



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 AM UTC

PDB ID : 3CDB / pdb\_00003cdb  
Title : Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors  
Authors : Pavlovsky, A.; Sarver, R.W.; Harris, M.S.; Finzel, B.C.  
Deposited on : 2008-02-26  
Resolution : 2.30 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

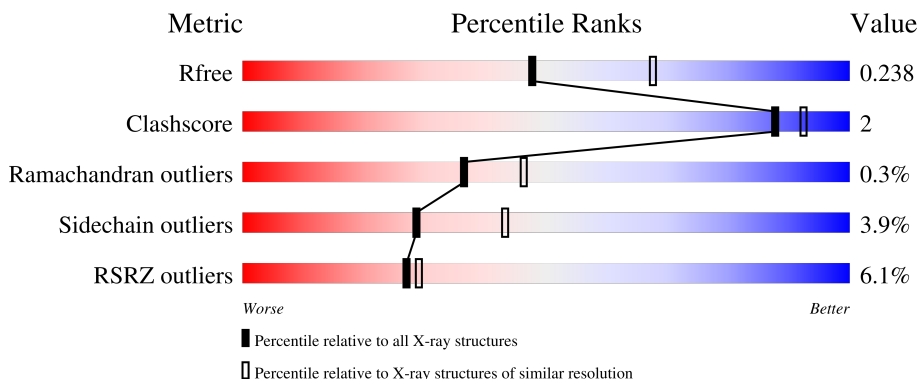
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	441	
1	B	441	
1	C	441	
1	D	441	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13109 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3133	1951	551	601	30	0	0	0
1	B	421	3139	1954	552	602	31	0	2	0
1	C	415	3086	1923	541	591	31	0	1	0
1	D	396	2934	1826	518	561	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

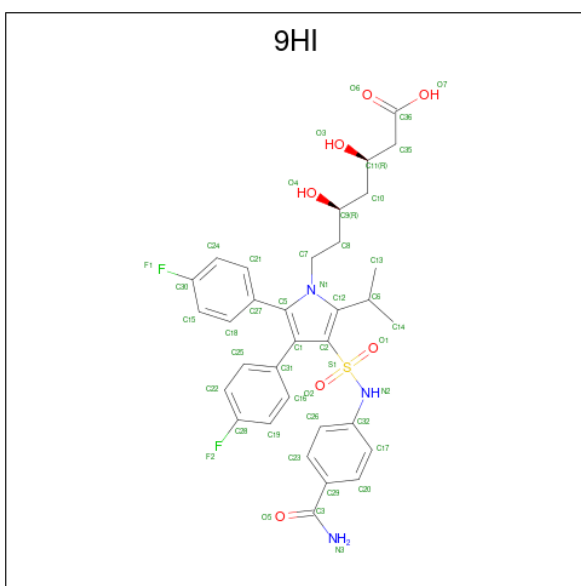
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	435	HIS	-	expression tag	UNP P04035
B	436	HIS	-	expression tag	UNP P04035
B	437	HIS	-	expression tag	UNP P04035
B	438	HIS	-	expression tag	UNP P04035
B	439	HIS	-	expression tag	UNP P04035
B	440	HIS	-	expression tag	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	435	HIS	-	expression tag	UNP P04035
C	436	HIS	-	expression tag	UNP P04035
C	437	HIS	-	expression tag	UNP P04035
C	438	HIS	-	expression tag	UNP P04035
C	439	HIS	-	expression tag	UNP P04035
C	440	HIS	-	expression tag	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035

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Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is (3R,5R)-7-{3-[(4-carbamoylphenyl)sulfamoyl]-4,5-bis(4-fluorophenyl)-2-(1-methylethyl)-1H-pyrrol-1-yl}-3,5-dihydroxyheptanoic acid (CCD ID: 9HI) (formula: C<sub>33</sub>H<sub>35</sub>F<sub>2</sub>N<sub>3</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	A	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		

