



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:46 PM UTC

PDB ID : 5Y5R / pdb_00005y5r
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

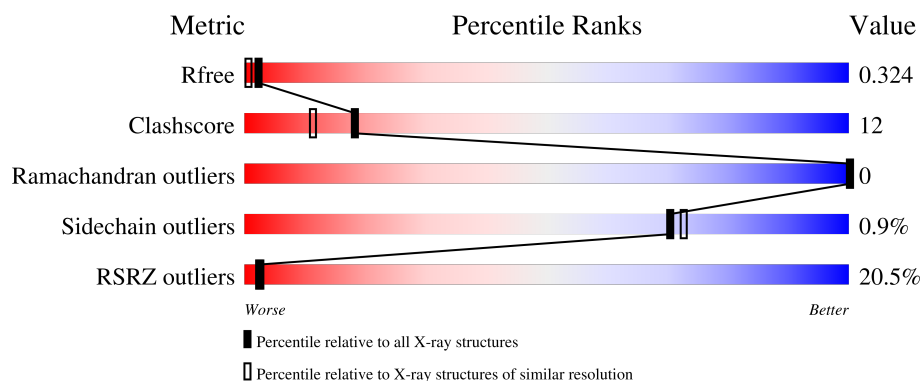
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	6% 77% 10% 12%
1	B	288	74% 12% 12%
1	C	288	6% 70% 17% 12%
1	D	288	6% 72% 16% 12%
1	E	288	34% 60% 26% 13%

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Mol	Chain	Length	Quality of chain
1	F	288	58% 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
1	A	252	Total	C	N	O	S	Se	0	0	0
			1914	1218	331	358	1	6			
1	B	252	Total	C	N	O	S	Se	0	0	0
			1914	1218	331	358	1	6			
1	C	252	Total	C	N	O	S	Se	0	0	0
			1908	1215	328	358	1	6			
1	D	253	Total	C	N	O	S	Se	0	0	0
			1917	1220	329	361	1	6			
1	E	251	Total	C	N	O	S	Se	0	0	0
			1887	1201	326	353	1	6			
1	F	251	Total	C	N	O	S	Se	0	0	0
			1827	1158	320	342	1	6			

There are 54 discrepancies between the modelled and reference sequences:

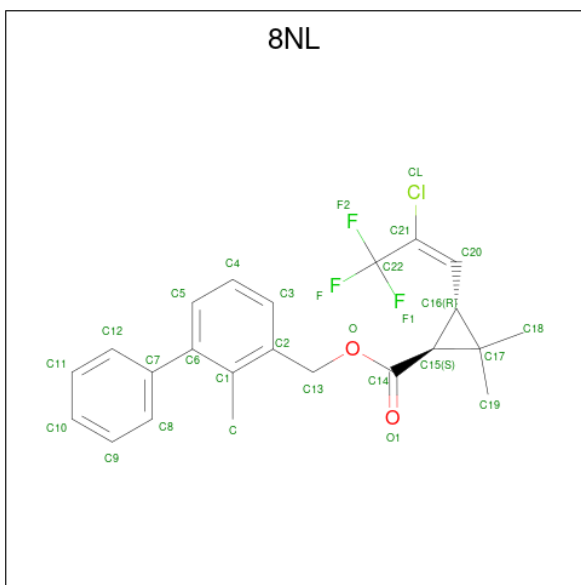
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP D0VUS3
A	281	LEU	-	expression tag	UNP D0VUS3
A	282	GLU	-	expression tag	UNP D0VUS3
A	283	HIS	-	expression tag	UNP D0VUS3
A	284	HIS	-	expression tag	UNP D0VUS3
A	285	HIS	-	expression tag	UNP D0VUS3
A	286	HIS	-	expression 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 (CCD ID: 8NL) (formula: $C_{23}H_{22}ClF_3O_2$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



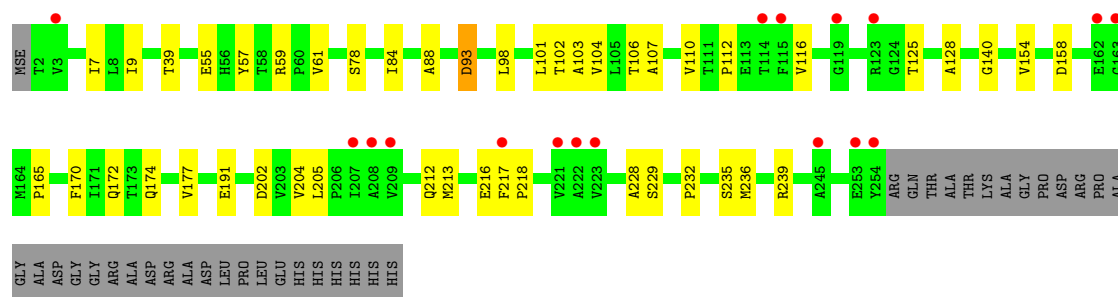
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

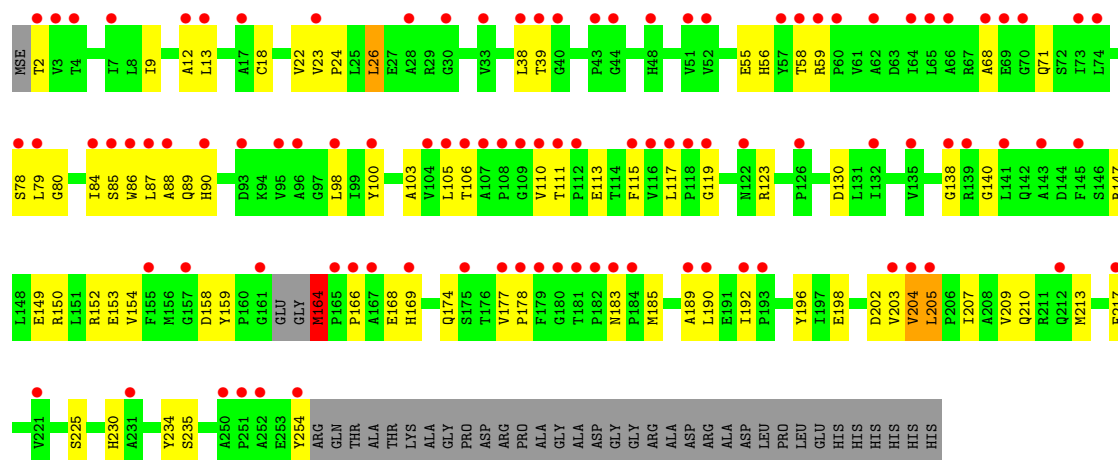
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	108	Total	O	0	0
			108	108		
4	C	74	Total	O	0	0
			74	74		
4	D	82	Total	O	0	0
			82	82		
4	E	57	Total	O	0	0
			57	57		
4	F	42	Total	O	0	0
			42	42		

- Molecule 1: Pyrethroid hydrolase

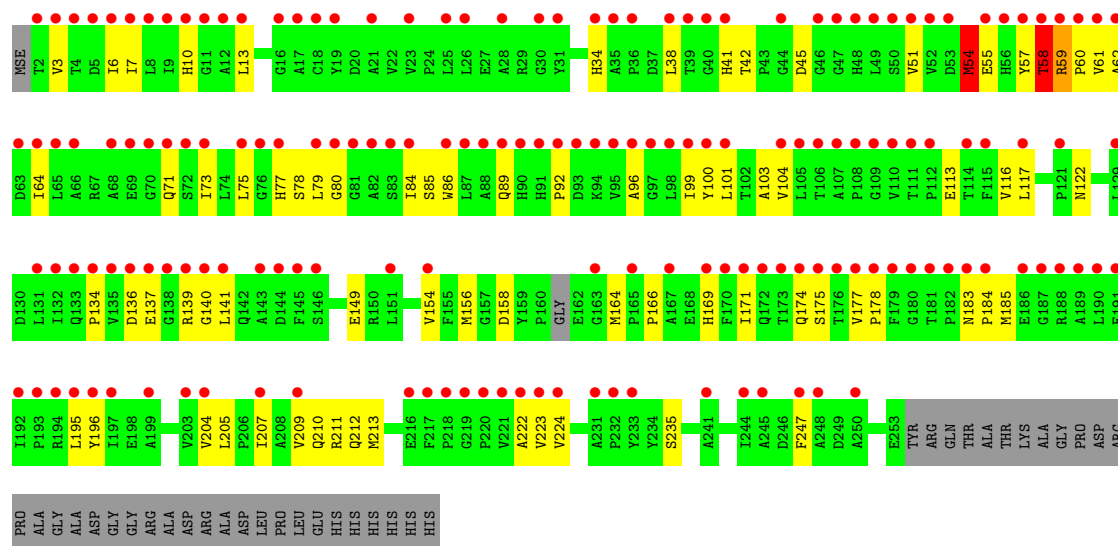




• Molecule 1: Pyrethroid hydrolase



• Molecule 1: Pyrethroid hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.4 (19.91-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.90Å)	Xtriage
Refinement program	PHENIX (dev_2247: ???)	Depositor
R, R_{free}	0.273 , 0.322 0.277 , 0.324	Depositor DCC
R_{free} test set	7014 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12042	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/1960	0.72	0/2672
1	B	0.52	0/1960	0.69	1/2672 (0.0%)
1	C	0.48	0/1954	0.66	1/2665 (0.0%)
1	D	0.52	0/1964	0.69	0/2680
1	E	0.53	2/1934 (0.1%)	0.74	4/2642 (0.2%)
1	F	0.55	0/1872	0.81	3/2559 (0.1%)
All	All	0.53	2/11644 (0.0%)	0.72	9/15890 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	VAL	C-O	-6.83	1.16	1.23
1	E	205	LEU	C-N	5.24	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	204	VAL	N-CA-C	-6.89	105.04	111.45
1	F	54	MSE	N-CA-C	6.24	118.08	111.28
1	C	188	ARG	N-CA-C	6.09	117.92	111.28
1	B	164	MSE	N-CA-C	5.85	122.73	109.81
1	F	80	GLY	N-CA-C	-5.76	105.69	113.24
1	F	58	THR	CB-CA-C	-5.55	100.90	110.72
1	E	164	MSE	CA-C-N	-5.21	115.01	120.38
1	E	164	MSE	C-N-CA	-5.21	115.01	120.38
1	E	205	LEU	O-C-N	5.12	125.98	121.32

