



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:47 pm BST

PDB ID : 5Y5R  
Title : Crystal structure of a novel Pyrethroid Hydrolase PytH with BIF  
Authors : Xu, D.Q.; Ran, T.T.; Wang, W.W.  
Deposited on : 2017-08-09  
Resolution : 1.90 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 : 2.11  
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) : 2.11

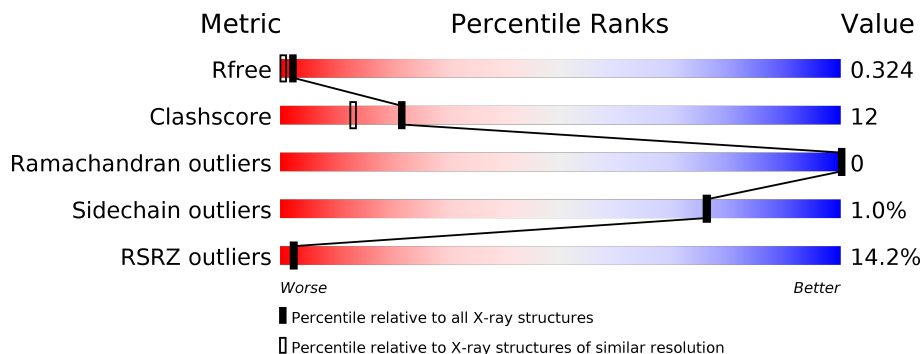
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	288	 2% 76% 11% 13%
1	B	288	 74% 13% 13%
1	C	288	 6% 70% 17% 13%
1	D	288	 5% 72% 15% 12%
1	E	288	 23% 59% 27% 13%
1	F	288	 36% 60% 26% 13%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12042 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 Pyrethroid hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	252	1914	1218	331	358	1	6	0	0	0
1	B	252	1914	1218	331	358	1	6	0	0	0
1	C	252	1908	1215	328	358	1	6	0	0	0
1	D	253	1917	1220	329	361	1	6	0	0	0
1	E	251	1887	1201	326	353	1	6	0	0	0
1	F	251	1827	1158	320	342	1	6	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

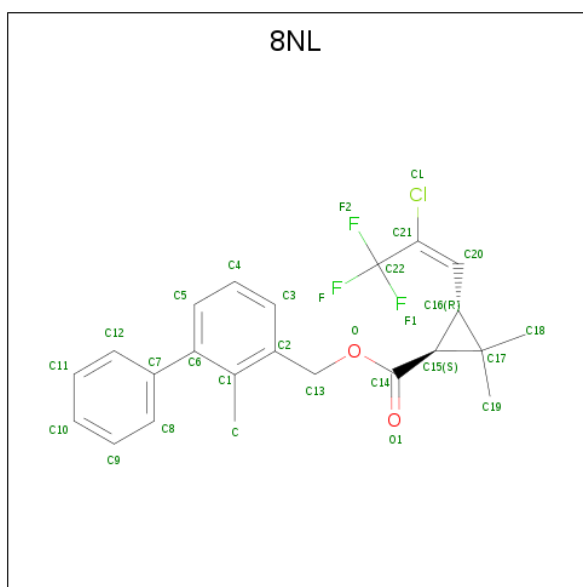
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP D0VUS3
A	281	LEU	-	expression tag	UNP D0VUS3
A	282	GLU	-	expression tag	UNP D0VUS3
A	283	HIS	-	expression tag	UNP D0VUS3
A	284	HIS	-	expression tag	UNP D0VUS3
A	285	HIS	-	expression tag	UNP D0VUS3
A	286	HIS	-	expression tag	UNP D0VUS3
A	287	HIS	-	expression tag	UNP D0VUS3
A	288	HIS	-	expression tag	UNP D0VUS3
B	1	MSE	-	initiating methionine	UNP D0VUS3
B	281	LEU	-	expression tag	UNP D0VUS3
B	282	GLU	-	expression tag	UNP D0VUS3
B	283	HIS	-	expression tag	UNP D0VUS3
B	284	HIS	-	expression tag	UNP D0VUS3
B	285	HIS	-	expression tag	UNP D0VUS3
B	286	HIS	-	expression tag	UNP D0VUS3
B	287	HIS	-	expression tag	UNP D0VUS3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	288	HIS	-	expression tag	UNP D0VUS3
C	1	MSE	-	initiating methionine	UNP D0VUS3
C	281	LEU	-	expression tag	UNP D0VUS3
C	282	GLU	-	expression tag	UNP D0VUS3
C	283	HIS	-	expression tag	UNP D0VUS3
C	284	HIS	-	expression tag	UNP D0VUS3
C	285	HIS	-	expression tag	UNP D0VUS3
C	286	HIS	-	expression tag	UNP D0VUS3
C	287	HIS	-	expression tag	UNP D0VUS3
C	288	HIS	-	expression tag	UNP D0VUS3
D	1	MSE	-	initiating methionine	UNP D0VUS3
D	281	LEU	-	expression tag	UNP D0VUS3
D	282	GLU	-	expression tag	UNP D0VUS3
D	283	HIS	-	expression tag	UNP D0VUS3
D	284	HIS	-	expression tag	UNP D0VUS3
D	285	HIS	-	expression tag	UNP D0VUS3
D	286	HIS	-	expression tag	UNP D0VUS3
D	287	HIS	-	expression tag	UNP D0VUS3
D	288	HIS	-	expression tag	UNP D0VUS3
E	1	MSE	-	initiating methionine	UNP D0VUS3
E	281	LEU	-	expression tag	UNP D0VUS3
E	282	GLU	-	expression tag	UNP D0VUS3
E	283	HIS	-	expression tag	UNP D0VUS3
E	284	HIS	-	expression tag	UNP D0VUS3
E	285	HIS	-	expression tag	UNP D0VUS3
E	286	HIS	-	expression tag	UNP D0VUS3
E	287	HIS	-	expression tag	UNP D0VUS3
E	288	HIS	-	expression tag	UNP D0VUS3
F	1	MSE	-	initiating methionine	UNP D0VUS3
F	281	LEU	-	expression tag	UNP D0VUS3
F	282	GLU	-	expression tag	UNP D0VUS3
F	283	HIS	-	expression tag	UNP D0VUS3
F	284	HIS	-	expression tag	UNP D0VUS3
F	285	HIS	-	expression tag	UNP D0VUS3
F	286	HIS	-	expression tag	UNP D0VUS3
F	287	HIS	-	expression tag	UNP D0VUS3
F	288	HIS	-	expression tag	UNP D0VUS3

- Molecule 2 is (2-methyl-3-phenyl-phenyl)methyl (1 {S})-3-[( {E})-2-chloranyl-3,3,3-tris(fluoranyl)prop-1-enyl]-2,2-dimethyl-cyclopropane-1-carboxylate (three-letter code: 8NL) (formula: C<sub>23</sub>H<sub>22</sub>ClF<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	F	O		
2	A	1	29	23	1	3	2	0	0
2	B	1	29	23	1	3	2	0	0
2	C	1	29	23	1	3	2	0	0
2	D	1	29	23	1	3	2	0	0
2	E	1	29	23	1	3	2	0	0
2	F	1	29	23	1	3	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

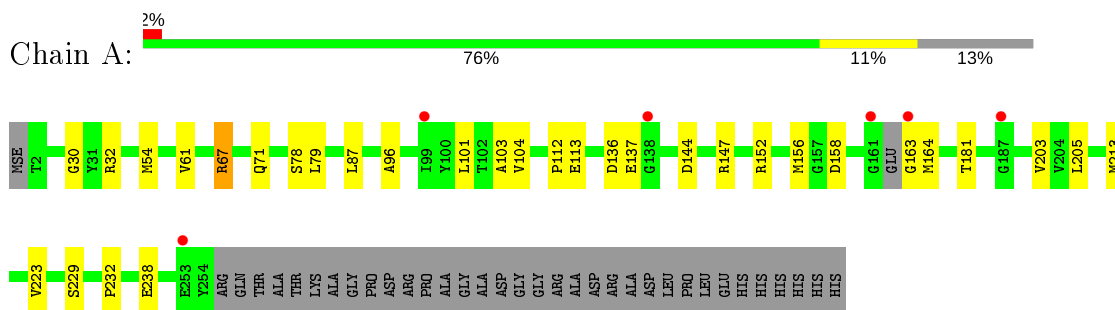
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	108	Total	O	0	0
			108	108		
4	C	74	Total	O	0	0
			74	74		
4	D	82	Total	O	0	0
			82	82		
4	E	57	Total	O	0	0
			57	57		
4	F	42	Total	O	0	0
			42	42		

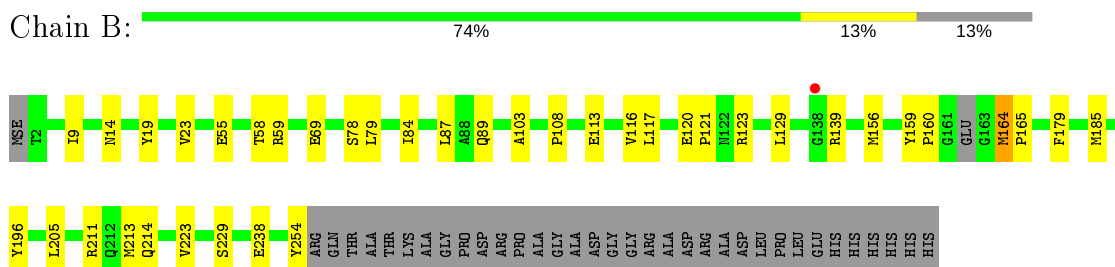
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