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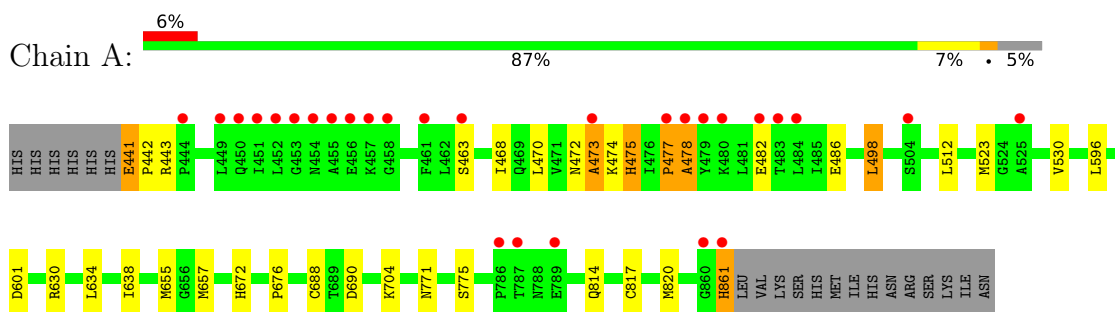
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	159	Total 159	O 159	0	0
3	C	122	Total 122	O 122	0	0
3	D	172	Total 172	O 172	0	0

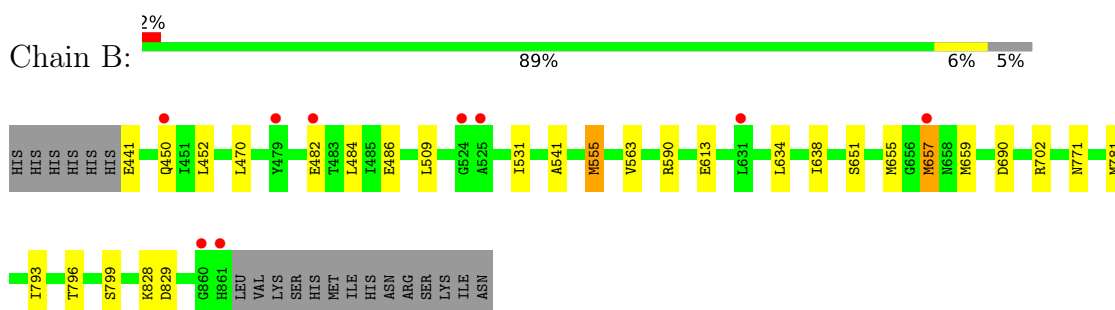
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

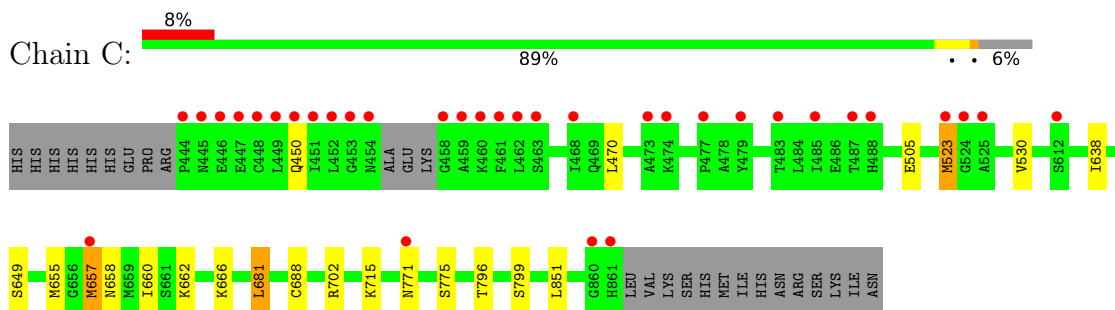
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



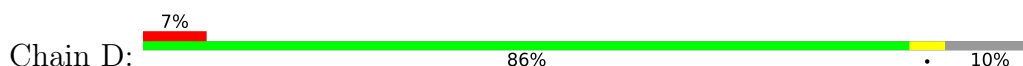
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

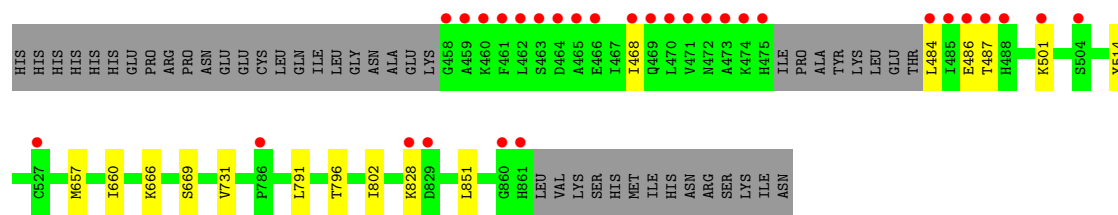


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.58Å 173.48Å 75.99Å 90.00° 118.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.30) 92.9 (50.00-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.202 , 0.239 0.204 , 0.238	Depositor DCC
$R_{free}$ test set	3509 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.021 for -h-l,-k,l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: 9HI