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	1914	0	1876	20	0
1	B	1914	0	1876	29	0
1	C	1908	0	1865	34	0
1	D	1917	0	1872	35	0
1	E	1887	0	1827	74	1
1	F	1827	0	1706	83	1
2	A	29	0	0	2	0
2	B	29	0	0	2	0
2	C	29	0	0	1	0
2	D	29	0	0	4	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	273	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 (273) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:F:54:MSE:HA	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: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
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:HG	2:F:301:8NL:C19	1.99	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:HE3	1:F:54:MSE:CA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ALA:HB2	1:C:98:LEU:HD21	1.79	0.64
1:E:198:GLU:OE2	1:E:225:SER:OG	2.15	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: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
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:N	1:A:137:GLU:OE1	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:OD1	1:D:93:ASP:N	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:E:106:THR:OG1	4:E:402:HOH:O	2.12	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: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:CE	1:F:54:MSE:HA	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:106:THR:HB	1:D:110:VAL:HB	1.90	0.53
1:E:205:LEU:C	1:E:205:LEU:HD12	2.34	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:15:ARG:HD3	1:C:168:GLU:O	2.09	0.52
1:C:158:ASP:HB3	1:C:235:SER:HB3	1.92	0.52
1:F:175:SER:OG	1:F:177:VAL:HG22	2.10	0.52
1:B:254:TYR:C	4:B:464:HOH:O	2.51	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:3:VAL:HG11	1:F:73:ILE:HG12	1.91	0.52
1:F:158:ASP:HB3	1:F:235:SER:HB3	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:88:ALA:HB1	1:E:192:ILE:HD12	1.91	0.51
1:E:113:GLU:O	1:E:117:LEU:HD23	2.09	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:58:THR:HB	1:E:87:LEU:HD11	1.91	0.51
1:E:205:LEU:HD12	1:E:209:VAL:HB	1.89	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:CE	1:F:54:MSE:CA	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:A:78:SER:OG	1:A:79:LEU:N	2.41	0.49
1:D:104:VAL:HG11	1:D:112:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:GLY:O	1:E:84:ILE:HG23	2.13	0.48
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:A:163:GLY:C	1:A:164:MSE:HG3	2.39	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: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:88:ALA:HB2	1:E:98:LEU:HD21	1.97	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: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:7:ILE:HG21	1:C:61:VAL:HG13	1.96	0.47
1:C:67:ARG:HG2	1:C:67:ARG:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:TRP:O	1:E:90:HIS:ND1	2.39	0.46
1:E:149:GLU:O	1:E:153:GLU:HG3	2.15	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:23:VAL:HG23	1:E:24:PRO:CD	2.46	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:F:207:ILE:HA	1:F:210:GLN:NE2	2.30	0.46
1:F:77:HIS:HA	1:F:101:LEU:O	2.16	0.45
1:F:156:MSE:SE	1:F:164:MSE:HE2	2.66	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:E:39:THR:OG1	1:E:56:HIS:O	2.27	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:F:99:ILE:HD11	1:F:247:PHE:CE2	2.51	0.45
1:D:140:GLY:HA2	1:D:174:GLN:O	2.16	0.45
1:E:202:ASP:CG	1:E:205:LEU:H	2.25	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:D:101:LEU:O	1:D:102:THR:C	2.60	0.44
1:B:205:LEU:HD21	1:B:213:MSE:HE1	1.99	0.44
1:C:90:HIS:C	1:C:92:PRO:HD3	2.42	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:HD23	1:E:190:LEU:HA	1.70	0.43
1:B:159:TYR:CD1	1:B:160:PRO:HD2	2.53	0.43
1:D:78:SER:HG	2:D:301:8NL:C14	2.28	0.43
1:F:59:ARG:C	1:F:61:VAL:N	2.76	0.43
1:A:205:LEU:HD21	1:A:213:MSE:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD13	1:F:99:ILE:HA	1.80	0.42
1:F:38:LEU:O	1:F:41:HIS:HB2	2.20	0.42
1:F:79:LEU:CB	2:F:301:8NL:C18	2.97	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
1:B:238:GLU:HB2	3:B:302:SO4:S	2.60	0.42
1:C:13:LEU:HA	1:C:13:LEU:HD23	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:E:168:GLU:H	1:E:168:GLU:CD	2.24	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:55:GLU:OE1	1:E:59:ARG:NH1	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:78:SER:OG	2:B:301:8NL:O1	2.38	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:6:ILE:HG12	1:F:73:ILE:HB	2.03	0.40
1:F:41:HIS:ND1	1:F:171:ILE:HD13	2.36	0.40
1:F:54:MSE:CE	1:F:54:MSE:O	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 ⓘ

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	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 ⓘ

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%)	200 (100%)	1 (0%)	81	84
1	B	201/220 (91%)	199 (99%)	2 (1%)	68	70
1	C	200/220 (91%)	199 (100%)	1 (0%)	81	84
1	D	201/220 (91%)	200 (100%)	1 (0%)	81	84
1	E	195/220 (89%)	193 (99%)	2 (1%)	68	70
1	F	178/220 (81%)	174 (98%)	4 (2%)	45	42
All	All	1176/1320 (89%)	1165 (99%)	11 (1%)	70	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	B	113	GLU
1	B	164	MSE
1	C	78	SER

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Mol	Chain	Res	Type
1	D	93	ASP
1	E	26	LEU
1	E	164	MSE
1	F	54	MSE
1	F	58	THR
1	F	59	ARG
1	F	60	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	C	122	ASN
1	D	14	ASN
1	E	14	ASN
1	E	122	ASN
1	F	34	HIS
1	F	48	HIS
1	F	77	HIS
1	F	122	ASN
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 oligosaccharides 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	4.75	16 (34%)
2	8NL	D	301	-	31,31,31	1.69	2 (6%)	46,47,47	3.24	16 (34%)
3	SO4	B	302	-	4,4,4	0.34	0	6,6,6	0.47	0
2	8NL	A	301	-	31,31,31	1.74	3 (9%)	46,47,47	3.35	23 (50%)
3	SO4	C	302	-	4,4,4	0.29	0	6,6,6	0.46	0
3	SO4	A	302	-	4,4,4	0.30	0	6,6,6	0.35	0
3	SO4	F	302	-	4,4,4	0.25	0	6,6,6	0.43	0
2	8NL	E	301	-	31,31,31	1.39	4 (12%)	46,47,47	3.72	22 (47%)
2	8NL	B	301	-	31,31,31	1.65	2 (6%)	46,47,47	3.16	15 (32%)
3	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.24	0
3	SO4	E	302	-	4,4,4	0.27	0	6,6,6	0.11	0
2	8NL	C	301	-	31,31,31	1.76	3 (9%)	46,47,47	3.37	19 (41%)