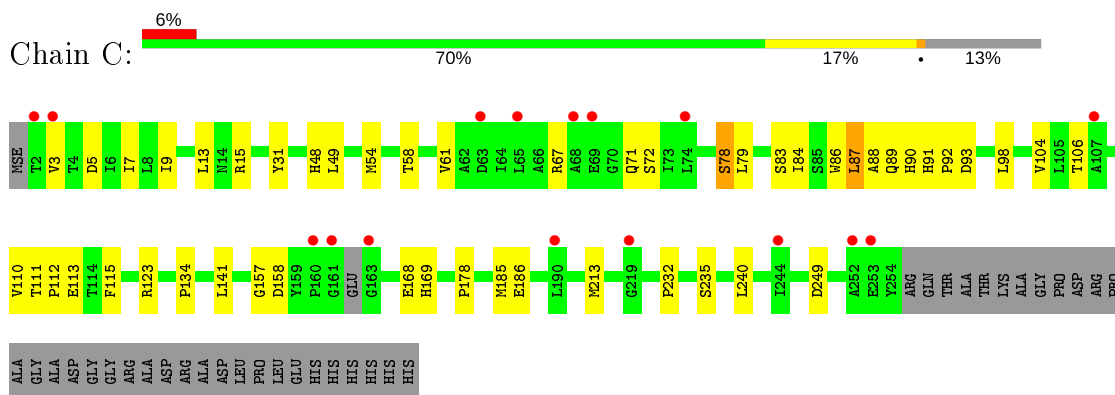
- Molecule 1: Pyrethroid hydrolase



- Molecule 1: Pyrethroid hydrolase

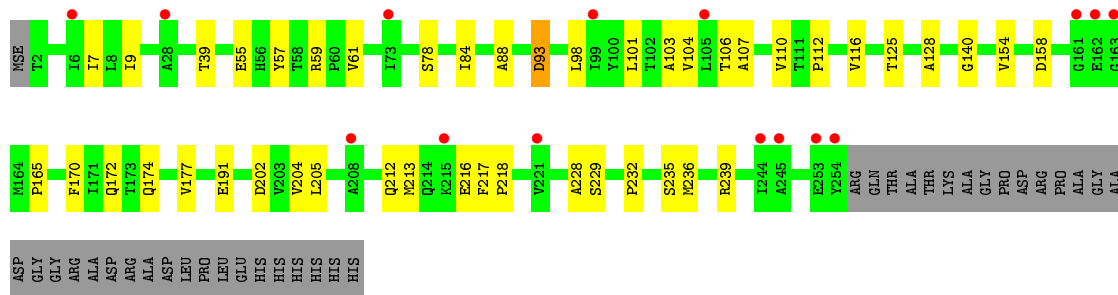


- Molecule 1: Pyrethroid hydrolase

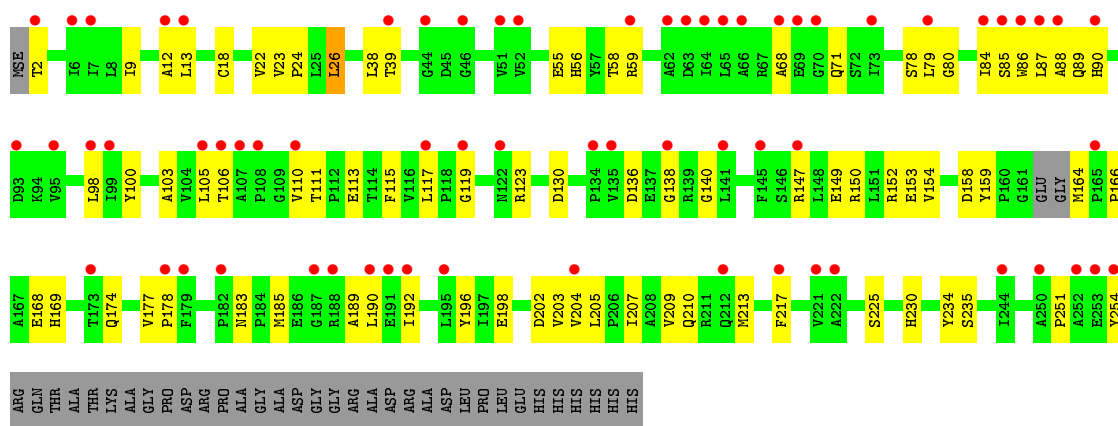


- Molecule 1: Pyrethroid hydrolase

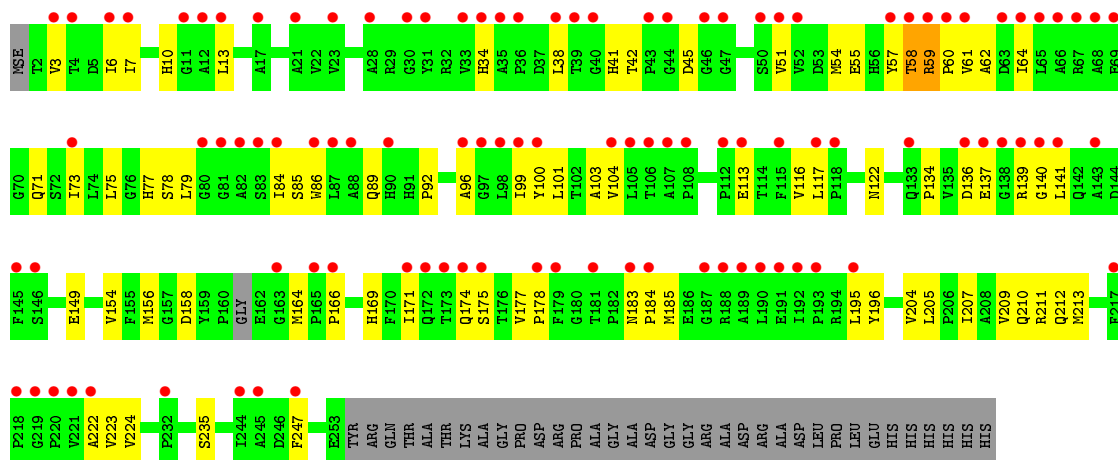




• Molecule 1: Pyrethroid hydrolase



• Molecule 1: Pyrethroid hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.86Å 168.86Å 123.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.90 19.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.91-1.90) 99.5 (19.91-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (dev_2247: ???)	Depositor
R, $R_{free}$	0.273 , 0.322 0.277 , 0.324	Depositor DCC
$R_{free}$ test set	7013 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 8NL

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	0.57	0/1960	0.71	0/2672
1	B	0.56	0/1960	0.68	0/2672
1	C	0.48	0/1954	0.66	0/2665
1	D	0.55	0/1964	0.72	0/2680
1	E	0.50	0/1934	0.71	0/2642
1	F	0.49	0/1872	0.71	0/2559
All	All	0.53	0/11644	0.70	0/15890

There are no bond length outliers.

There are no bond angle outliers.

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	1914	0	1876	21	0
1	B	1914	0	1876	29	0
1	C	1908	0	1865	33	0
1	D	1917	0	1872	33	0
1	E	1887	0	1827	72	1
1	F	1827	0	1706	82	1
2	A	29	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	0	2	0
2	C	29	0	0	1	0
2	D	29	0	0	3	0
2	E	29	0	0	2	0
2	F	29	0	0	6	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	108	0	0	4	0
4	B	108	0	0	6	1
4	C	74	0	0	4	0
4	D	82	0	0	5	0
4	E	57	0	0	8	0
4	F	42	0	0	5	1
All	All	12042	0	11022	268	2

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 12.