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	0.49	0/3179	0.78	0/4298
1	B	0.50	1/3195 (0.0%)	0.78	0/4319
1	C	0.47	0/3135	0.77	0/4236
1	D	0.48	0/2975	0.78	0/4019
All	All	0.48	1/12484 (0.0%)	0.78	0/16872

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-6.69	1.62	1.79

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	3133	0	3167	18	0
1	B	3139	0	3174	12	0
1	C	3086	0	3122	10	0
1	D	2934	0	2967	3	0
2	A	92	0	68	8	0
2	C	46	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	46	0	34	3	0
3	A	180	0	0	0	0
3	B	159	0	0	1	0
3	C	122	0	0	1	0
3	D	172	0	0	0	0
All	All	13109	0	12566	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (50) 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)
2:A:2:9HI:H13B	2:A:2:9HI:H7	1.71	0.70
1:A:655:MET:SD	1:A:657:MET:HG3	2.32	0.69
2:D:3:9HI:H13B	2:D:3:9HI:H7	1.76	0.67
2:A:1:9HI:H7	2:A:1:9HI:H13B	1.77	0.66
2:C:4:9HI:H13B	2:C:4:9HI:H7	1.79	0.64
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.79	0.64
1:C:771:ASN:OD1	1:C:775:SER:OG	2.15	0.63
2:A:1:9HI:C2	2:A:1:9HI:H26	2.31	0.60
2:A:1:9HI:H26	2:A:1:9HI:C12	2.32	0.59
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.35	0.56
1:A:861:HIS:HA	2:A:1:9HI:F2	1.96	0.55
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.92	0.52
2:D:3:9HI:H8A	2:D:3:9HI:H14B	1.93	0.51
2:C:4:9HI:O1	2:C:4:9HI:H6	2.10	0.51
1:B:655:MET:SD	1:B:657[B]:MET:HG3	2.51	0.51
1:A:820:MET:HE2	1:B:509:LEU:CD2	2.40	0.51
1:A:441:GLU:N	1:A:442:PRO:CD	2.73	0.50
2:D:3:9HI:O1	2:D:3:9HI:H6	2.12	0.50
1:A:472:ASN:O	1:A:473:ALA:HB3	2.13	0.49
1:A:657:MET:HE1	1:A:690:ASP:OD2	2.12	0.49
1:C:655:MET:HE1	1:C:657[A]:MET:HG3	1.95	0.49
2:A:2:9HI:O1	2:A:2:9HI:H6	2.14	0.48
1:C:657[B]:MET:HG3	1:C:658:ASN:N	2.28	0.48
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.48	0.48
1:A:472:ASN:O	1:A:473:ALA:CB	2.62	0.48
1:A:638:ILE:O	1:D:796:THR:HG21	2.13	0.48
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.96	0.47
1:B:638:ILE:O	1:C:796:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:MET:HE1	1:B:531:ILE:HD11	1.97	0.47
1:A:474:LYS:O	1:A:475:HIS:HB2	2.15	0.46
1:A:477:PRO:O	1:A:478:ALA:HB2	2.17	0.45
1:A:596:LEU:HB3	1:A:601:ASP:HB2	1.99	0.45
1:B:590:ARG:HD2	3:B:984:HOH:O	2.17	0.45
1:B:657[B]:MET:HE1	1:B:690:ASP:OD2	2.17	0.45
1:B:541:ALA:HB2	1:B:555:MET:HE2	1.99	0.45
1:B:702:ARG:O	1:B:799:SER:HA	2.17	0.45
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.48	0.44
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.43
1:A:771:ASN:OD1	1:A:775:SER:OG	2.36	0.43
1:A:817:CYS:HA	1:A:820:MET:HE3	2.01	0.42
1:B:796:THR:HG21	1:C:638:ILE:O	2.19	0.42
2:A:1:9HI:H14B	2:A:1:9HI:H8A	2.01	0.42
1:A:474:LYS:O	1:A:475:HIS:CB	2.67	0.42
1:C:523:MET:HE2	3:C:919:HOH:O	2.19	0.41
2:C:4:9HI:H14B	2:C:4:9HI:H8A	2.02	0.41
1:B:651:SER:HA	1:B:659:MET:HE2	2.02	0.41
1:D:468:ILE:HG21	1:D:501:LYS:NZ	2.36	0.41
2:A:1:9HI:C2	2:A:1:9HI:C26	2.99	0.41
1:C:655:MET:SD	1:C:657[A]:MET:HG3	2.61	0.41
1:B:781:MET:HE2	1:B:793:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	419/441 (95%)	395 (94%)	20 (5%)	4 (1%)	12 15
1	B	421/441 (96%)	409 (97%)	12 (3%)	0	100 100
1	C	412/441 (93%)	396 (96%)	16 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	392/441 (89%)	378 (96%)	13 (3%)	1 (0%)	36	46
All	All	1644/1764 (93%)	1578 (96%)	61 (4%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	475	HIS
1	A	478	ALA
1	D	514	TYR
1	A	477	PRO