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	-	-	12/23/36/36	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	B	301	-	-	9/23/36/36	0/3/3/3
2	8NL	C	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	7.98	1.50	1.33
2	A	301	8NL	O-C14	7.81	1.49	1.33
2	B	301	8NL	O-C14	7.64	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	8NL	O-C14	7.49	1.49	1.33
2	E	301	8NL	O-C14	5.97	1.45	1.33
2	F	301	8NL	O-C14	5.15	1.44	1.33
2	F	301	8NL	C22-C21	3.40	1.52	1.49
2	D	301	8NL	C20-C21	3.37	1.34	1.31
2	B	301	8NL	C20-C21	3.28	1.34	1.31
2	C	301	8NL	C20-C21	3.15	1.34	1.31
2	C	301	8NL	C22-C21	2.76	1.52	1.49
2	E	301	8NL	C22-C21	2.64	1.51	1.49
2	E	301	8NL	C20-C21	2.34	1.33	1.31
2	A	301	8NL	C20-C21	2.33	1.33	1.31
2	F	301	8NL	O-C13	-2.32	1.40	1.45
2	F	301	8NL	C2-C1	-2.26	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 (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	8NL	C17-C16-C20	-19.12	88.47	122.62
2	F	301	8NL	C22-C21-CL	16.49	125.14	112.52
2	A	301	8NL	C18-C17-C16	-12.14	90.68	117.95
2	F	301	8NL	C20-C21-CL	-11.97	111.51	123.58
2	D	301	8NL	C17-C16-C20	-10.72	103.47	122.62
2	B	301	8NL	C17-C16-C20	-10.37	104.10	122.62
2	E	301	8NL	C22-C21-CL	9.89	120.09	112.52
2	D	301	8NL	C18-C17-C16	-9.80	95.93	117.95
2	A	301	8NL	C17-C16-C20	-9.28	106.05	122.62
2	C	301	8NL	C17-C16-C20	-8.92	106.69	122.62
2	C	301	8NL	C22-C21-CL	8.80	119.25	112.52
2	F	301	8NL	C18-C17-C16	-8.53	98.79	117.95
2	E	301	8NL	C16-C15-C14	-8.32	102.24	120.36
2	E	301	8NL	C20-C21-CL	-8.05	115.46	123.58
2	E	301	8NL	O-C14-C15	8.04	125.32	110.86
2	B	301	8NL	C22-C21-CL	7.68	118.40	112.52
2	C	301	8NL	C20-C21-CL	-7.38	116.14	123.58
2	E	301	8NL	C18-C17-C16	-7.33	101.48	117.95
2	C	301	8NL	C18-C17-C16	-7.26	101.64	117.95
2	C	301	8NL	O-C14-C15	6.96	123.38	110.86
2	E	301	8NL	C16-C20-C21	-6.92	119.28	125.48
2	B	301	8NL	O-C13-C2	6.87	124.16	108.73
2	E	301	8NL	C17-C16-C20	-6.66	110.74	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	8NL	C16-C15-C14	-6.64	105.89	120.36
2	A	301	8NL	C22-C21-CL	6.54	117.52	112.52
2	D	301	8NL	C22-C21-CL	6.40	117.42	112.52
2	B	301	8NL	O-C14-C15	6.19	121.99	110.86
2	C	301	8NL	O-C13-C2	5.95	122.10	108.73
2	C	301	8NL	C16-C15-C14	-5.85	107.63	120.36
2	D	301	8NL	C-C1-C2	-5.63	115.14	120.94
2	F	301	8NL	C16-C20-C21	-5.51	120.55	125.48
2	B	301	8NL	C20-C21-CL	-5.37	118.17	123.58
2	E	301	8NL	O-C14-O1	-5.31	114.42	124.14
2	A	301	8NL	C13-O-C14	5.29	126.20	116.28
2	D	301	8NL	C16-C20-C21	-5.21	120.81	125.48
2	F	301	8NL	C17-C15-C14	-4.89	110.13	122.40
2	A	301	8NL	C16-C15-C14	-4.83	109.84	120.36
2	D	301	8NL	O-C14-C15	4.78	119.45	110.86
2	E	301	8NL	C-C1-C2	-4.77	116.02	120.94
2	F	301	8NL	O-C14-O1	-4.69	115.57	124.14
2	E	301	8NL	O-C13-C2	4.54	118.92	108.73
2	A	301	8NL	C16-C20-C21	-4.49	121.45	125.48
2	D	301	8NL	O-C13-C2	4.46	118.75	108.73
2	A	301	8NL	O-C13-C2	4.39	118.59	108.73
2	B	301	8NL	C19-C17-C16	-4.32	108.24	117.95
2	C	301	8NL	O-C14-O1	-4.23	116.40	124.14
2	B	301	8NL	C-C1-C2	-4.11	116.71	120.94
2	C	301	8NL	C15-C16-C20	-4.07	115.34	121.07
2	D	301	8NL	C16-C15-C14	-4.02	111.60	120.36
2	F	301	8NL	C3-C2-C1	4.00	122.35	119.49
2	C	301	8NL	C18-C17-C15	3.93	130.36	117.97
2	A	301	8NL	O-C14-C15	3.92	117.92	110.86
2	D	301	8NL	C13-C2-C1	-3.89	114.95	122.64
2	D	301	8NL	C18-C17-C15	3.88	130.19	117.97
2	E	301	8NL	C13-C2-C1	-3.86	115.02	122.64
2	E	301	8NL	C19-C17-C18	3.83	118.55	113.46
2	F	301	8NL	O-C14-C15	3.78	117.65	110.86
2	D	301	8NL	F-C22-C21	-3.77	106.42	112.50
2	A	301	8NL	C20-C21-CL	-3.74	119.81	123.58
2	C	301	8NL	C-C1-C2	-3.66	117.17	120.94
2	F	301	8NL	C13-O-C14	-3.51	109.69	116.28
2	B	301	8NL	O1-C14-C15	-3.51	118.90	125.25
2	B	301	8NL	F-C22-C21	-3.51	106.84	112.50
2	D	301	8NL	C20-C21-CL	-3.51	120.04	123.58
2	C	301	8NL	C13-C2-C1	-3.51	115.71	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	8NL	C17-C15-C14	-3.51	113.60	122.40
2	F	301	8NL	C13-C2-C1	-3.44	115.84	122.64
2	E	301	8NL	C15-C16-C20	-3.42	116.25	121.07
2	A	301	8NL	C18-C17-C15	3.32	128.41	117.97
2	B	301	8NL	C13-C2-C1	-3.27	116.19	122.64
2	A	301	8NL	F-C22-C21	-3.22	107.31	112.50
2	B	301	8NL	C19-C17-C15	3.15	127.90	117.97
2	A	301	8NL	C3-C2-C1	-3.07	117.30	119.49
2	F	301	8NL	C18-C17-C15	3.02	127.48	117.97
2	C	301	8NL	C17-C15-C14	2.99	129.91	122.40
2	A	301	8NL	C-C1-C2	-2.94	117.91	120.94
2	C	301	8NL	O1-C14-C15	-2.83	120.13	125.25
2	B	301	8NL	C16-C20-C21	2.81	127.99	125.48
2	E	301	8NL	O1-C14-C15	-2.79	120.20	125.25
2	B	301	8NL	O-C14-O1	-2.79	119.05	124.14
2	A	301	8NL	O1-C14-C15	-2.77	120.24	125.25
2	A	301	8NL	F2-C22-C21	-2.75	108.08	112.50
2	F	301	8NL	F-C22-C21	-2.73	108.11	112.50
2	D	301	8NL	C13-C2-C3	2.65	125.25	119.51
2	A	301	8NL	C12-C7-C6	2.61	125.22	120.91
2	B	301	8NL	C13-C2-C3	2.57	125.08	119.51
2	A	301	8NL	C15-C16-C20	2.57	124.69	121.07
2	C	301	8NL	F1-C22-C21	-2.52	108.44	112.50
2	E	301	8NL	F1-C22-C21	-2.48	108.50	112.50
2	A	301	8NL	C7-C6-C1	2.48	126.56	122.47
2	F	301	8NL	C-C1-C2	-2.46	118.41	120.94
2	D	301	8NL	O1-C14-C15	-2.45	120.83	125.25
2	D	301	8NL	O-C14-O1	-2.42	119.72	124.14
2	E	301	8NL	C3-C2-C1	2.38	121.19	119.49
2	C	301	8NL	C5-C6-C1	-2.33	117.50	119.92
2	C	301	8NL	C17-C16-C15	2.30	61.48	59.96
2	E	301	8NL	C13-O-C14	-2.29	111.98	116.28
2	A	301	8NL	C9-C8-C7	2.27	123.12	120.54
2	F	301	8NL	C4-C3-C2	-2.21	117.64	120.88
2	A	301	8NL	C13-C2-C1	2.18	126.94	122.64
2	E	301	8NL	F2-C22-C21	-2.15	109.03	112.50
2	E	301	8NL	C12-C7-C6	2.12	124.42	120.91
2	E	301	8NL	C5-C6-C1	-2.11	117.74	119.92
2	A	301	8NL	C11-C10-C9	-2.10	116.99	119.87
2	C	301	8NL	C19-C17-C16	-2.10	113.23	117.95
2	F	301	8NL	F2-C22-C21	-2.07	109.17	112.50
2	E	301	8NL	C8-C7-C6	-2.07	117.48	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	8NL	C4-C3-C2	-2.06	117.86	120.88
2	A	301	8NL	C17-C16-C15	2.06	61.32	59.96
2	A	301	8NL	C5-C6-C7	-2.03	114.66	118.70
2	D	301	8NL	C17-C15-C14	-2.03	117.31	122.40

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
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	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	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	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