All (268) 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:F:78:SER:OG	2:F:301:8NL:C17	2.00	1.09
1:F:78:SER:OG	2:F:301:8NL:C19	2.01	1.08
1:F:54:MSE:CE	1:F:57:TYR:HB3	1.91	1.00
1:F:104:VAL:HG23	1:F:213:MSE:HE1	1.42	0.98
1:F:54:MSE:O	1:F:58:THR:OG1	1.85	0.93
1:F:54:MSE:HA	1:F:54:MSE:HE3	1.52	0.92
1:E:204:VAL:HG21	1:E:230:HIS:CD2	2.07	0.88
1:E:202:ASP:OD1	1:E:204:VAL:HG22	1.74	0.88
1:F:54:MSE:HE3	1:F:57:TYR:HB3	1.56	0.86
1:F:177:VAL:HG23	1:F:178:PRO:HD3	1.59	0.84
1:F:54:MSE:HE1	1:F:57:TYR:HB3	1.60	0.82
1:F:104:VAL:HG23	1:F:213:MSE:CE	2.10	0.81
1:E:205:LEU:CD1	1:E:209:VAL:HB	2.11	0.80
1:F:78:SER:HG	2:F:301:8NL:C19	1.92	0.80
1:E:204:VAL:HG21	1:E:230:HIS:CG	2.18	0.78
1:F:222:ALA:HA	4:F:405:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:GLN:HB3	1:F:96:ALA:HB2	1.68	0.76
1:E:9:ILE:HD12	1:E:84:ILE:HG22	1.66	0.75
1:F:78:SER:OG	2:F:301:8NL:C15	2.35	0.74
1:F:122:ASN:HD22	1:F:212:GLN:NE2	1.88	0.72
1:D:228:ALA:HB2	1:D:236:MSE:HE3	1.71	0.72
1:F:209:VAL:O	1:F:213:MSE:HG3	1.90	0.72
1:E:12:ALA:HB3	2:E:301:8NL:O1	1.90	0.71
1:F:51:VAL:HG11	1:F:177:VAL:HG21	1.74	0.70
1:B:55:GLU:OE1	1:B:59:ARG:NH2	2.18	0.70
1:F:185:MSE:O	4:F:401:HOH:O	2.11	0.69
1:E:78:SER:HA	1:E:103:ALA:HA	1.73	0.69
1:F:55:GLU:HA	1:F:86:TRP:CH2	2.28	0.69
1:F:58:THR:HG21	1:F:86:TRP:CE3	2.27	0.69
1:D:9:ILE:HD12	1:D:84:ILE:HG22	1.73	0.69
1:F:86:TRP:CD1	1:F:184:PRO:HG3	2.28	0.69
1:E:89:GLN:HB2	1:E:185:MSE:HA	1.75	0.68
1:A:30:GLY:O	4:A:401:HOH:O	2.09	0.68
1:F:205:LEU:CD2	1:F:210:GLN:HG3	2.24	0.68
1:F:42:THR:O	1:F:45:ASP:HB2	1.93	0.68
1:E:106:THR:HB	1:E:110:VAL:HB	1.76	0.67
1:F:99:ILE:HD11	1:F:247:PHE:CD2	2.29	0.67
1:E:254:TYR:O	4:E:401:HOH:O	2.11	0.67
1:F:104:VAL:CG2	1:F:213:MSE:HE1	2.22	0.66
1:C:78:SER:OG	2:C:301:8NL:C14	2.43	0.66
1:F:54:MSE:CA	1:F:54:MSE:HE3	2.26	0.66
1:B:9:ILE:HD12	1:B:84:ILE:HG22	1.78	0.65
1:E:111:THR:HG23	4:E:405:HOH:O	1.95	0.64
1:F:223:VAL:N	4:F:405:HOH:O	2.26	0.64
1:C:88:ALA:HB2	1:C:98:LEU:HD21	1.79	0.64
1:B:113:GLU:HB2	1:B:117:LEU:HD12	1.79	0.63
1:C:83:SER:O	1:C:87:LEU:HD12	1.98	0.63
1:F:45:ASP:OD1	4:F:402:HOH:O	2.15	0.63
1:E:23:VAL:HG23	1:E:24:PRO:HD3	1.81	0.62
1:E:204:VAL:CG2	1:E:230:HIS:CG	2.82	0.62
1:B:164:MSE:HB2	1:B:165:PRO:CD	2.29	0.62
1:D:239:ARG:HG3	3:D:302:SO4:O2	1.99	0.62
1:E:85:SER:HB2	1:E:185:MSE:SE	2.50	0.61
1:D:55:GLU:O	4:D:401:HOH:O	2.16	0.61
1:E:198:GLU:OE2	1:E:225:SER:OG	2.15	0.61
1:E:204:VAL:HG21	1:E:230:HIS:CE1	2.34	0.61
1:F:57:TYR:CE2	1:F:178:PRO:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ASP:HB3	1:E:235:SER:HB3	1.82	0.61
1:F:86:TRP:HA	1:F:184:PRO:HG2	1.81	0.60
1:E:100:TYR:HB3	1:E:103:ALA:HB3	1.82	0.59
1:E:2:THR:HG22	1:E:71:GLN:HG3	1.85	0.59
1:F:104:VAL:HA	1:F:213:MSE:HE1	1.83	0.59
1:A:137:GLU:OE1	1:A:137:GLU:N	2.36	0.59
1:B:78:SER:HA	1:B:103:ALA:HA	1.84	0.59
1:F:137:GLU:O	4:F:403:HOH:O	2.17	0.58
1:B:156:MSE:SE	1:B:164:MSE:HE3	2.52	0.58
1:F:207:ILE:HA	1:F:210:GLN:HE21	1.66	0.58
1:B:164:MSE:HB2	1:B:165:PRO:HD2	1.86	0.57
1:D:93:ASP:N	1:D:93:ASP:OD1	2.26	0.57
1:F:205:LEU:HD23	1:F:210:GLN:HG3	1.85	0.57
1:C:79:LEU:HD21	1:C:178:PRO:HG2	1.87	0.57
1:B:58:THR:HB	1:B:87:LEU:HD21	1.86	0.57
1:E:204:VAL:HG21	1:E:230:HIS:NE2	2.19	0.57
1:C:104:VAL:HG11	1:C:112:PRO:HB3	1.87	0.57
1:E:130:ASP:OD2	1:E:147:ARG:NH1	2.28	0.56
1:F:99:ILE:HD12	1:F:195:LEU:HD23	1.86	0.56
1:C:48:HIS:ND1	4:C:405:HOH:O	2.33	0.56
1:F:34:HIS:CD2	1:F:64:ILE:HD11	2.41	0.56
1:B:19:TYR:O	1:B:23:VAL:HG23	2.06	0.56
1:E:106:THR:OG1	4:E:402:HOH:O	2.12	0.56
1:E:89:GLN:HA	1:E:189:ALA:HB2	1.88	0.56
1:E:150:ARG:NH1	1:E:153:GLU:OE1	2.38	0.55
1:D:202:ASP:OD1	1:D:204:VAL:N	2.38	0.55
1:E:22:VAL:HG12	1:E:26:LEU:HD22	1.88	0.55
1:F:54:MSE:HA	1:F:54:MSE:CE	2.32	0.55
1:F:116:VAL:HG22	2:F:301:8NL:CL	2.44	0.55
1:E:22:VAL:HG12	1:E:26:LEU:CD2	2.36	0.55
1:B:78:SER:HB2	2:B:301:8NL:C19	2.37	0.54
1:E:115:PHE:CB	1:E:213:MSE:HE2	2.38	0.54
1:F:54:MSE:HE2	1:F:58:THR:OG1	2.07	0.54
1:F:75:LEU:HA	1:F:99:ILE:HB	1.91	0.53
1:A:78:SER:OG	1:A:79:LEU:N	2.41	0.53
1:D:106:THR:HB	1:D:110:VAL:HB	1.90	0.53
1:A:54:MSE:HG3	1:A:181:THR:HG21	1.91	0.53
1:D:191:GLU:OE1	1:F:59:ARG:NH2	2.42	0.53
1:D:128:ALA:HB3	2:D:301:8NL:CL	2.46	0.52
1:C:158:ASP:HB3	1:C:235:SER:HB3	1.92	0.52
1:C:15:ARG:HD3	1:C:168:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:SER:OG	1:F:177:VAL:HG22	2.10	0.52
1:D:205:LEU:HD21	1:D:213:MSE:HE1	1.91	0.52
1:F:166:PRO:HG2	1:F:169:HIS:CD2	2.44	0.52
1:A:104:VAL:HG11	1:A:112:PRO:HB3	1.92	0.52
1:D:78:SER:HB2	2:D:301:8NL:C17	2.40	0.52
1:E:68:ALA:HA	4:E:436:HOH:O	2.08	0.52
1:A:101:LEU:HD11	1:A:232:PRO:HG2	1.91	0.52
1:F:158:ASP:HB3	1:F:235:SER:HB3	1.91	0.52
1:F:3:VAL:HG11	1:F:73:ILE:HG12	1.91	0.52
1:C:115:PHE:CE2	1:C:213:MSE:HG2	2.46	0.51
1:C:123:ARG:O	4:C:401:HOH:O	2.18	0.51
1:E:113:GLU:O	1:E:117:LEU:HD23	2.09	0.51
1:E:88:ALA:HB1	1:E:192:ILE:HD12	1.91	0.51
1:F:136:ASP:O	1:F:139:ARG:HB3	2.11	0.51
1:D:158:ASP:OD1	1:D:229:SER:OG	2.24	0.51
1:E:205:LEU:HD12	1:E:209:VAL:HB	1.89	0.51
1:E:58:THR:HB	1:E:87:LEU:HD11	1.91	0.51
1:A:136:ASP:OD1	4:A:403:HOH:O	2.19	0.50
1:E:78:SER:CA	1:E:103:ALA:HA	2.41	0.50
1:F:54:MSE:CA	1:F:54:MSE:CE	2.90	0.50
1:C:111:THR:OG1	1:C:113:GLU:HG2	2.12	0.50
1:F:154:VAL:HG12	1:F:204:VAL:HG22	1.92	0.50
1:D:165:PRO:HG2	1:D:170:PHE:HZ	1.76	0.50
1:F:84:ILE:HD11	1:F:100:TYR:CZ	2.47	0.50
1:F:134:PRO:HA	1:F:141:LEU:HD23	1.93	0.49
1:D:104:VAL:HG11	1:D:112:PRO:HB3	1.94	0.49
1:D:212:GLN:NE2	1:D:216:GLU:OE1	2.42	0.49
1:C:91:HIS:N	1:C:92:PRO:HD3	2.27	0.49
1:D:158:ASP:HB3	1:D:235:SER:HB3	1.94	0.49
1:F:10:HIS:HE1	1:F:41:HIS:CE1	2.31	0.49
1:F:58:THR:HG21	1:F:86:TRP:HE3	1.75	0.49
1:B:108:PRO:HD2	4:B:495:HOH:O	2.12	0.49
1:E:9:ILE:HG23	1:E:38:LEU:HD11	1.95	0.49
1:F:195:LEU:HD11	1:F:224:VAL:HG22	1.93	0.49
1:E:205:LEU:O	1:E:210:GLN:NE2	2.43	0.48
1:B:79:LEU:HD22	1:B:179:PHE:CE1	2.48	0.48
1:B:89:GLN:HB2	1:B:185:MSE:HA	1.94	0.48
1:A:238:GLU:HB2	3:A:302:SO4:S	2.54	0.48
1:D:7:ILE:HG21	1:D:61:VAL:HG13	1.96	0.48
1:E:205:LEU:HD12	1:E:205:LEU:C	2.34	0.48
1:E:80:GLY:O	1:E:84:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:SER:HB2	4:B:471:HOH:O	2.12	0.48
1:E:115:PHE:HB2	1:E:213:MSE:HE2	1.96	0.48
1:F:78:SER:HA	1:F:103:ALA:HA	1.96	0.48
1:D:177:VAL:HG23	4:D:405:HOH:O	2.13	0.48
1:F:89:GLN:O	1:F:92:PRO:HD3	2.13	0.48
1:D:107:ALA:HA	1:D:217:PHE:CD1	2.48	0.48
1:F:122:ASN:HD22	1:F:212:GLN:HE21	1.61	0.48
1:D:172:GLN:NE2	4:D:407:HOH:O	2.36	0.48
1:B:254:TYR:C	4:B:464:HOH:O	2.51	0.47
1:E:152:ARG:HG3	1:E:164:MSE:HG2	1.95	0.47
1:C:3:VAL:HG23	1:C:31:TYR:HE1	1.79	0.47
1:D:39:THR:HB	1:D:57:TYR:HA	1.95	0.47
1:E:12:ALA:HB2	1:E:79:LEU:HD22	1.96	0.47
1:A:78:SER:HA	1:A:103:ALA:HA	1.97	0.47
1:C:115:PHE:CZ	1:C:213:MSE:HG2	2.50	0.47
1:F:51:VAL:CG1	1:F:177:VAL:HG21	2.43	0.47
1:E:154:VAL:HG12	1:E:204:VAL:CG1	2.44	0.47
1:E:204:VAL:HG21	1:E:230:HIS:ND1	2.30	0.47
1:E:88:ALA:HB2	1:E:98:LEU:HD21	1.97	0.47
1:F:196:TYR:O	1:F:223:VAL:HA	2.15	0.47
1:E:207:ILE:HD12	1:E:207:ILE:HA	1.72	0.47
1:C:67:ARG:O	1:C:67:ARG:HG2	2.15	0.47
1:C:7:ILE:HG21	1:C:61:VAL:HG13	1.96	0.47
1:D:101:LEU:HD11	1:D:232:PRO:HG2	1.97	0.47
1:B:116:VAL:HG12	1:B:129:LEU:HD21	1.97	0.46
1:F:134:PRO:HA	1:F:140:GLY:O	2.15	0.46
1:D:125:THR:OG1	2:D:301:8NL:CL	2.58	0.46
1:E:149:GLU:O	1:E:153:GLU:HG3	2.15	0.46
1:E:86:TRP:O	1:E:90:HIS:ND1	2.39	0.46
1:D:116:VAL:HG13	1:D:125:THR:OG1	2.15	0.46
1:D:229:SER:HB2	4:D:451:HOH:O	2.15	0.46
1:F:207:ILE:HD11	1:F:211:ARG:HH21	1.80	0.46
1:B:14:ASN:ND2	4:B:409:HOH:O	2.41	0.46
1:C:89:GLN:OE1	1:C:185:MSE:HA	2.16	0.46
1:E:18:CYS:HA	1:E:169:HIS:ND1	2.31	0.46
1:F:13:LEU:HD12	1:F:174:GLN:HB2	1.98	0.46
1:C:79:LEU:O	1:C:79:LEU:HG	2.15	0.46
1:E:154:VAL:HG13	1:E:203:VAL:HG23	1.98	0.46
1:E:111:THR:N	4:E:405:HOH:O	2.49	0.46
1:E:113:GLU:HB2	1:E:117:LEU:HD23	1.98	0.46
1:E:23:VAL:HG23	1:E:24:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ILE:HA	1:F:210:GLN:NE2	2.30	0.46
1:F:156:MSE:SE	1:F:164:MSE:HE2	2.66	0.45
1:F:77:HIS:HA	1:F:101:LEU:O	2.16	0.45
1:C:72:SER:N	4:C:410:HOH:O	2.50	0.45
1:C:157:GLY:N	4:C:411:HOH:O	2.49	0.45
1:F:174:GLN:HG3	1:F:175:SER:O	2.16	0.45
1:A:78:SER:HB2	2:A:301:8NL:C18	2.46	0.45
1:B:196:TYR:O	1:B:223:VAL:HA	2.17	0.45
1:B:78:SER:HG	2:B:301:8NL:C14	2.25	0.45
1:F:99:ILE:HD11	1:F:247:PHE:CE2	2.51	0.45
1:A:158:ASP:OD2	1:A:229:SER:OG	2.22	0.45
1:D:140:GLY:HA2	1:D:174:GLN:O	2.16	0.45
1:E:177:VAL:N	1:E:178:PRO:HD2	2.32	0.44
1:D:128:ALA:HB2	1:D:204:VAL:HG13	1.99	0.44
1:E:204:VAL:CG2	1:E:230:HIS:ND1	2.81	0.44
1:B:205:LEU:HD21	1:B:213:MSE:HE1	1.99	0.44
1:A:144:ASP:OD2	1:A:147:ARG:NH2	2.46	0.44
1:B:214:GLN:NE2	4:B:404:HOH:O	2.30	0.44
1:E:140:GLY:HA2	1:E:174:GLN:O	2.18	0.43
1:D:110:VAL:HA	4:D:416:HOH:O	2.18	0.43
1:E:190:LEU:HA	1:E:190:LEU:HD23	1.70	0.43
1:B:159:TYR:CD1	1:B:160:PRO:HD2	2.53	0.43
1:A:205:LEU:HD21	1:A:213:MSE:HE1	1.99	0.43
1:C:86:TRP:CE2	1:C:90:HIS:CE1	3.06	0.43
1:F:104:VAL:HA	1:F:213:MSE:CE	2.48	0.43
1:F:177:VAL:HG23	1:F:178:PRO:CD	2.40	0.43
1:A:163:GLY:C	1:A:164:MSE:HG3	2.39	0.43
1:D:88:ALA:HB2	1:D:98:LEU:HD21	2.01	0.43
1:F:85:SER:HB2	1:F:185:MSE:SE	2.69	0.43
1:A:78:SER:HB2	2:A:301:8NL:C17	2.49	0.43
1:F:61:VAL:O	1:F:64:ILE:HG22	2.18	0.43
1:A:32:ARG:NH2	1:A:67:ARG:NH1	2.67	0.43
1:C:9:ILE:HD12	1:C:84:ILE:HG22	2.00	0.42
1:F:183:ASN:HA	1:F:184:PRO:HD2	1.81	0.42
1:B:120:GLU:HA	1:B:121:PRO:HA	1.78	0.42
1:F:99:ILE:HA	1:F:99:ILE:HD13	1.80	0.42
1:F:79:LEU:CB	2:F:301:8NL:C18	2.97	0.42
1:F:38:LEU:O	1:F:41:HIS:HB2	2.20	0.42
1:E:13:LEU:HD12	2:E:301:8NL:C	2.49	0.42
1:E:59:ARG:NH2	4:E:411:HOH:O	2.52	0.42
1:F:156:MSE:SE	1:F:164:MSE:CE	3.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLU:HB2	3:B:302:SO4:S	2.60	0.42
1:C:13:LEU:HD23	1:C:13:LEU:HA	1.73	0.42
1:C:134:PRO:HA	1:C:141:LEU:HD23	2.02	0.42
1:C:71:GLN:NE2	1:C:93:ASP:O	2.53	0.42
1:F:7:ILE:HD13	1:F:64:ILE:HG21	2.01	0.42
1:E:39:THR:HG21	1:E:56:HIS:NE2	2.35	0.42
1:E:150:ARG:O	1:E:154:VAL:HG23	2.20	0.42
1:E:159:TYR:HA	1:E:234:TYR:HB3	2.02	0.42
1:E:55:GLU:OE1	1:E:59:ARG:NH1	2.53	0.42
1:C:15:ARG:N	1:C:169:HIS:O	2.53	0.41
1:E:106:THR:O	1:E:217:PHE:HE2	2.02	0.41
1:E:138:GLY:N	4:E:410:HOH:O	2.49	0.41
1:A:223:VAL:HG11	4:A:507:HOH:O	2.18	0.41
1:E:166:PRO:HB2	1:E:168:GLU:OE1	2.21	0.41
1:C:106:THR:HB	1:C:110:VAL:HB	2.02	0.41
1:E:89:GLN:HA	1:E:189:ALA:CB	2.51	0.41
1:F:113:GLU:O	1:F:117:LEU:HD12	2.20	0.41
1:A:152:ARG:HA	1:A:156:MSE:HE3	2.01	0.41
1:B:121:PRO:O	1:B:123:ARG:HG3	2.21	0.41
1:B:164:MSE:CB	1:B:165:PRO:CD	2.96	0.41
1:D:154:VAL:HG12	1:D:204:VAL:HG22	2.02	0.41
1:D:217:PHE:CD1	1:D:218:PRO:HD2	2.56	0.41
1:E:106:THR:O	1:E:183:ASN:ND2	2.38	0.41
1:F:59:ARG:O	1:F:62:ALA:N	2.54	0.41
1:A:71:GLN:HB3	1:A:96:ALA:HB2	2.03	0.41
1:B:78:SER:CA	1:B:103:ALA:HA	2.49	0.41
1:E:105:LEU:N	4:E:413:HOH:O	2.53	0.41
1:E:136:ASP:N	1:E:136:ASP:OD1	2.53	0.41
1:E:204:VAL:CG2	1:E:230:HIS:CE1	3.03	0.41
1:A:61:VAL:HG11	1:A:87:LEU:HD13	2.02	0.41
1:B:211:ARG:HB3	4:B:470:HOH:O	2.21	0.41
1:C:232:PRO:HB2	1:C:240:LEU:HD22	2.03	0.41
1:E:115:PHE:CE1	1:E:213:MSE:HG2	2.56	0.41
1:F:41:HIS:NE2	1:F:57:TYR:OH	2.48	0.41
1:C:5:ASP:HB2	1:C:72:SER:OG	2.21	0.41
1:E:119:GLY:O	1:E:123:ARG:HB2	2.21	0.41
1:D:55:GLU:OE2	1:D:59:ARG:HD3	2.21	0.40
1:A:203:VAL:HG22	4:A:472:HOH:O	2.20	0.40
1:C:54:MSE:O	1:C:58:THR:OG1	2.23	0.40
1:C:89:GLN:OE1	1:C:186:GLU:HG3	2.21	0.40
1:F:41:HIS:ND1	1:F:171:ILE:HD13	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:ILE:HG12	1:F:73:ILE:HB	2.03	0.40
1:F:54:MSE:O	1:F:54:MSE:CE	2.70	0.40
1:B:139:ARG:HD2	1:C:49:LEU:HD13	2.04	0.40
1:C:31:TYR:OH	1:C:249:ASP:OD1	2.28	0.40
1:D:78:SER:HA	1:D:103:ALA:HA	2.04	0.40
1:E:196:TYR:OH	1:E:210:GLN:HG2	2.21	0.40