### 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	335/355 (94%)	321 (96%)	14 (4%)	26	40
1	B	337/355 (95%)	322 (96%)	15 (4%)	24	37
1	C	331/355 (93%)	317 (96%)	14 (4%)	26	40
1	D	313/355 (88%)	302 (96%)	11 (4%)	32	48
All	All	1316/1420 (93%)	1262 (96%)	54 (4%)	28	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	463	SER
1	A	470	LEU
1	A	482	GLU
1	A	486	GLU
1	A	498	LEU
1	A	512	LEU
1	A	630	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	634	LEU
1	A	688	CYS
1	A	704	LYS
1	A	814	GLN
1	A	861	HIS
1	B	441	GLU
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	482	GLU
1	B	484	LEU
1	B	486	GLU
1	B	613	GLU
1	B	634	LEU
1	B	657[A]	MET
1	B	657[B]	MET
1	B	771[A]	ASN
1	B	771[B]	ASN
1	B	828	LYS
1	B	829	ASP
1	C	450	GLN
1	C	470	LEU
1	C	505	GLU
1	C	523	MET
1	C	649	SER
1	C	657[A]	MET
1	C	657[B]	MET
1	C	660	ILE
1	C	662	LYS
1	C	666	LYS
1	C	681	LEU
1	C	688	CYS
1	C	715	LYS
1	C	851	LEU
1	D	484	LEU
1	D	486	GLU
1	D	487	THR
1	D	657	MET
1	D	660	ILE
1	D	666	LYS
1	D	669	SER
1	D	791	LEU

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Mol	Chain	Res	Type
1	D	802	ILE
1	D	828	LYS
1	D	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	518	ASN
1	A	567	ASN
1	A	679	GLN
1	A	788	ASN
1	A	861	HIS
1	B	472	ASN
1	B	529	ASN
1	B	632	GLN
1	B	635	HIS
1	B	819	GLN
1	C	469	GLN
1	C	472	ASN
1	C	497	GLN
1	C	679	GLN
1	C	736	ASN
1	C	819	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	736	ASN
1	D	788	ASN
1	D	819	GLN
1	D	861	HIS

### 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](#)

4 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	9HI	A	2	-	48,49,49	1.21	4 (8%)	60,71,71	1.80	12 (20%)
2	9HI	A	1	-	48,49,49	1.19	4 (8%)	60,71,71	1.86	7 (11%)
2	9HI	D	3	-	48,49,49	1.23	4 (8%)	60,71,71	1.69	8 (13%)
2	9HI	C	4	-	48,49,49	1.23	4 (8%)	60,71,71	1.78	9 (15%)