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

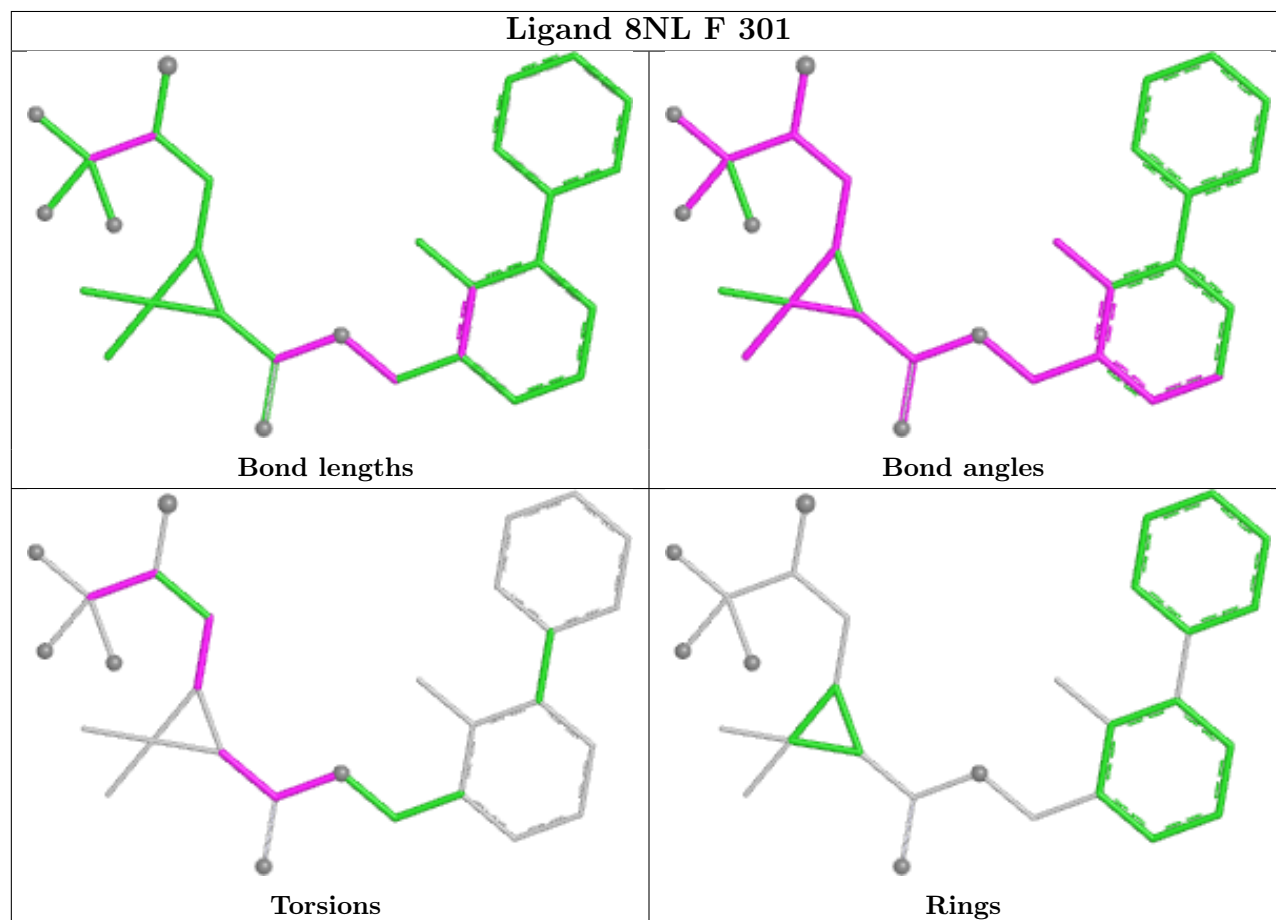
There are no ring outliers.

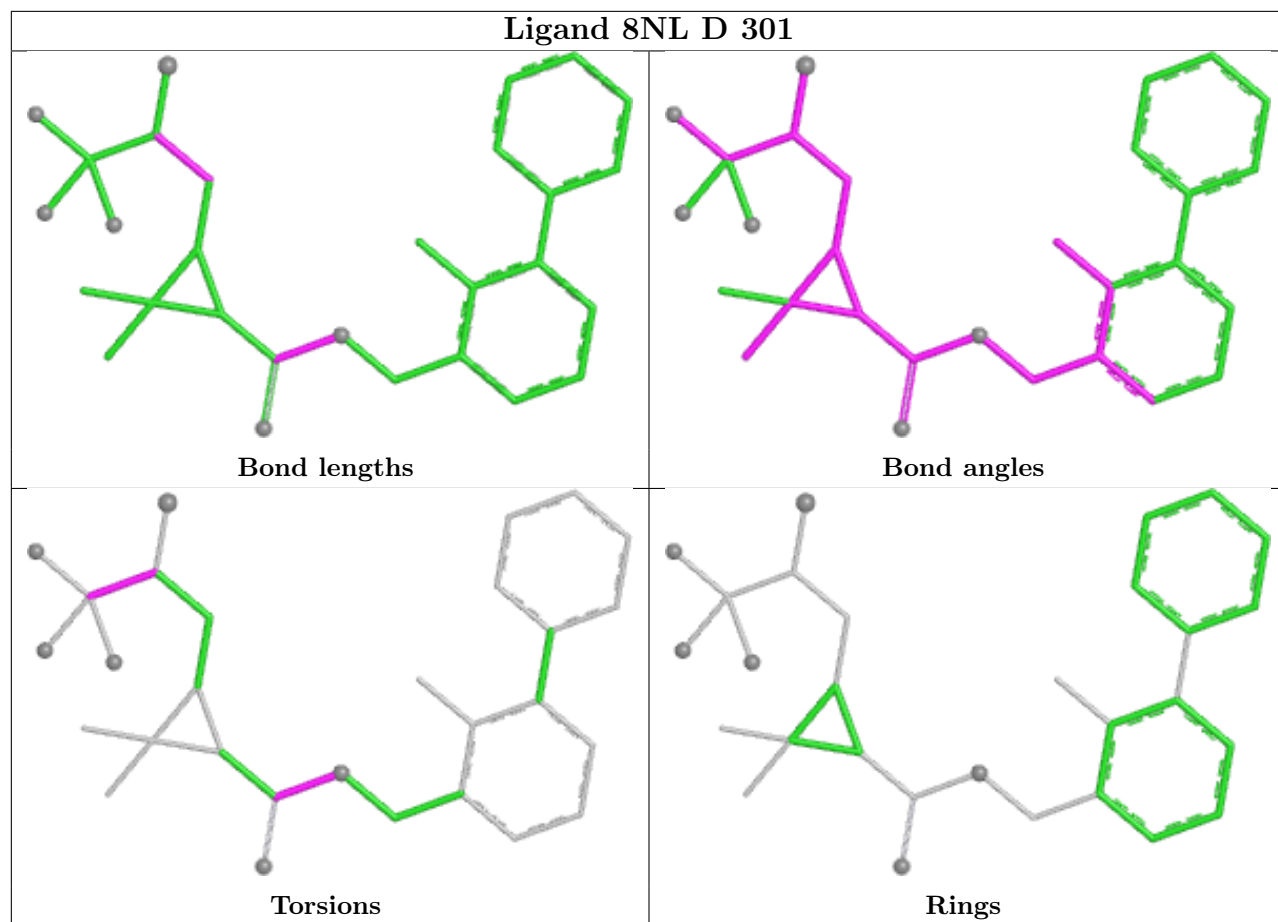
9 monomers are involved in 20 short contacts:

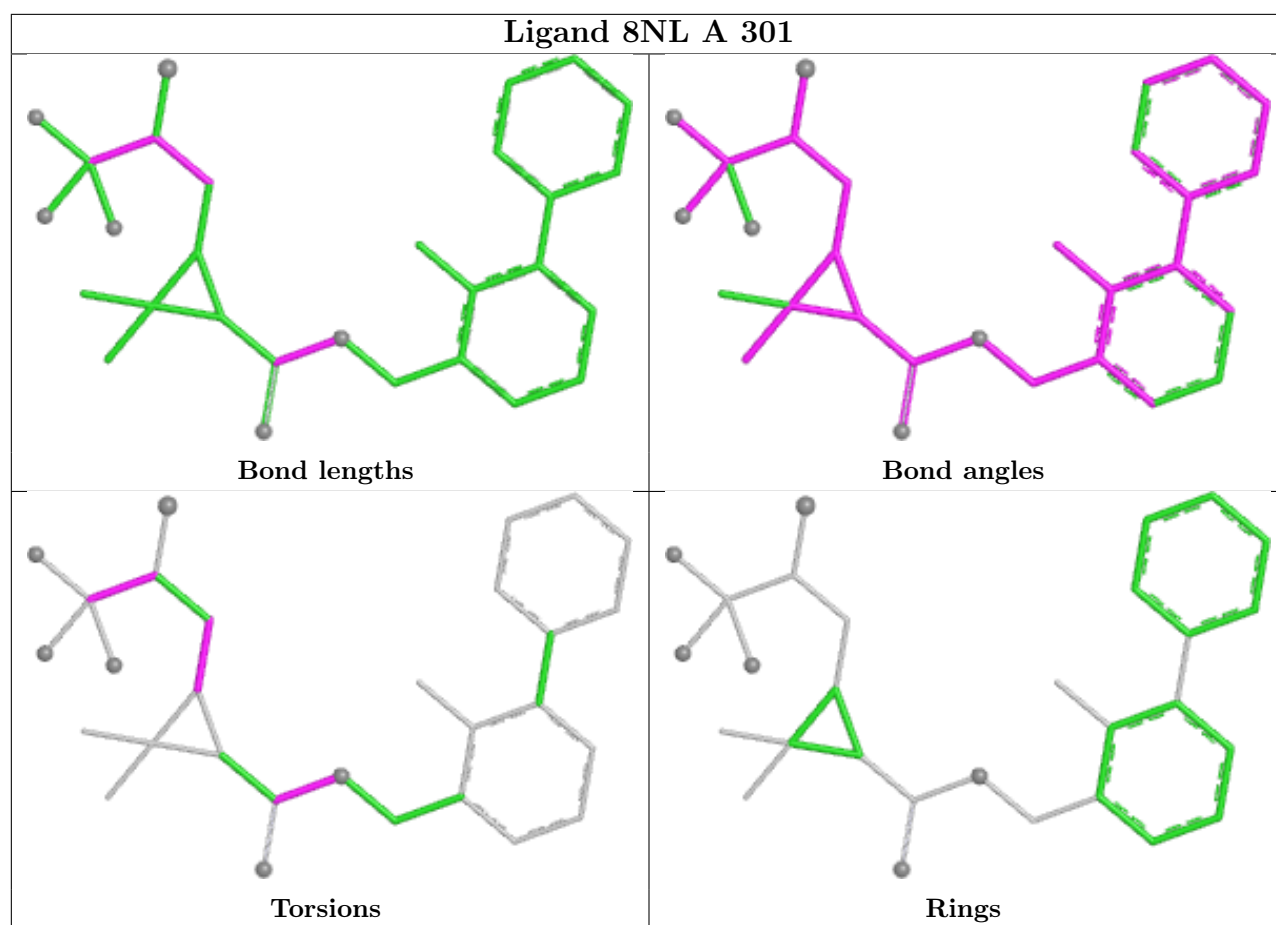
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	8NL	6	0
2	D	301	8NL	4	0
3	B	302	SO4	1	0
2	A	301	8NL	2	0
3	A	302	SO4	1	0
2	E	301	8NL	2	0
2	B	301	8NL	2	0
3	D	302	SO4	1	0
2	C	301	8NL	1	0

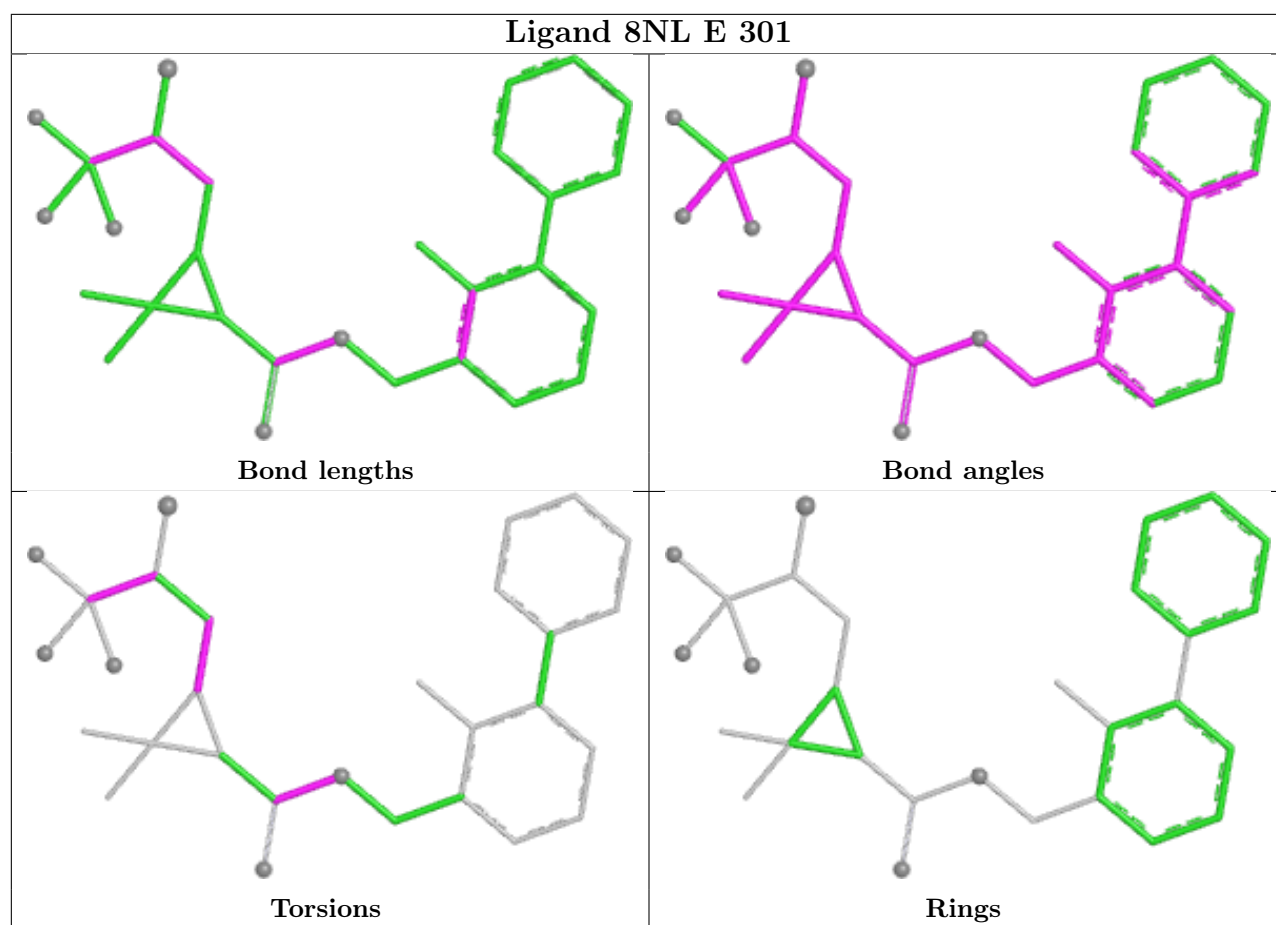
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

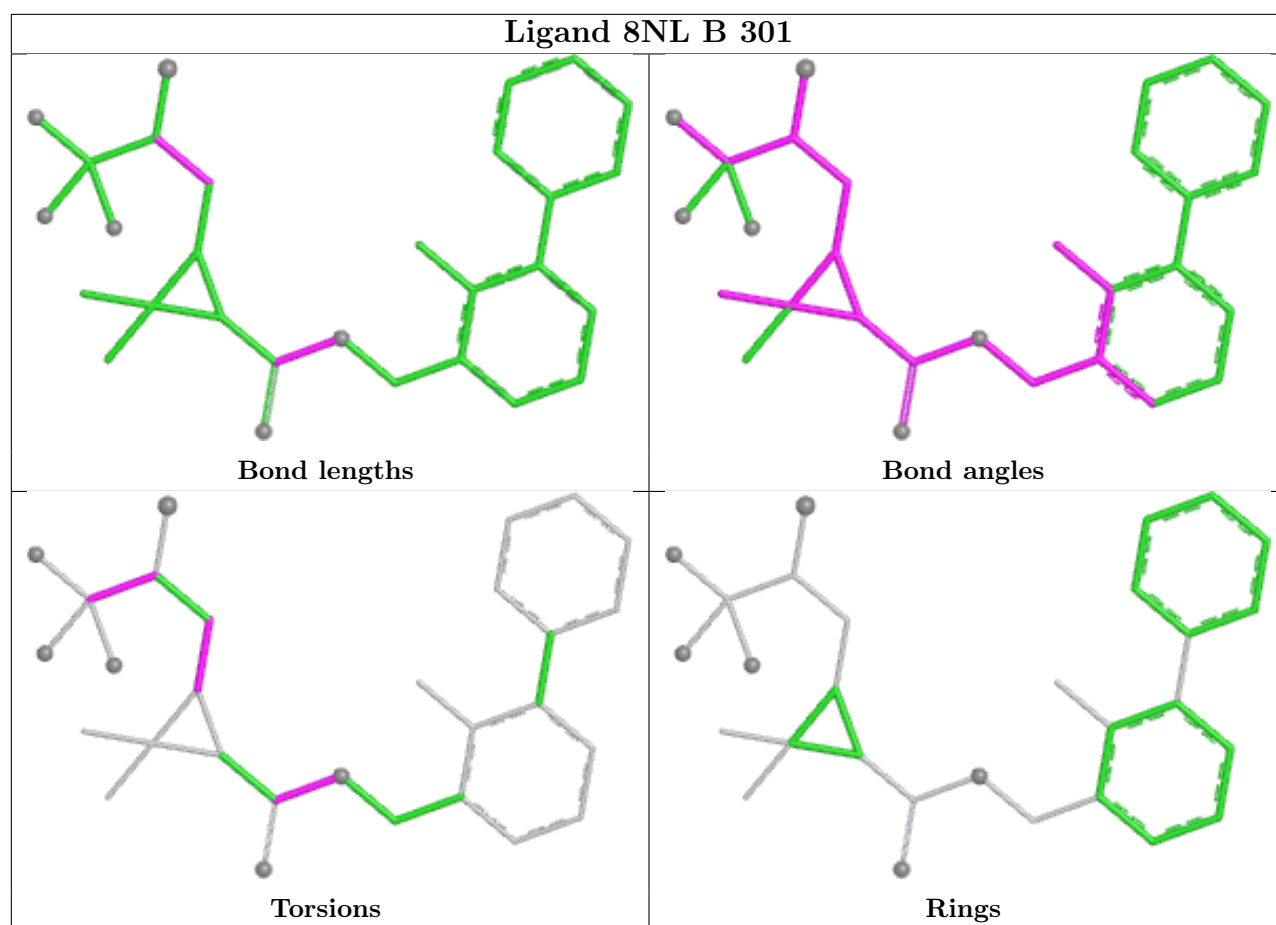
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