All (2) 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:E:164:MSE:N	1:F:149:GLU:OE1[8_554]	1.95	0.25
4:B:415:HOH:O	4:F:404:HOH:O[3_555]	2.17	0.03

## 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	248/288 (86%)	243 (98%)	5 (2%)	0	100	100
1	B	248/288 (86%)	240 (97%)	8 (3%)	0	100	100
1	C	248/288 (86%)	242 (98%)	6 (2%)	0	100	100
1	D	251/288 (87%)	245 (98%)	6 (2%)	0	100	100
1	E	247/288 (86%)	238 (96%)	9 (4%)	0	100	100
1	F	247/288 (86%)	239 (97%)	8 (3%)	0	100	100
All	All	1489/1728 (86%)	1447 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	201/220 (91%)	199 (99%)	2 (1%)	76	76
1	B	201/220 (91%)	199 (99%)	2 (1%)	76	76
1	C	200/220 (91%)	198 (99%)	2 (1%)	76	76
1	D	201/220 (91%)	200 (100%)	1 (0%)	88	89
1	E	195/220 (89%)	193 (99%)	2 (1%)	76	76
1	F	178/220 (81%)	175 (98%)	3 (2%)	60	57
All	All	1176/1320 (89%)	1164 (99%)	12 (1%)	76	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	113	GLU
1	B	69	GLU
1	B	164	MSE
1	C	78	SER
1	C	87	LEU
1	D	93	ASP
1	E	26	LEU
1	E	251	PRO
1	F	58	THR
1	F	59	ARG
1	F	60	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	34	HIS
1	F	212	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	8NL	F	301	-	31,31,31	1.39	4 (12%)	46,47,47	5.88	14 (30%)
2	8NL	A	301	-	31,31,31	1.76	3 (9%)	46,47,47	3.67	22 (47%)
2	8NL	D	301	-	31,31,31	1.72	2 (6%)	46,47,47	3.60	15 (32%)
3	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.24	0
3	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.52	0
3	SO4	A	302	-	4,4,4	0.20	0	6,6,6	0.38	0
2	8NL	E	301	-	31,31,31	1.41	4 (12%)	46,47,47	4.30	22 (47%)
3	SO4	C	302	-	4,4,4	0.20	0	6,6,6	0.46	0
2	8NL	C	301	-	31,31,31	1.78	3 (9%)	46,47,47	3.86	19 (41%)
3	SO4	E	302	-	4,4,4	0.16	0	6,6,6	0.09	0
2	8NL	B	301	-	31,31,31	1.68	2 (6%)	46,47,47	3.56	15 (32%)
3	SO4	F	302	-	4,4,4	0.13	0	6,6,6	0.43	0

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	8NL	F	301	-	-	13/23/36/36	0/3/3/3
2	8NL	D	301	-	-	8/23/36/36	0/3/3/3
2	8NL	A	301	-	-	8/23/36/36	0/3/3/3
2	8NL	E	301	-	-	9/23/36/36	0/3/3/3
2	8NL	C	301	-	-	9/23/36/36	0/3/3/3
2	8NL	B	301	-	-	9/23/36/36	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	8NL	O-C14	8.11	1.50	1.33
2	A	301	8NL	O-C14	7.94	1.49	1.33
2	B	301	8NL	O-C14	7.77	1.49	1.33
2	D	301	8NL	O-C14	7.62	1.49	1.33
2	E	301	8NL	O-C14	6.08	1.45	1.33
2	F	301	8NL	O-C14	5.24	1.44	1.33
2	D	301	8NL	C20-C21	3.57	1.34	1.31
2	B	301	8NL	C20-C21	3.47	1.34	1.31
2	F	301	8NL	C22-C21	3.37	1.52	1.49
2	C	301	8NL	C20-C21	3.34	1.34	1.31
2	C	301	8NL	C22-C21	2.74	1.52	1.49
2	E	301	8NL	C22-C21	2.63	1.51	1.49
2	E	301	8NL	C20-C21	2.51	1.33	1.31
2	A	301	8NL	C20-C21	2.50	1.33	1.31
2	F	301	8NL	O-C13	-2.38	1.40	1.45
2	F	301	8NL	C2-C1	-2.27	1.38	1.40
2	A	301	8NL	C22-C21	2.23	1.51	1.49
2	E	301	8NL	C2-C1	-2.08	1.38	1.40

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	8NL	C17-C16-C20	-23.45	88.47	122.46
2	F	301	8NL	C20-C21-CL	-22.26	111.51	123.75
2	F	301	8NL	C22-C21-CL	16.26	125.14	112.47
2	E	301	8NL	C20-C21-CL	-15.07	115.46	123.75
2	C	301	8NL	C20-C21-CL	-13.84	116.14	123.75
2	D	301	8NL	C17-C16-C20	-13.10	103.47	122.46
2	B	301	8NL	C17-C16-C20	-12.67	104.10	122.46
2	A	301	8NL	C18-C17-C16	-12.16	90.68	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	8NL	C17-C16-C20	-11.32	106.05	122.46
2	C	301	8NL	C17-C16-C20	-10.88	106.69	122.46
2	E	301	8NL	C16-C20-C21	-10.36	119.28	125.68
2	B	301	8NL	C20-C21-CL	-10.15	118.17	123.75
2	D	301	8NL	C18-C17-C16	-9.81	95.93	117.94
2	E	301	8NL	C22-C21-CL	9.78	120.09	112.47
2	C	301	8NL	C22-C21-CL	8.70	119.25	112.47
2	F	301	8NL	C18-C17-C16	-8.54	98.79	117.94
2	F	301	8NL	C16-C20-C21	-8.31	120.55	125.68
2	E	301	8NL	C17-C16-C20	-8.09	110.74	122.46
2	D	301	8NL	C16-C20-C21	-7.87	120.81	125.68
2	E	301	8NL	O-C14-C15	7.78	125.32	110.89
2	B	301	8NL	C22-C21-CL	7.60	118.40	112.47
2	E	301	8NL	C16-C15-C14	-7.52	102.24	120.33
2	B	301	8NL	O-C13-C2	7.43	124.16	108.72
2	E	301	8NL	C18-C17-C16	-7.34	101.48	117.94
2	C	301	8NL	C18-C17-C16	-7.27	101.64	117.94
2	A	301	8NL	C20-C21-CL	-7.16	119.81	123.75
2	A	301	8NL	C16-C20-C21	-6.84	121.45	125.68
2	D	301	8NL	C20-C21-CL	-6.74	120.04	123.75
2	C	301	8NL	O-C14-C15	6.74	123.38	110.89
2	A	301	8NL	C22-C21-CL	6.48	117.52	112.47
2	C	301	8NL	O-C13-C2	6.43	122.10	108.72
2	D	301	8NL	C22-C21-CL	6.35	117.42	112.47
2	B	301	8NL	C16-C15-C14	-6.00	105.89	120.33
2	B	301	8NL	O-C14-C15	5.99	121.99	110.89
2	D	301	8NL	C-C1-C2	-5.63	115.14	120.94
2	A	301	8NL	C13-O-C14	5.59	126.20	116.32
2	C	301	8NL	C16-C15-C14	-5.28	107.63	120.33
2	E	301	8NL	O-C14-O1	-5.13	114.42	124.13
2	E	301	8NL	O-C13-C2	4.91	118.92	108.72
2	D	301	8NL	O-C13-C2	4.82	118.75	108.72
2	F	301	8NL	C17-C15-C14	-4.81	110.13	122.42
2	E	301	8NL	C-C1-C2	-4.77	116.02	120.94
2	A	301	8NL	O-C13-C2	4.75	118.59	108.72
2	D	301	8NL	O-C14-C15	4.61	119.45	110.89
2	F	301	8NL	O-C14-O1	-4.52	115.57	124.13
2	A	301	8NL	C16-C15-C14	-4.36	109.84	120.33
2	B	301	8NL	C19-C17-C16	-4.32	108.24	117.94
2	B	301	8NL	C-C1-C2	-4.10	116.71	120.94
2	C	301	8NL	O-C14-O1	-4.08	116.40	124.13
2	C	301	8NL	C15-C16-C20	-4.07	115.34	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	8NL	C3-C2-C1	4.00	122.35	119.48
2	C	301	8NL	C18-C17-C15	3.95	130.36	117.96
2	D	301	8NL	C18-C17-C15	3.90	130.19	117.96
2	A	301	8NL	O-C14-C15	3.79	117.92	110.89
2	F	301	8NL	C13-O-C14	-3.75	109.69	116.32
2	B	301	8NL	C16-C20-C21	3.74	127.99	125.68
2	E	301	8NL	C19-C17-C18	3.69	118.55	113.47
2	C	301	8NL	C-C1-C2	-3.65	117.17	120.94
2	F	301	8NL	O-C14-C15	3.65	117.65	110.89
2	D	301	8NL	C16-C15-C14	-3.63	111.60	120.33
2	D	301	8NL	F-C22-C21	-3.59	106.42	112.52
2	B	301	8NL	O1-C14-C15	-3.49	118.90	125.25
2	E	301	8NL	C17-C15-C14	-3.45	113.60	122.42
2	E	301	8NL	C15-C16-C20	-3.42	116.25	121.07
2	B	301	8NL	F-C22-C21	-3.35	106.84	112.52
2	A	301	8NL	C18-C17-C15	3.33	128.41	117.96
2	B	301	8NL	C19-C17-C15	3.17	127.90	117.96
2	B	301	8NL	C6-C1-C2	3.07	122.14	118.77
2	A	301	8NL	F-C22-C21	-3.07	107.31	112.52
2	A	301	8NL	C3-C2-C1	-3.05	117.30	119.48
2	F	301	8NL	C18-C17-C15	3.03	127.48	117.96
2	D	301	8NL	C6-C1-C2	3.02	122.08	118.77
2	A	301	8NL	C-C1-C2	-2.93	117.91	120.94
2	C	301	8NL	C17-C15-C14	2.93	129.91	122.42
2	C	301	8NL	O1-C14-C15	-2.81	120.13	125.25
2	E	301	8NL	O1-C14-C15	-2.78	120.20	125.25
2	A	301	8NL	O1-C14-C15	-2.75	120.24	125.25
2	B	301	8NL	O-C14-O1	-2.69	119.05	124.13
2	A	301	8NL	C12-C7-C6	2.66	125.22	120.91
2	D	301	8NL	C13-C2-C3	2.64	125.25	119.52
2	A	301	8NL	F2-C22-C21	-2.62	108.08	112.52
2	F	301	8NL	F-C22-C21	-2.60	108.11	112.52
2	A	301	8NL	C15-C16-C20	2.56	124.69	121.07
2	B	301	8NL	C13-C2-C3	2.56	125.08	119.52
2	F	301	8NL	C-C1-C2	-2.46	118.41	120.94
2	E	301	8NL	C13-O-C14	-2.45	111.98	116.32
2	D	301	8NL	O1-C14-C15	-2.43	120.83	125.25
2	C	301	8NL	F1-C22-C21	-2.41	108.44	112.52
2	E	301	8NL	C3-C2-C1	2.38	121.19	119.48
2	E	301	8NL	F1-C22-C21	-2.37	108.50	112.52
2	C	301	8NL	C17-C16-C15	2.36	61.48	59.91
2	D	301	8NL	O-C14-O1	-2.33	119.72	124.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	8NL	C6-C1-C2	2.33	121.32	118.77
2	A	301	8NL	C7-C6-C1	2.30	126.56	122.42
2	A	301	8NL	C6-C1-C2	2.29	121.27	118.77
2	C	301	8NL	C6-C1-C2	2.27	121.26	118.77
2	C	301	8NL	C5-C6-C1	-2.27	117.50	119.92
2	F	301	8NL	C4-C3-C2	-2.18	117.64	120.89
2	E	301	8NL	C12-C7-C6	2.17	124.42	120.91
2	A	301	8NL	C17-C16-C15	2.12	61.32	59.91
2	E	301	8NL	C8-C7-C6	-2.11	117.48	120.91
2	C	301	8NL	C19-C17-C16	-2.10	113.23	117.94
2	E	301	8NL	F2-C22-C21	-2.06	109.03	112.52
2	E	301	8NL	C5-C6-C1	-2.05	117.74	119.92
2	A	301	8NL	C9-C8-C7	2.04	123.12	120.56
2	A	301	8NL	C5-C6-C7	-2.03	114.66	118.68
2	C	301	8NL	C4-C3-C2	-2.03	117.86	120.89

