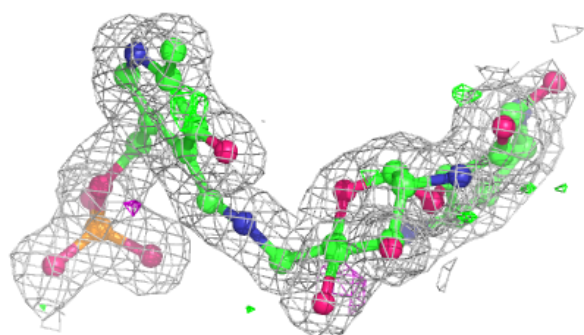
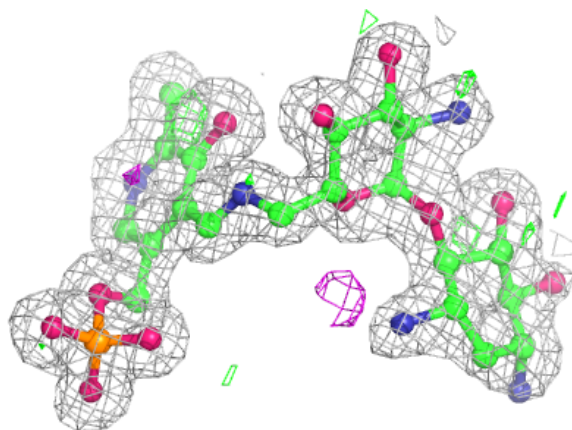


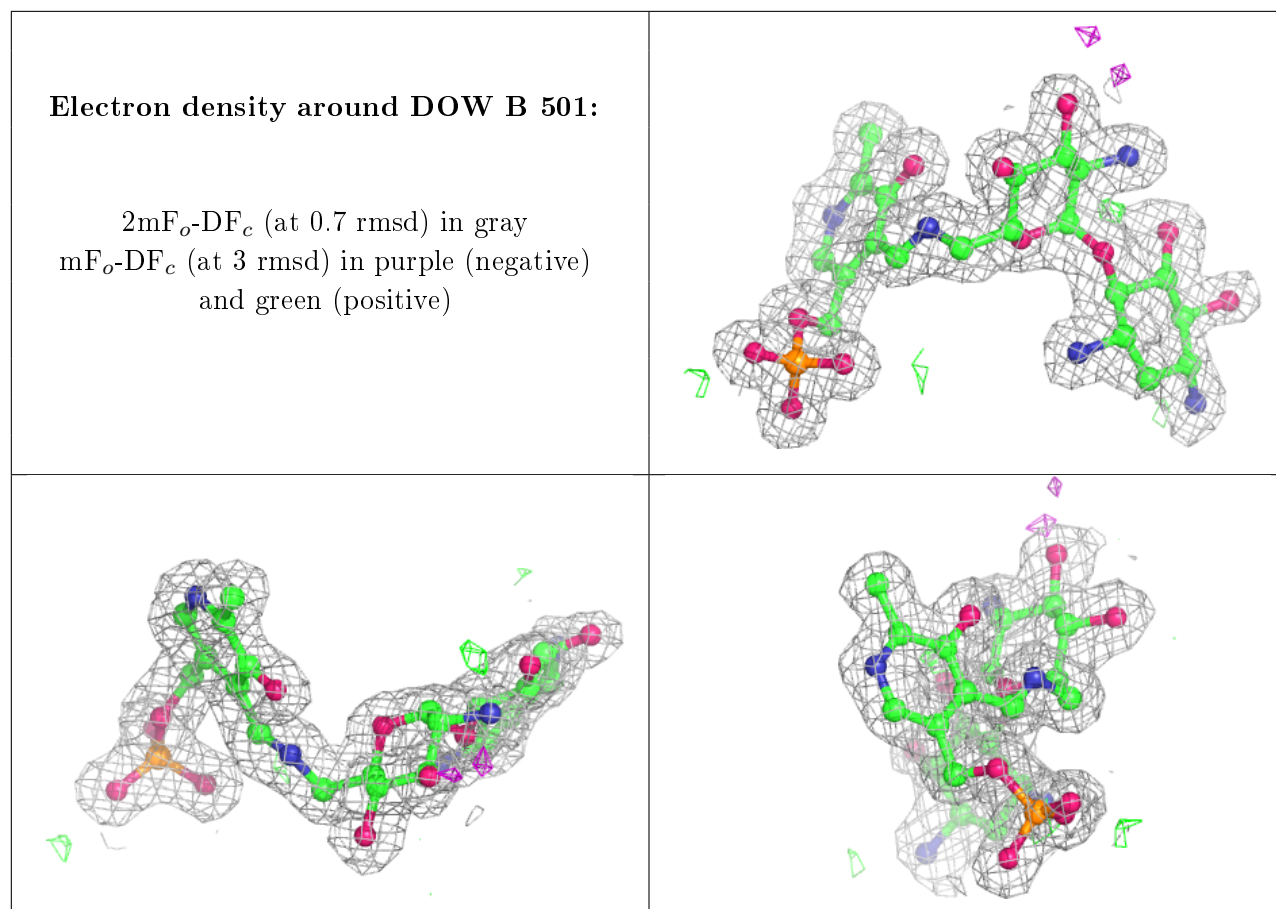
**Electron density around DOW D 501:**

$2mF_o-DF_c$  (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.