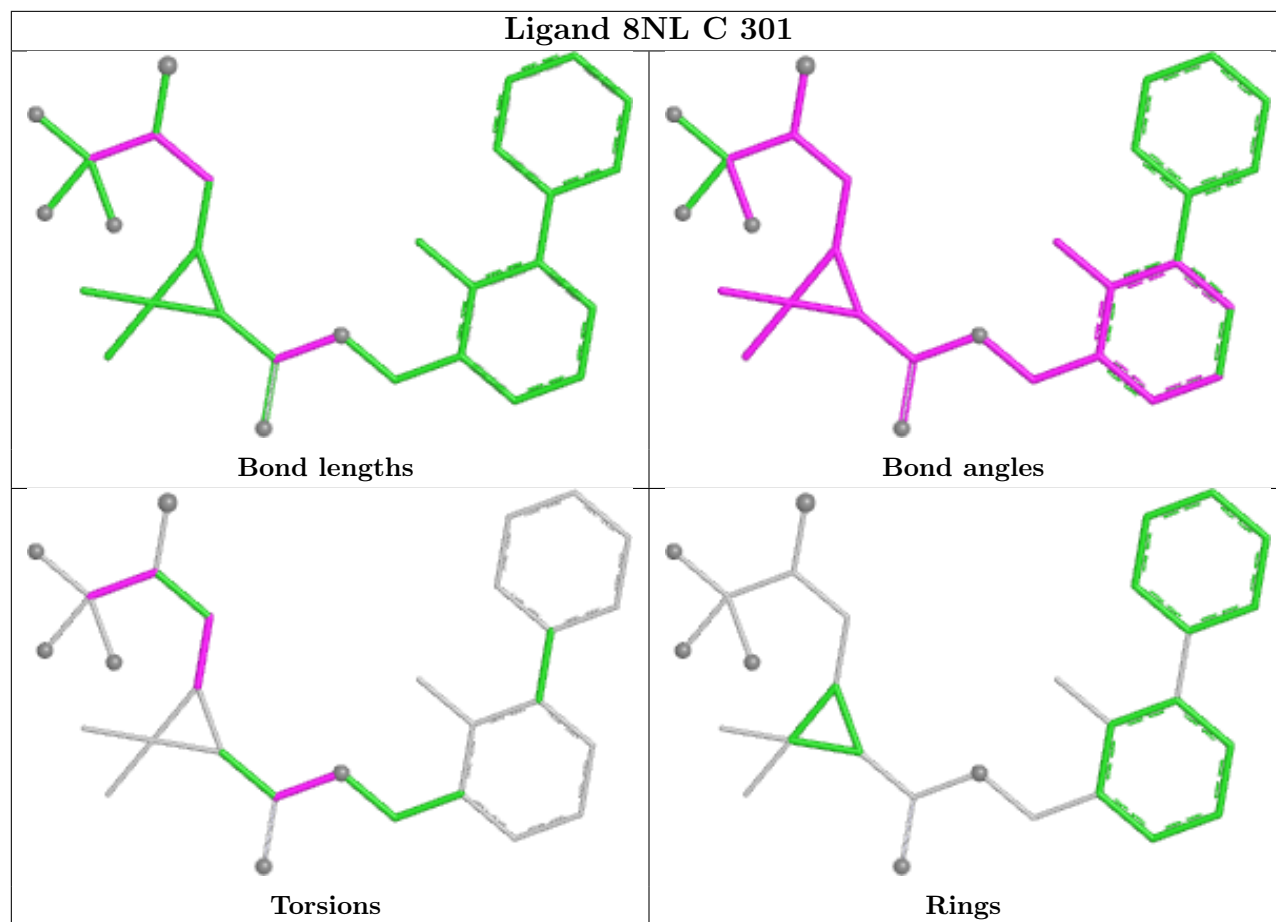












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	246/288 (85%)	0.04	3 (1%) 76 79	13, 24, 38, 50	0
1	B	246/288 (85%)	0.08	1 (0%) 88 90	14, 24, 37, 49	0
1	C	246/288 (85%)	0.66	16 (6%) 25 26	18, 33, 50, 60	0
1	D	247/288 (85%)	0.56	17 (6%) 23 24	17, 28, 44, 54	0
1	E	245/288 (85%)	1.89	99 (40%) 0 0	25, 43, 59, 71	0
1	F	245/288 (85%)	2.62	167 (68%) 0 0	30, 56, 74, 90	0
All	All	1475/1728 (85%)	0.97	303 (20%) 2 2	13, 33, 65, 90	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	87	LEU	6.3
1	F	86	TRP	6.1
1	F	189	ALA	6.1
1	F	84	ILE	6.0
1	E	86	TRP	5.5
1	F	83	SER	5.4
1	F	218	PRO	5.2
1	F	3	VAL	5.0
1	F	188	ARG	4.9
1	F	82	ALA	4.9
1	F	190	LEU	4.9
1	E	190	LEU	4.9
1	F	221	VAL	4.8
1	F	108	PRO	4.8
1	F	217	PHE	4.8
1	F	51	VAL	4.8
1	F	80	GLY	4.8
1	F	179	PHE	4.7
1	F	112	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	110	VAL	4.6
1	F	220	PRO	4.6
1	E	107	ALA	4.5
1	F	57	TYR	4.5
1	F	38	LEU	4.5
1	F	100	TYR	4.4
1	F	143	ALA	4.4
1	E	179	PHE	4.3
1	F	105	LEU	4.3
1	F	175	SER	4.3
1	F	178	PRO	4.2
1	F	12	ALA	4.2
1	F	88	ALA	4.2
1	F	60	PRO	4.2
1	F	184	PRO	4.2
1	E	135	VAL	4.1
1	F	65	LEU	4.1
1	F	247	PHE	4.1
1	F	181	THR	4.1
1	F	183	ASN	4.1
1	F	134	PRO	4.1
1	E	117	LEU	4.0
1	F	121	PRO	4.0
1	E	88	ALA	4.0
1	E	192	ILE	4.0
1	E	221	VAL	4.0
1	E	66	ALA	3.9
1	F	107	ALA	3.9
1	F	139	ARG	3.9
1	F	141	LEU	3.8
1	F	195	LEU	3.8
1	E	189	ALA	3.8
1	F	17	ALA	3.8
1	F	39	THR	3.7
1	E	217	PHE	3.7
1	F	44	GLY	3.7
1	F	81	GLY	3.7
1	F	219	GLY	3.7
1	F	50	SER	3.7
1	F	111	THR	3.7
1	F	222	ALA	3.7
1	F	52	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	95	VAL	3.7
1	E	2	THR	3.6
1	F	140	GLY	3.6
1	F	61	VAL	3.6
1	F	176	THR	3.6
1	F	6	ILE	3.6
1	F	192	ILE	3.6
1	F	163	GLY	3.5
1	C	2	THR	3.5
1	F	58	THR	3.5
1	F	177	VAL	3.5
1	F	96	ALA	3.5
1	E	106	THR	3.4
1	F	49	LEU	3.4
1	F	64	ILE	3.4
1	F	187	GLY	3.4
1	F	104	VAL	3.4
1	F	23	VAL	3.3
1	C	65	LEU	3.3
1	F	99	ILE	3.3
1	E	74	LEU	3.3
1	F	36	PRO	3.3
1	E	44	GLY	3.3
1	C	66	ALA	3.2
1	F	106	THR	3.2
1	F	145	PHE	3.2
1	F	109	GLY	3.2
1	F	191	GLU	3.2
1	F	216	GLU	3.2
1	E	141	LEU	3.2
1	B	161	GLY	3.2
1	F	2	THR	3.1
1	E	110	VAL	3.1
1	E	108	PRO	3.1
1	F	47	GLY	3.1
1	E	115	PHE	3.1
1	E	70	GLY	3.1
1	F	7	ILE	3.1
1	F	193	PRO	3.1
1	F	68	ALA	3.1
1	E	73	ILE	3.0
1	F	53	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	157	GLY	3.0
1	E	13	LEU	3.0
1	C	163	GLY	3.0
1	D	208	ALA	3.0
1	F	76	GLY	3.0
1	E	165	PRO	3.0
1	F	250	ALA	3.0
1	F	9	ILE	3.0
1	E	65	LEU	2.9
1	E	51	VAL	2.9
1	F	16	GLY	2.9
1	E	182	PRO	2.9
1	F	232	PRO	2.9
1	F	241	ALA	2.9
1	C	252	ALA	2.9
1	F	167	ALA	2.9
1	F	245	ALA	2.9
1	E	98	LEU	2.9
1	F	79	LEU	2.9
1	A	138	GLY	2.9
1	C	3	VAL	2.9
1	F	197	ILE	2.9
1	F	40	GLY	2.9
1	E	3	VAL	2.8
1	E	95	VAL	2.8
1	E	184	PRO	2.8
1	F	41	HIS	2.8
1	F	170	PHE	2.8
1	F	248	ALA	2.8
1	F	63	ASP	2.8
1	E	64	ILE	2.8
1	E	79	LEU	2.8
1	E	122	ASN	2.8
1	F	138	GLY	2.8
1	E	251	PRO	2.8
1	F	66	ALA	2.8
1	F	26	LEU	2.8
1	F	34	HIS	2.8
1	E	118	PRO	2.8
1	E	126	PRO	2.8
1	F	182	PRO	2.8
1	F	224	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	68	ALA	2.8
1	E	38	LEU	2.8
1	E	105	LEU	2.8
1	F	171	ILE	2.8
1	F	244	ILE	2.8
1	E	112	PRO	2.8
1	F	72	SER	2.7
1	F	19	TYR	2.7
1	C	107	ALA	2.7
1	F	94	LYS	2.7
1	F	173	THR	2.7