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	8NL	C15-C14-O-C13
2	F	301	8NL	O1-C14-O-C13
2	F	301	8NL	CL-C21-C22-F2
2	F	301	8NL	CL-C21-C22-F1
2	F	301	8NL	CL-C21-C22-F
2	F	301	8NL	C20-C21-C22-F2
2	F	301	8NL	C20-C21-C22-F1
2	F	301	8NL	C20-C21-C22-F
2	D	301	8NL	C15-C14-O-C13
2	D	301	8NL	CL-C21-C22-F2
2	D	301	8NL	CL-C21-C22-F1
2	D	301	8NL	CL-C21-C22-F
2	D	301	8NL	C20-C21-C22-F2
2	D	301	8NL	C20-C21-C22-F1
2	D	301	8NL	C20-C21-C22-F
2	A	301	8NL	CL-C21-C22-F2
2	A	301	8NL	CL-C21-C22-F1
2	A	301	8NL	CL-C21-C22-F
2	A	301	8NL	C20-C21-C22-F2
2	A	301	8NL	C20-C21-C22-F1
2	A	301	8NL	C20-C21-C22-F
2	A	301	8NL	C15-C16-C20-C21

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Mol	Chain	Res	Type	Atoms
2	E	301	8NL	CL-C21-C22-F2
2	E	301	8NL	CL-C21-C22-F1
2	E	301	8NL	CL-C21-C22-F
2	E	301	8NL	C20-C21-C22-F2
2	E	301	8NL	C20-C21-C22-F1
2	E	301	8NL	C20-C21-C22-F
2	E	301	8NL	C15-C16-C20-C21
2	C	301	8NL	C15-C14-O-C13
2	C	301	8NL	CL-C21-C22-F2
2	C	301	8NL	CL-C21-C22-F1
2	C	301	8NL	CL-C21-C22-F
2	C	301	8NL	C20-C21-C22-F2
2	C	301	8NL	C20-C21-C22-F1
2	C	301	8NL	C20-C21-C22-F
2	B	301	8NL	O1-C14-O-C13
2	B	301	8NL	CL-C21-C22-F2
2	B	301	8NL	CL-C21-C22-F1
2	B	301	8NL	CL-C21-C22-F
2	B	301	8NL	C20-C21-C22-F2
2	B	301	8NL	C20-C21-C22-F1
2	B	301	8NL	C20-C21-C22-F
2	B	301	8NL	C15-C16-C20-C21
2	D	301	8NL	O1-C14-O-C13
2	C	301	8NL	O1-C14-O-C13
2	E	301	8NL	C15-C14-O-C13
2	B	301	8NL	C15-C14-O-C13
2	E	301	8NL	O1-C14-O-C13
2	F	301	8NL	O1-C14-C15-C17
2	F	301	8NL	O-C14-C15-C17
2	F	301	8NL	C15-C16-C20-C21
2	C	301	8NL	C15-C16-C20-C21
2	A	301	8NL	O1-C14-O-C13
2	F	301	8NL	O1-C14-C15-C16
2	F	301	8NL	O-C14-C15-C16

There are no ring outliers.

9 monomers are involved in 19 short contacts:

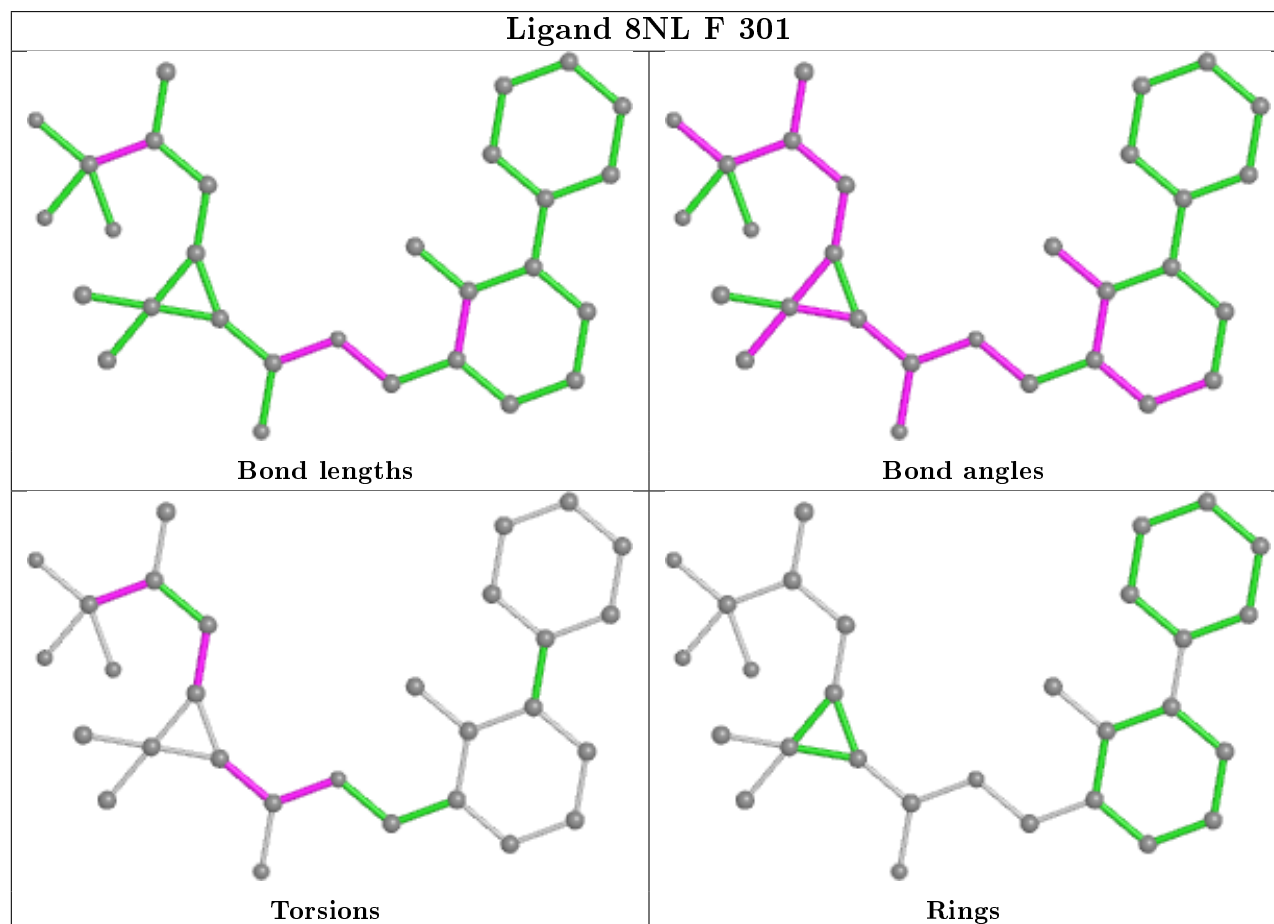
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	8NL	6	0
2	A	301	8NL	2	0
2	D	301	8NL	3	0