1	F	98	LEU	2.7
1	F	165	PRO	2.7
1	F	114	THR	2.7
1	F	75	LEU	2.7
1	E	203	VAL	2.7
1	F	169	HIS	2.7
1	E	68	ALA	2.7
1	E	143	ALA	2.7
1	E	167	ALA	2.7
1	F	115	PHE	2.7
1	F	35	ALA	2.6
1	F	144	ASP	2.6
1	F	55	GLU	2.6
1	E	177	VAL	2.6
1	F	11	GLY	2.6
1	F	97	GLY	2.6
1	E	212	GLN	2.6
1	E	69	GLU	2.6
1	F	31	TYR	2.6
1	E	4	THR	2.6
1	F	56	HIS	2.6
1	F	129	LEU	2.6
1	D	162	GLU	2.6
1	E	28	ALA	2.6
1	E	252	ALA	2.6
1	E	145	PHE	2.6
1	E	205	LEU	2.6
1	E	40	GLY	2.6
1	F	46	GLY	2.6
1	E	62	ALA	2.6
1	F	28	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	62	ALA	2.6
1	F	135	VAL	2.6
1	E	48	HIS	2.5
1	D	254	TYR	2.5
1	F	92	PRO	2.5
1	E	155	PHE	2.5
1	C	63	ASP	2.5
1	F	117	LEU	2.5
1	E	175	SER	2.5
1	F	18	CYS	2.5
1	F	196	TYR	2.5
1	E	87	LEU	2.5
1	F	8	LEU	2.5
1	F	25	LEU	2.5
1	A	163	GLY	2.5
1	E	109	GLY	2.5
1	E	132	ILE	2.5
1	F	73	ILE	2.5
1	F	132	ILE	2.5
1	E	39	THR	2.5
1	C	160	PRO	2.5
1	E	166	PRO	2.5
1	F	194	ARG	2.5
1	E	7	ILE	2.5
1	E	78	SER	2.5
1	E	43	PRO	2.5
1	E	60	PRO	2.5
1	D	119	GLY	2.4
1	F	233	TYR	2.4
1	E	52	VAL	2.4
1	E	161	GLY	2.4
1	F	172	GLN	2.4
1	C	31	TYR	2.4
1	F	13	LEU	2.4
1	F	4	THR	2.4
1	E	96	ALA	2.4
1	F	59	ARG	2.4
1	A	161	GLY	2.4
1	E	90	HIS	2.4
1	E	138	GLY	2.4
1	F	180	GLY	2.4
1	D	222	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	184	PRO	2.4
1	E	169	HIS	2.4
1	F	10	HIS	2.4
1	E	116	VAL	2.4
1	D	115	PHE	2.3
1	F	89	GLN	2.3
1	D	207	ILE	2.3
1	E	84	ILE	2.3
1	F	70	GLY	2.3
1	D	223	VAL	2.3
1	E	33	VAL	2.3
1	E	204	VAL	2.3
1	F	133	GLN	2.3
1	F	151	LEU	2.3
1	F	174	GLN	2.3
1	E	17	ALA	2.3
1	E	178	PRO	2.3
1	F	131	LEU	2.3
1	D	114	THR	2.3
1	E	231	ALA	2.3
1	E	250	ALA	2.3
1	F	21	ALA	2.3
1	E	30	GLY	2.3
1	D	221	VAL	2.3
1	E	23	VAL	2.3
1	F	101	LEU	2.3
1	F	30	GLY	2.2
1	E	85	SER	2.2
1	F	93	ASP	2.2
1	F	154	VAL	2.2
1	F	209	VAL	2.2
1	F	48	HIS	2.2
1	E	58	THR	2.2
1	F	203	VAL	2.2
1	E	181	THR	2.2
1	E	57	TYR	2.2
1	F	204	VAL	2.2
1	F	5	ASP	2.2
1	E	193	PRO	2.2
1	F	71	GLN	2.1
1	E	93	ASP	2.1
1	E	111	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	190	LEU	2.1
1	F	90	HIS	2.1
1	C	93	ASP	2.1
1	F	136	ASP	2.1
1	E	104	VAL	2.1
1	D	253	GLU	2.1
1	F	69	GLU	2.1
1	F	77	HIS	2.1
1	F	91	HIS	2.1
1	E	183	ASN	2.1
1	D	245	ALA	2.1
1	E	12	ALA	2.1
1	C	192	ILE	2.1
1	E	254	TYR	2.1
1	F	207	ILE	2.1
1	F	137	GLU	2.1
1	D	163	GLY	2.1
1	E	119	GLY	2.1
1	F	231	ALA	2.1
1	E	139	ARG	2.1
1	F	186	GLU	2.0
1	E	180	GLY	2.0
1	C	51	VAL	2.0
1	D	209	VAL	2.0
1	F	199	ALA	2.0
1	F	146	SER	2.0
1	D	217	PHE	2.0
1	E	100	TYR	2.0
1	D	3	VAL	2.0
1	D	123	ARG	2.0
1	E	59	ARG	2.0
1	F	223	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

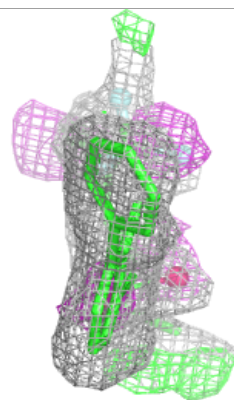
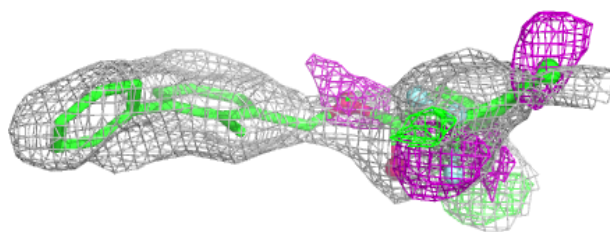
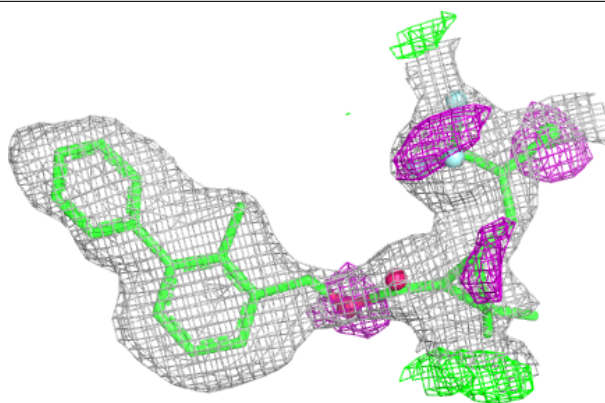
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8NL	E	301	29/29	0.69	0.15	26,41,57,74	0
2	8NL	F	301	29/29	0.75	0.14	40,50,61,64	0
2	8NL	D	301	29/29	0.82	0.12	19,26,37,83	0
2	8NL	A	301	29/29	0.84	0.11	16,24,36,67	0
2	8NL	B	301	29/29	0.84	0.11	20,26,38,73	0
2	8NL	C	301	29/29	0.84	0.11	20,27,36,47	0
3	SO4	F	302	5/5	0.88	0.12	37,45,52,53	0
3	SO4	B	302	5/5	0.91	0.11	26,31,39,43	0
3	SO4	D	302	5/5	0.92	0.09	39,39,50,52	0
3	SO4	E	302	5/5	0.93	0.11	36,38,43,44	0
3	SO4	C	302	5/5	0.96	0.08	31,33,37,38	0
3	SO4	A	302	5/5	0.98	0.06	25,27,33,34	0