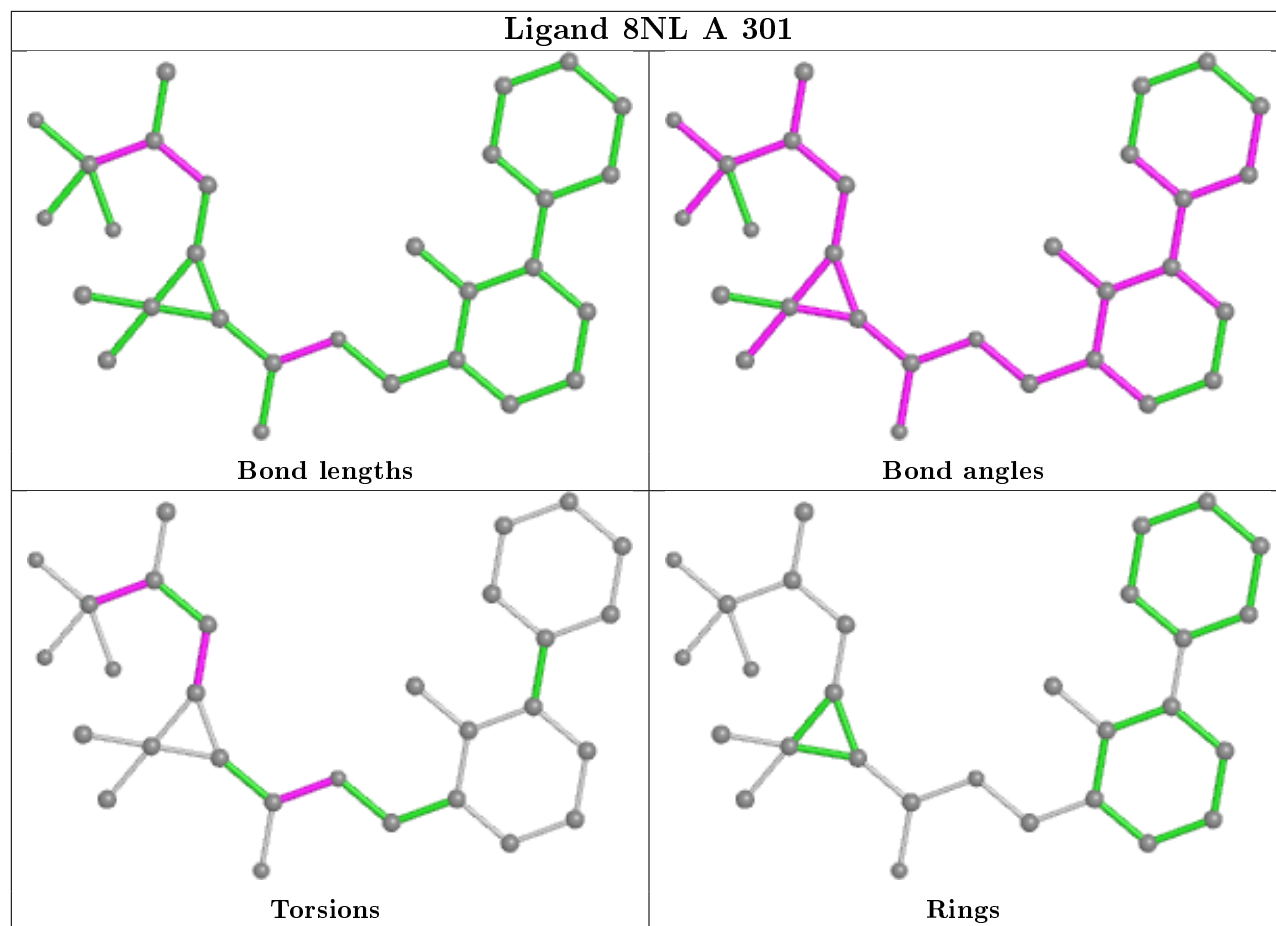
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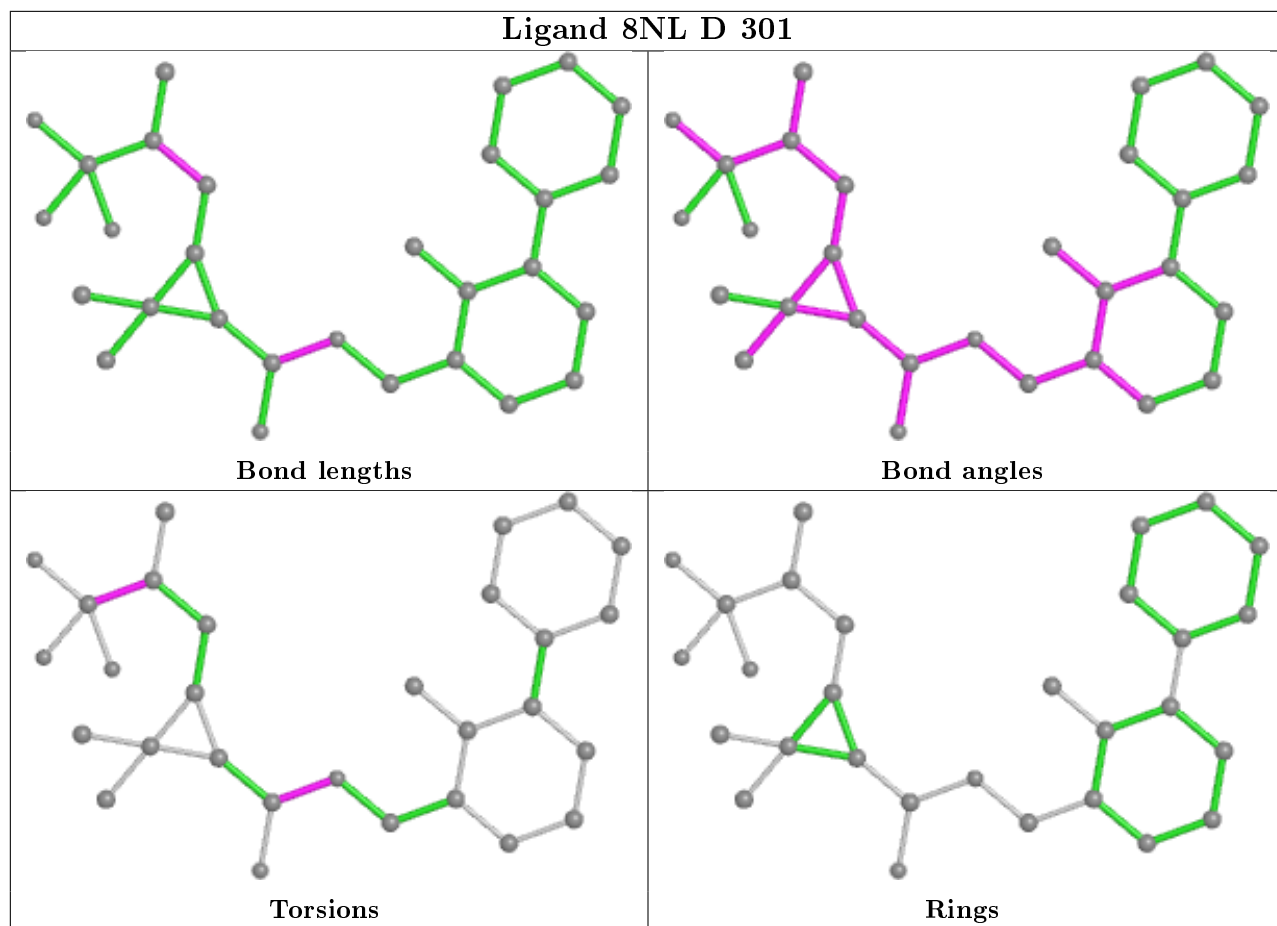
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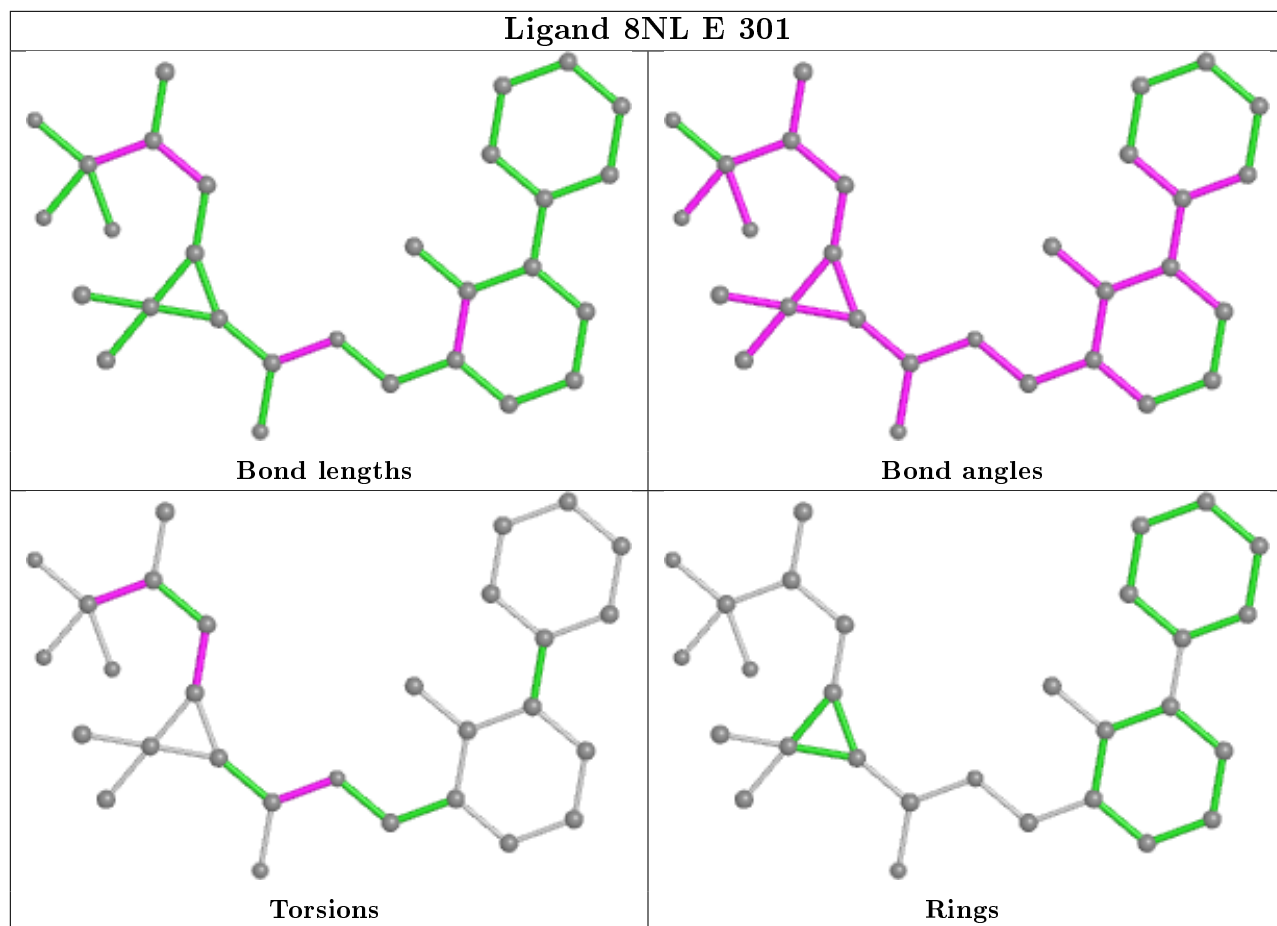
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	SO4	1	0
3	B	302	SO4	1	0
3	A	302	SO4	1	0
2	E	301	8NL	2	0
2	C	301	8NL	1	0
2	B	301	8NL	2	0

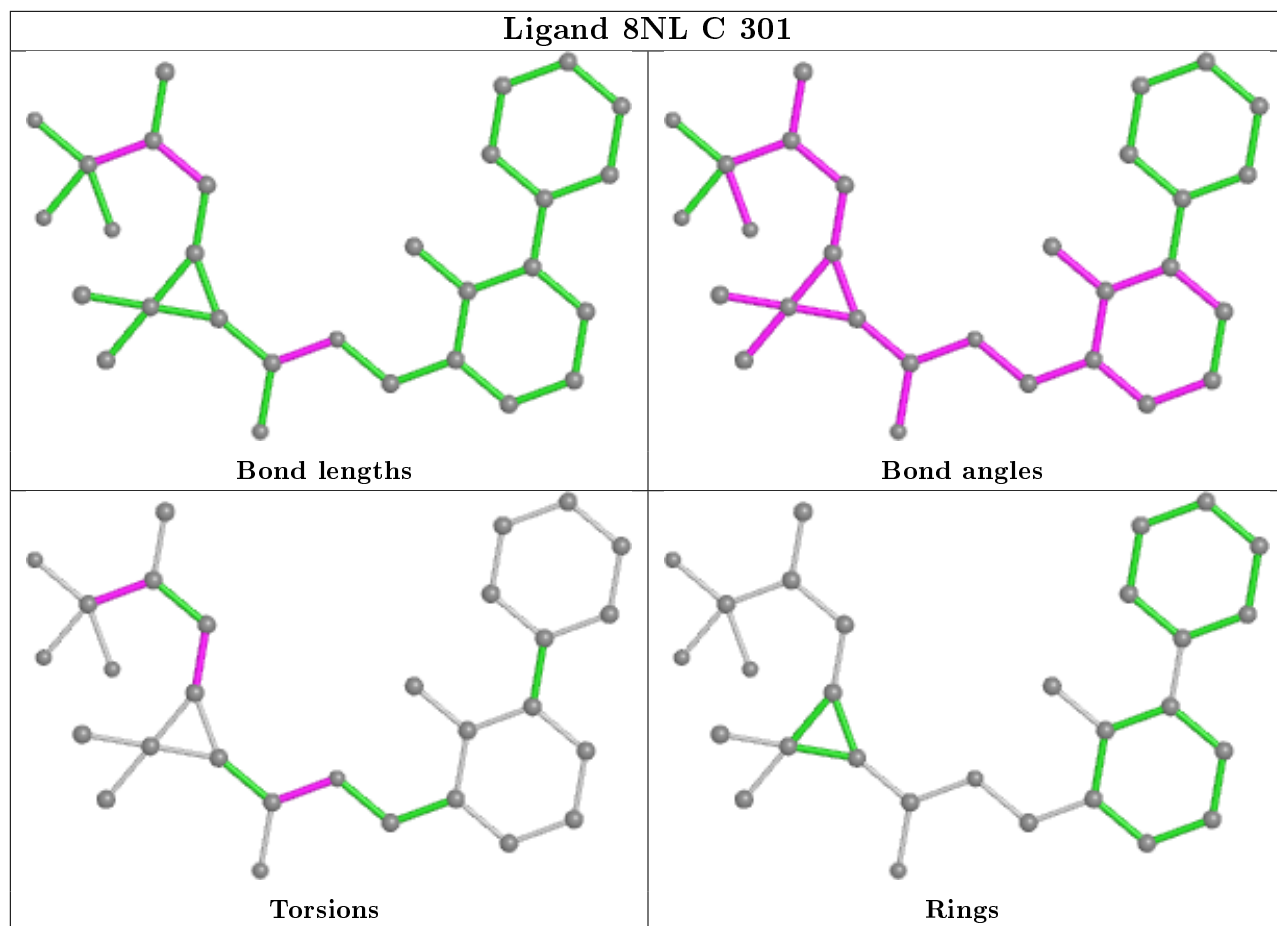
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