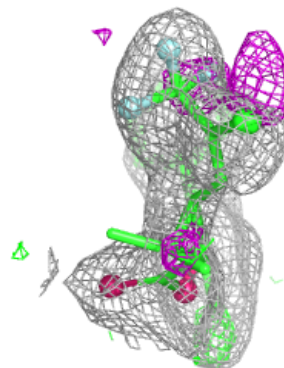
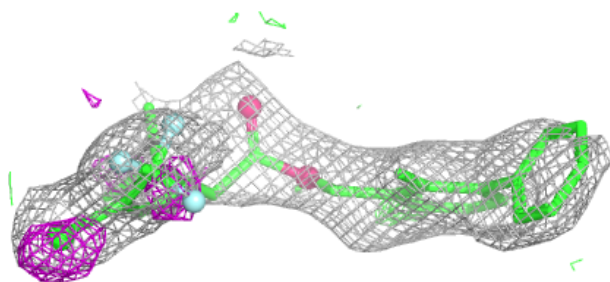
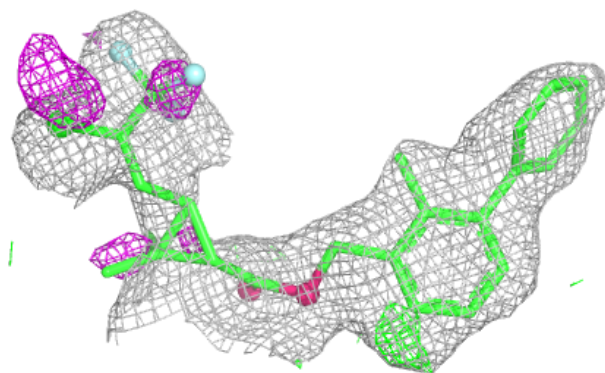
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8NL E 301:

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

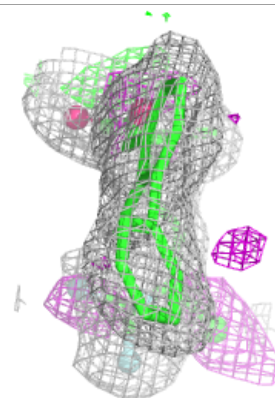
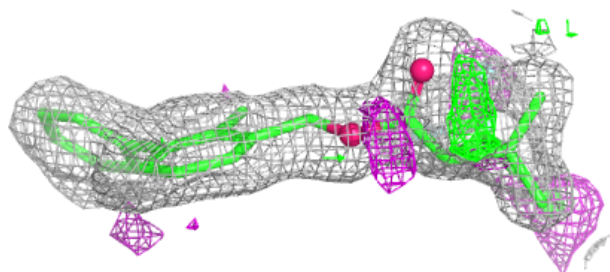
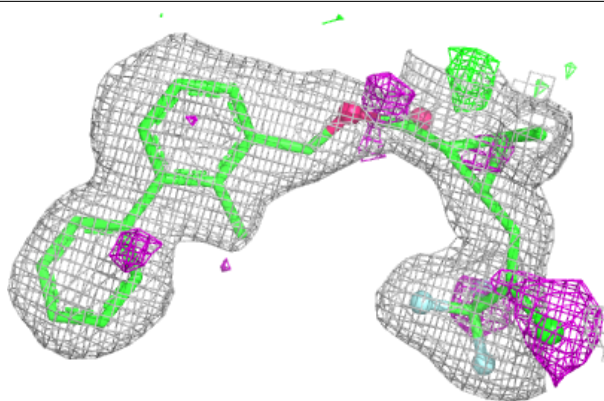
**Electron density around 8NL F 301:**

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

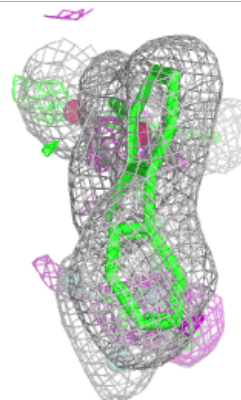
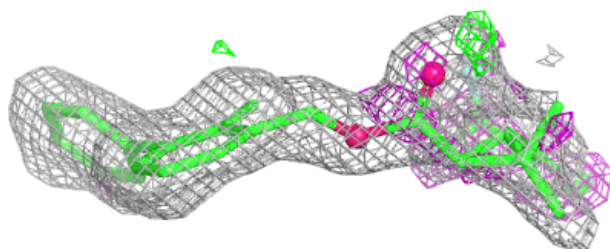
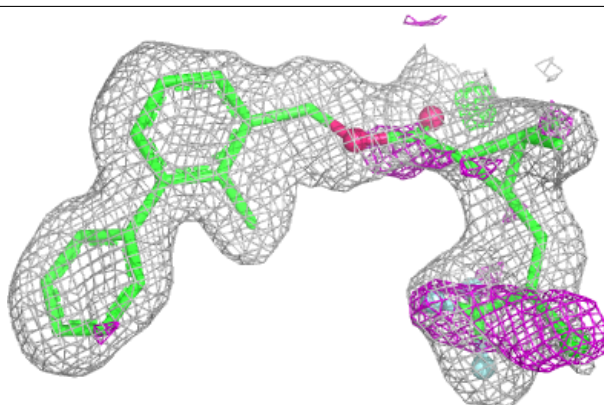


Electron density around 8NL D 301:

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

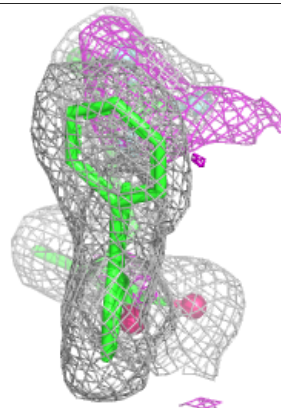
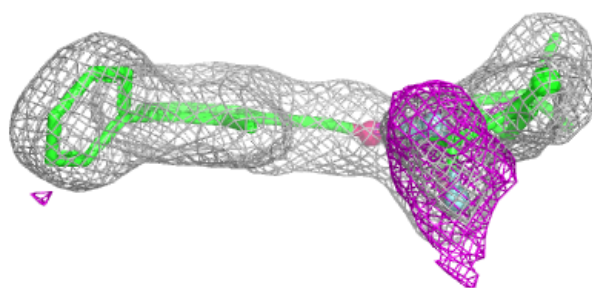
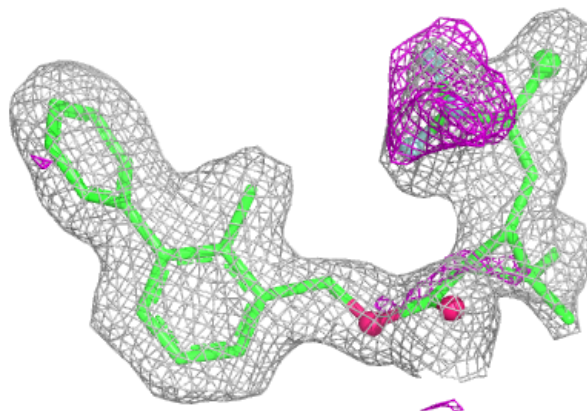
**Electron density around 8NL A 301:**

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

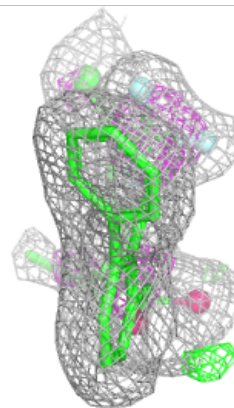
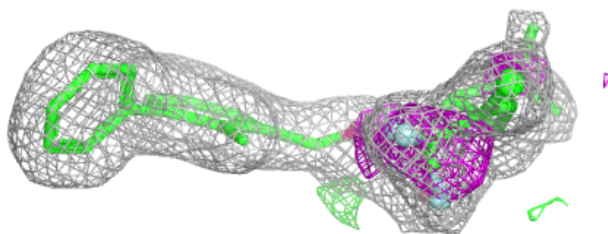
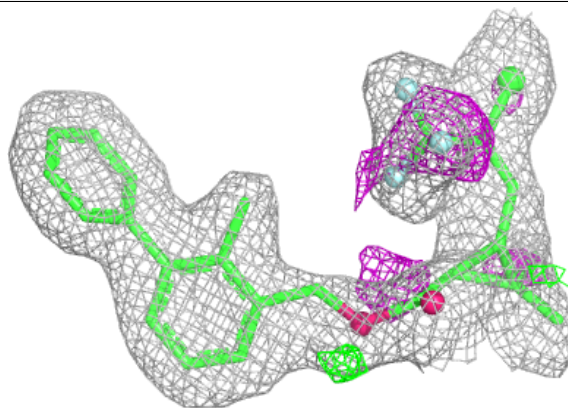


Electron density around 8NL B 301:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.