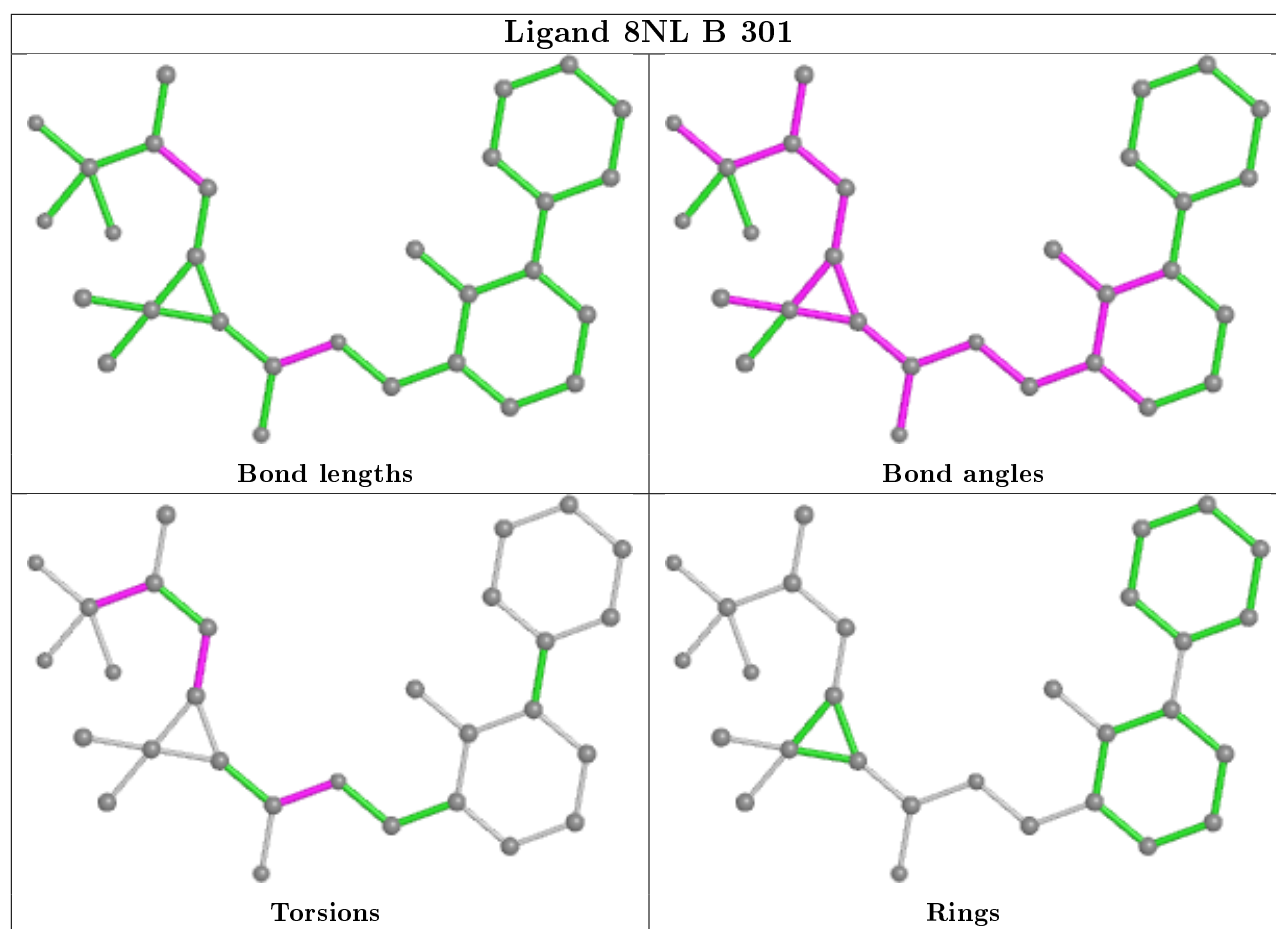












## 5.7 Other polymers [i](#)

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	246/288 (85%)	0.29	6 (2%) 59 62	13, 24, 38, 50	0
1	B	246/288 (85%)	0.29	1 (0%) 92 93	14, 24, 37, 49	0
1	C	246/288 (85%)	0.65	16 (6%) 18 21	18, 33, 50, 60	0
1	D	247/288 (85%)	0.59	15 (6%) 21 24	17, 28, 44, 54	0
1	E	245/288 (85%)	1.58	66 (26%) 0 0	25, 43, 59, 71	0
1	F	245/288 (85%)	2.03	105 (42%) 0 0	30, 56, 75, 90	0
All	All	1475/1728 (85%)	0.90	209 (14%) 2 2	13, 33, 65, 90	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	189	ALA	8.7
1	F	219	GLY	7.0
1	F	188	ARG	6.6
1	F	86	TRP	5.9
1	F	44	GLY	5.6
1	A	161	GLY	5.5
1	F	105	LEU	5.5
1	E	117	LEU	5.3
1	E	66	ALA	4.9
1	F	84	ILE	4.7
1	F	139	ARG	4.7
1	F	218	PRO	4.7
1	F	217	PHE	4.6
1	F	73	ILE	4.5
1	E	138	GLY	4.5
1	C	252	ALA	4.4
1	F	83	SER	4.3
1	E	86	TRP	4.3
1	F	68	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	52	VAL	4.2
1	F	138	GLY	4.1
1	E	252	ALA	4.1
1	F	179	PHE	4.0
1	E	108	PRO	4.0
1	C	161	GLY	4.0
1	F	222	ALA	4.0
1	E	222	ALA	4.0
1	D	162	GLU	4.0
1	F	140	GLY	3.9
1	F	100	TYR	3.9
1	F	60	PRO	3.9
1	A	138	GLY	3.9
1	F	141	LEU	3.9
1	D	161	GLY	3.8
1	F	39	THR	3.8
1	F	81	GLY	3.7
1	E	98	LEU	3.7
1	F	12	ALA	3.7
1	F	43	PRO	3.7
1	F	57	TYR	3.6
1	E	73	ILE	3.6
1	E	70	GLY	3.6
1	E	253	GLU	3.5
1	F	6	ILE	3.5
1	E	141	LEU	3.5
1	E	217	PHE	3.5
1	F	183	ASN	3.5
1	F	21	ALA	3.4
1	F	82	ALA	3.4
1	E	105	LEU	3.4
1	F	221	VAL	3.4
1	F	117	LEU	3.4
1	F	175	SER	3.3
1	F	23	VAL	3.3
1	F	80	GLY	3.2
1	E	212	GLN	3.2
1	E	65	LEU	3.2
1	C	65	LEU	3.2
1	F	67	ARG	3.2
1	F	220	PRO	3.2
1	F	13	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	50	SER	3.1
1	E	6	ILE	3.1
1	E	13	LEU	3.1
1	E	254	TYR	3.1
1	F	38	LEU	3.1
1	F	99	ILE	3.1
1	F	63	ASP	3.1
1	E	88	ALA	3.1
1	F	66	ALA	3.1
1	C	69	GLU	3.1
1	F	145	PHE	3.1
1	F	69	GLU	3.0
1	F	106	THR	3.0
1	E	51	VAL	3.0
1	F	3	VAL	3.0
1	F	104	VAL	3.0
1	C	107	ALA	3.0
1	E	250	ALA	3.0
1	E	135	VAL	3.0
1	F	181	THR	3.0
1	E	188	ARG	3.0
1	F	137	GLU	3.0
1	F	193	PRO	3.0
1	E	122	ASN	3.0
1	E	192	ILE	2.9
1	E	179	PHE	2.9
1	F	36	PRO	2.9
1	E	106	THR	2.9
1	F	51	VAL	2.9
1	E	95	VAL	2.8
1	F	112	PRO	2.8
1	D	254	TYR	2.8
1	E	221	VAL	2.8
1	C	190	LEU	2.8
1	E	190	LEU	2.8
1	F	195	LEU	2.8
1	A	163	GLY	2.8
1	F	178	PRO	2.8
1	F	65	LEU	2.8
1	F	96	ALA	2.8
1	E	2	THR	2.7
1	F	191	GLU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	219	GLY	2.7
1	F	98	LEU	2.7
1	F	165	PRO	2.7
1	F	46	GLY	2.7
1	E	62	ALA	2.7
1	F	34	HIS	2.7
1	F	146	SER	2.7
1	D	253	GLU	2.7
1	C	63	ASP	2.6
1	E	12	ALA	2.6
1	E	99	ILE	2.6
1	F	35	ALA	2.6
1	F	174	GLN	2.6
1	F	187	GLY	2.6
1	C	253	GLU	2.6
1	E	182	PRO	2.6
1	F	87	LEU	2.6
1	C	68	ALA	2.6
1	F	11	GLY	2.6
1	E	7	ILE	2.6
1	F	108	PRO	2.6
1	F	247	PHE	2.6
1	C	74	LEU	2.6
1	F	17	ALA	2.6
1	A	99	ILE	2.6
1	E	107	ALA	2.6
1	F	143	ALA	2.6
1	A	253	GLU	2.5
1	F	115	PHE	2.5
1	F	30	GLY	2.5
1	E	52	VAL	2.5
1	F	107	ALA	2.5
1	E	195	LEU	2.5
1	F	172	GLN	2.5
1	F	28	ALA	2.5
1	E	187	GLY	2.5
1	E	134	PRO	2.5
1	F	244	ILE	2.5
1	F	90	HIS	2.5
1	F	88	ALA	2.4
1	D	6	ILE	2.4
1	F	64	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	61	VAL	2.4
1	F	173	THR	2.4
1	F	190	LEU	2.4
1	E	119	GLY	2.4
1	E	68	ALA	2.4
1	F	113	GLU	2.4
1	F	58	THR	2.4
1	E	59	ARG	2.4
1	C	163	GLY	2.4
1	F	184	PRO	2.4
1	B	138	GLY	2.4
1	D	221	VAL	2.4
1	F	47	GLY	2.3
1	F	136	ASP	2.3
1	C	244	ILE	2.3
1	D	99	ILE	2.3
1	D	244	ILE	2.3
1	E	44	GLY	2.3
1	C	2	THR	2.3
1	F	192	ILE	2.3
1	E	147	ARG	2.3
1	C	3	VAL	2.3
1	E	173	THR	2.3
1	E	178	PRO	2.3
1	E	63	ASP	2.3
1	F	59	ARG	2.3
1	E	39	THR	2.2
1	E	84	ILE	2.2
1	E	87	LEU	2.2
1	F	166	PRO	2.2
1	E	244	ILE	2.2
1	A	187	GLY	2.2
1	E	46	GLY	2.2
1	E	93	ASP	2.2
1	E	69	GLU	2.2
1	E	90	HIS	2.2
1	F	232	PRO	2.2
1	D	245	ALA	2.2
1	E	64	ILE	2.2
1	D	105	LEU	2.2
1	F	245	ALA	2.2
1	D	215	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	165	PRO	2.1
1	F	118	PRO	2.1
1	F	171	ILE	2.1
1	D	208	ALA	2.1
1	D	73	ILE	2.1
1	C	160	PRO	2.1
1	F	133	GLN	2.1
1	D	163	GLY	2.1
1	E	191	GLU	2.1
1	F	33	VAL	2.1
1	D	28	ALA	2.1
1	E	85	SER	2.1
1	F	7	ILE	2.1
1	F	40	GLY	2.1
1	F	163	GLY	2.1
1	F	4	THR	2.1
1	F	97	GLY	2.1
1	F	31	TYR	2.0
1	E	110	VAL	2.0
1	E	145	PHE	2.0
1	E	204	VAL	2.0
1	E	79	LEU	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 carbohydrates 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.

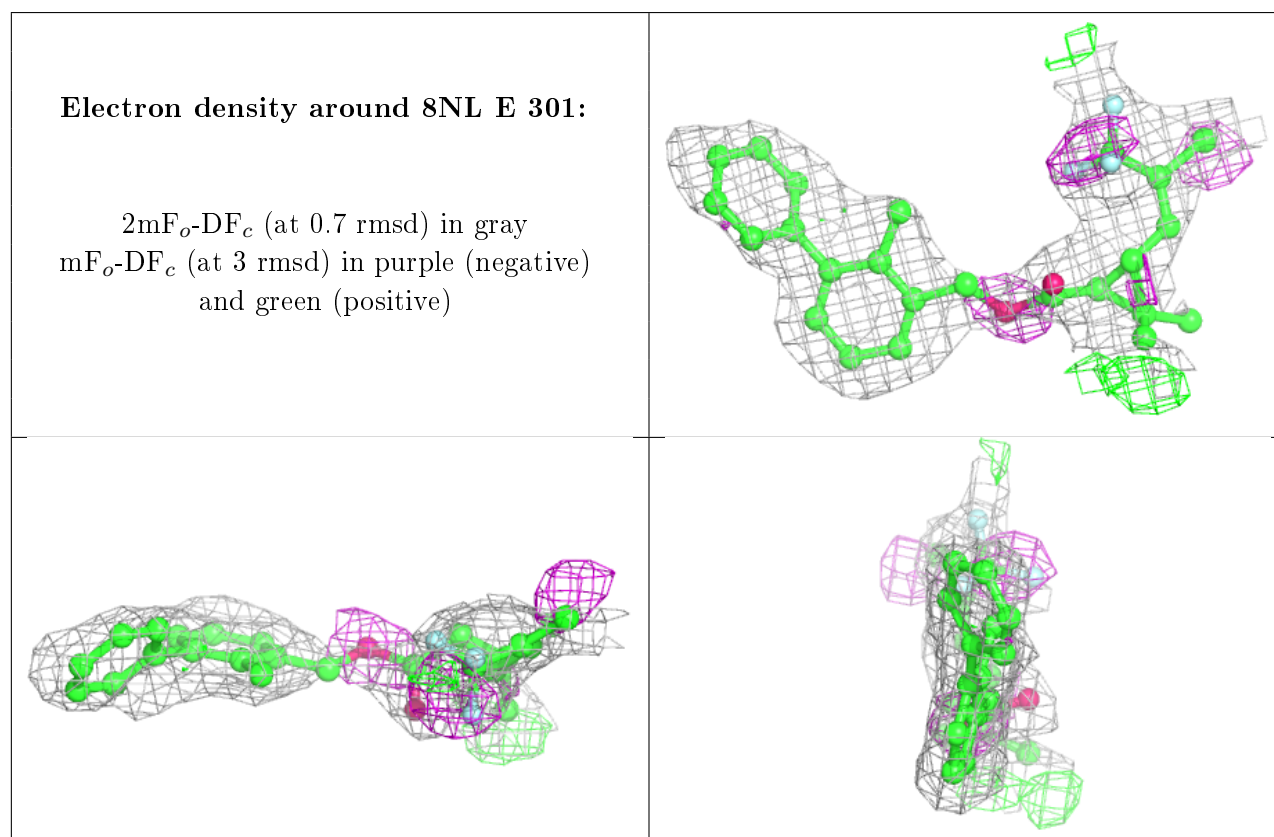
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	8NL	E	301	29/29	0.72	0.25	26,41,57,74	0

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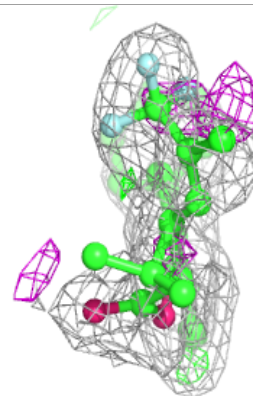
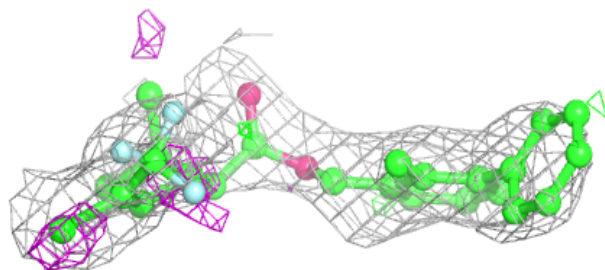
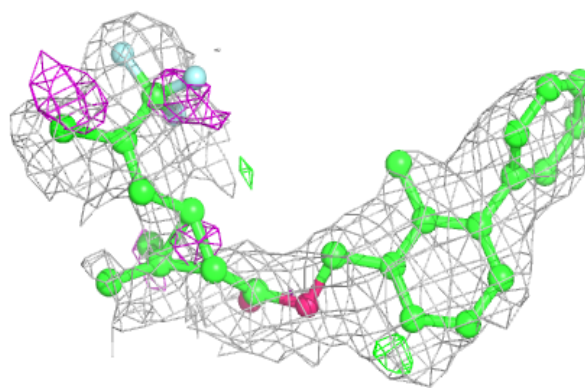
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	8NL	F	301	29/29	0.74	0.27	40,50,61,64	0
2	8NL	D	301	29/29	0.79	0.21	19,26,37,83	0
2	8NL	C	301	29/29	0.81	0.19	20,27,36,47	0
2	8NL	A	301	29/29	0.83	0.21	16,24,36,67	0
2	8NL	B	301	29/29	0.83	0.20	20,26,38,73	0
3	SO4	F	302	5/5	0.90	0.14	37,45,52,53	0
3	SO4	B	302	5/5	0.92	0.14	26,31,39,43	0
3	SO4	E	302	5/5	0.97	0.16	36,38,43,44	0
3	SO4	C	302	5/5	0.97	0.10	31,33,37,38	0
3	SO4	D	302	5/5	0.97	0.10	39,39,50,52	0
3	SO4	A	302	5/5	0.98	0.09	25,27,33,34	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.

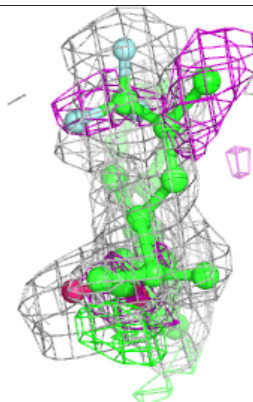
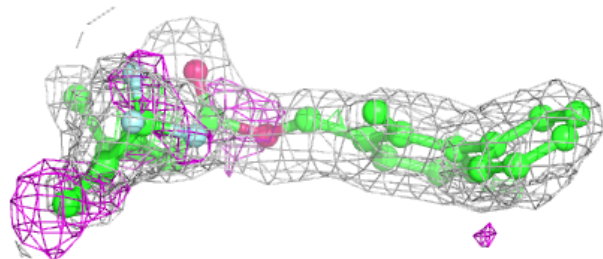
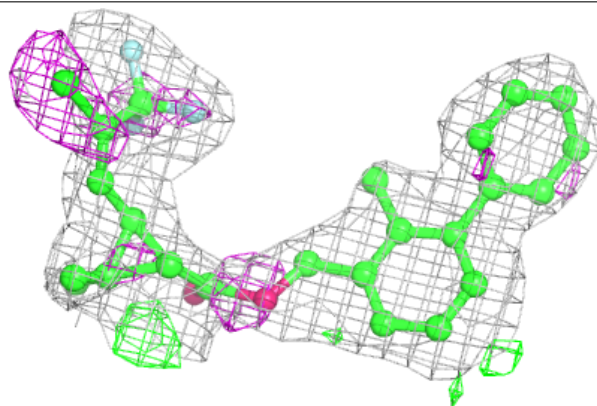


**Electron density around 8NL F 301:**

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

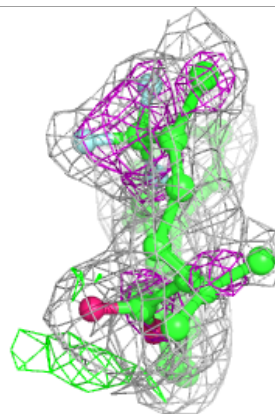
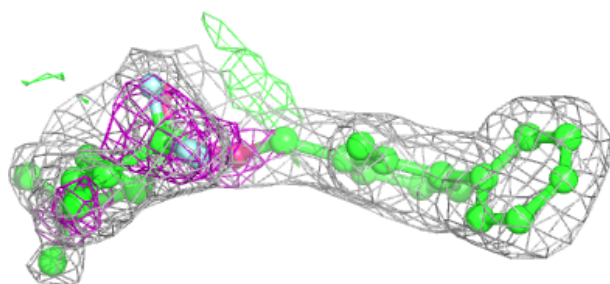
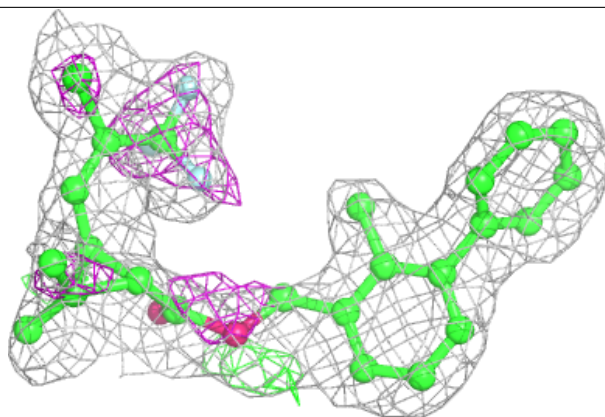
**Electron density around 8NL D 301:**

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

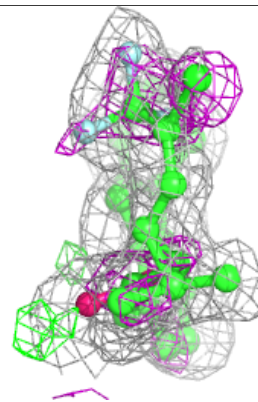
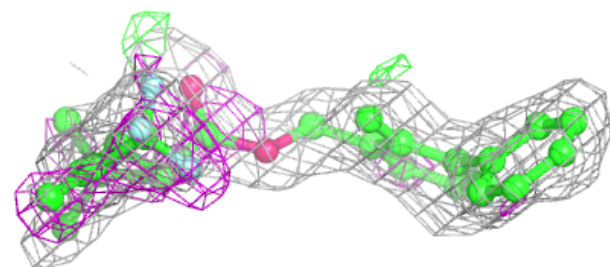
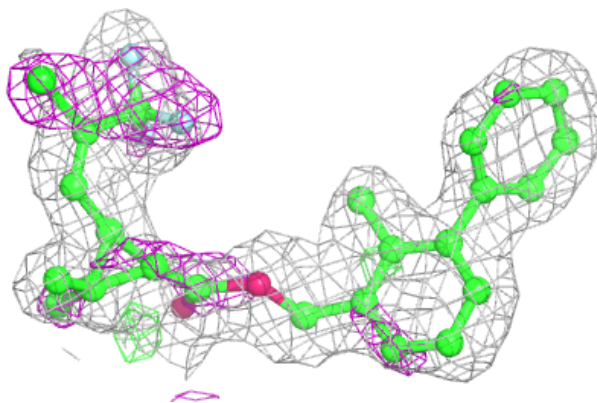


**Electron density around 8NL C 301:**

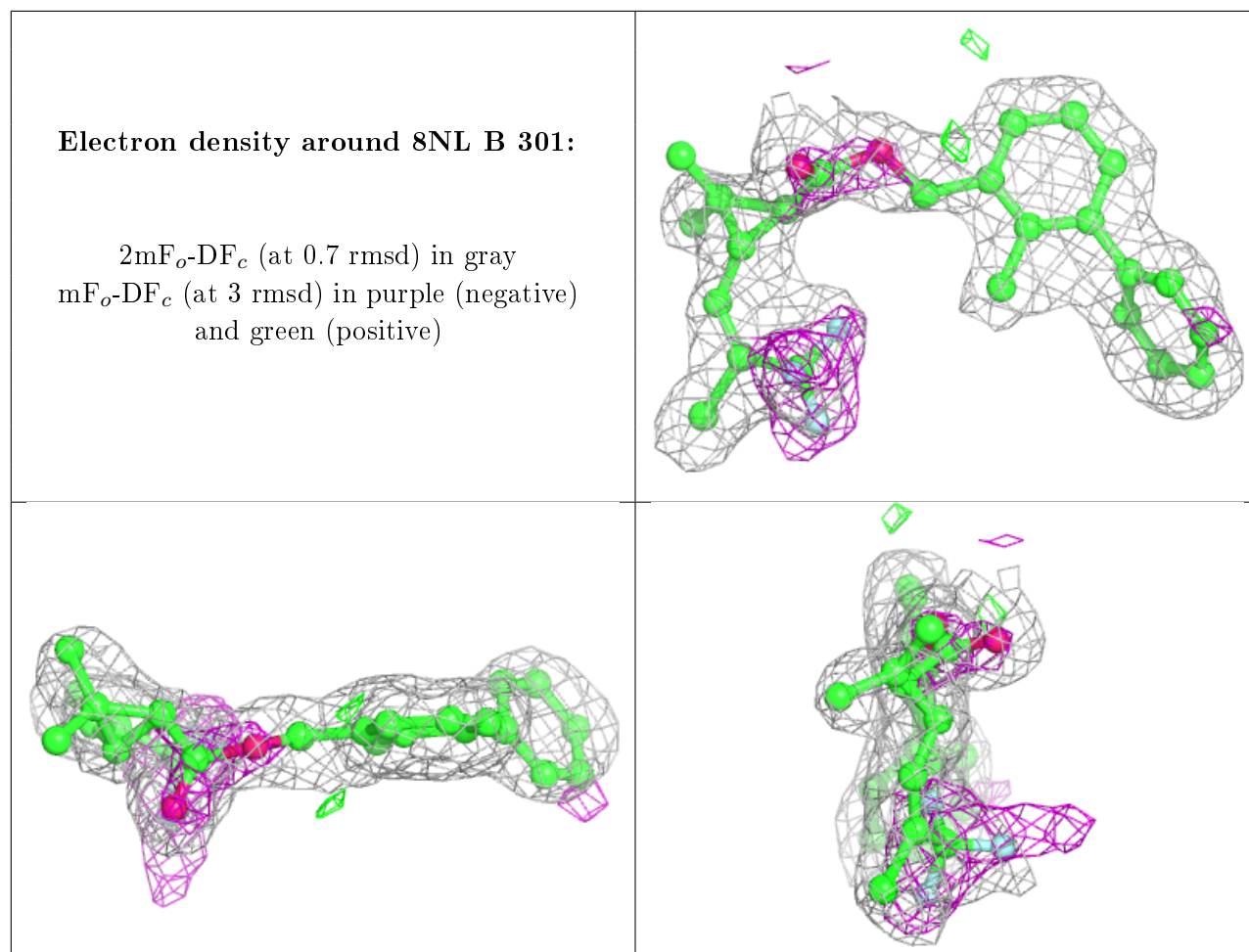
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 8NL A 301:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.