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	9HI	A	2	-	-	11/38/40/40	0/4/4/4
2	9HI	A	1	-	-	5/38/40/40	0/4/4/4
2	9HI	D	3	-	-	11/38/40/40	0/4/4/4
2	9HI	C	4	-	-	10/38/40/40	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	9HI	C1-C5	4.47	1.46	1.39
2	C	4	9HI	C32-N2	-4.37	1.36	1.43
2	D	3	9HI	C32-N2	-4.35	1.36	1.43
2	A	2	9HI	C1-C5	4.32	1.46	1.39
2	C	4	9HI	C1-C5	4.14	1.46	1.39
2	A	2	9HI	C32-N2	-4.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	9HI	C1-C5	3.91	1.45	1.39
2	A	1	9HI	C32-N2	-3.79	1.37	1.43
2	A	1	9HI	C1-C2	-3.70	1.36	1.43
2	C	4	9HI	C1-C2	-3.39	1.36	1.43
2	A	2	9HI	C1-C2	-3.16	1.37	1.43
2	D	3	9HI	C1-C2	-3.01	1.37	1.43
2	A	1	9HI	C5-N1	-2.93	1.34	1.39
2	C	4	9HI	C5-N1	-2.77	1.35	1.39
2	D	3	9HI	C5-N1	-2.62	1.35	1.39
2	A	2	9HI	C5-N1	-2.54	1.35	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	9HI	O2-S1-O1	-7.47	106.11	119.82
2	C	4	9HI	C27-C5-N1	6.90	135.96	122.89
2	A	1	9HI	C27-C5-N1	6.69	135.56	122.89
2	D	3	9HI	O2-S1-O1	-6.45	108.00	119.82
2	A	2	9HI	O2-S1-O1	-6.43	108.03	119.82
2	C	4	9HI	O2-S1-O1	-6.36	108.15	119.82
2	D	3	9HI	C27-C5-N1	5.88	134.03	122.89
2	A	2	9HI	C27-C5-N1	5.58	133.46	122.89
2	C	4	9HI	C27-C5-C1	-5.49	116.56	128.66
2	A	1	9HI	C27-C5-C1	-5.27	117.06	128.66
2	D	3	9HI	C27-C5-C1	-4.88	117.91	128.66
2	A	2	9HI	C27-C5-C1	-4.49	118.76	128.66
2	A	2	9HI	C7-N1-C5	-3.14	120.87	126.72
2	D	3	9HI	C19-C28-C22	-2.71	119.25	122.80
2	D	3	9HI	C7-N1-C5	-2.64	121.80	126.72
2	D	3	9HI	C25-C22-C28	2.61	121.06	118.38
2	A	1	9HI	C7-N1-C5	-2.60	121.88	126.72
2	C	4	9HI	C7-N1-C5	-2.48	122.11	126.72
2	A	2	9HI	C7-C8-C9	-2.43	108.30	113.31
2	A	2	9HI	C11-C10-C9	-2.41	110.47	114.28
2	A	2	9HI	C14-C6-C12	-2.35	108.31	112.92
2	A	1	9HI	C25-C31-C1	-2.34	117.11	120.79
2	A	2	9HI	C21-C27-C5	-2.28	117.12	120.56
2	A	2	9HI	C25-C22-C28	2.26	120.70	118.38
2	C	4	9HI	C19-C28-C22	-2.25	119.85	122.80
2	A	2	9HI	C26-C32-N2	2.24	124.73	120.02
2	A	1	9HI	C10-C11-C35	-2.21	108.45	112.96
2	A	2	9HI	C19-C28-C22	-2.14	119.99	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	9HI	C10-C11-C35	-2.08	108.71	112.96
2	C	4	9HI	C14-C6-C12	-2.07	108.86	112.92
2	D	3	9HI	C10-C11-C35	-2.06	108.75	112.96
2	A	1	9HI	C26-C32-N2	2.05	124.34	120.02
2	C	4	9HI	C25-C22-C28	2.04	120.48	118.38
2	C	4	9HI	C24-C30-C15	-2.03	120.14	122.80
2	A	2	9HI	C16-C31-C1	-2.02	117.61	120.79
2	D	3	9HI	C24-C30-C15	-2.01	120.16	122.80

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	9HI	C32-N2-S1-O1
2	A	1	9HI	C32-N2-S1-C2
2	A	2	9HI	C2-C12-C6-C13
2	D	3	9HI	C32-N2-S1-O1
2	A	2	9HI	C20-C29-C3-N3
2	A	2	9HI	C23-C29-C3-N3
2	A	2	9HI	C20-C29-C3-O5
2	A	2	9HI	C23-C29-C3-O5
2	C	4	9HI	C20-C29-C3-N3
2	C	4	9HI	C20-C29-C3-O5
2	D	3	9HI	C20-C29-C3-N3
2	D	3	9HI	C23-C29-C3-N3
2	D	3	9HI	C20-C29-C3-O5
2	C	4	9HI	C23-C29-C3-N3
2	C	4	9HI	C23-C29-C3-O5
2	D	3	9HI	C23-C29-C3-O5
2	A	2	9HI	N1-C12-C6-C13
2	A	2	9HI	C1-C2-S1-O2
2	C	4	9HI	C1-C2-S1-O2
2	A	2	9HI	C12-C2-S1-O2
2	C	4	9HI	C12-C2-S1-O2
2	D	3	9HI	C12-C2-S1-O2
2	A	1	9HI	C32-N2-S1-O2
2	C	4	9HI	C32-N2-S1-O1
2	D	3	9HI	C2-C1-C31-C25
2	C	4	9HI	C11-C35-C36-O7
2	D	3	9HI	C11-C35-C36-O7
2	A	2	9HI	C2-C1-C31-C16
2	D	3	9HI	C2-C1-C31-C16

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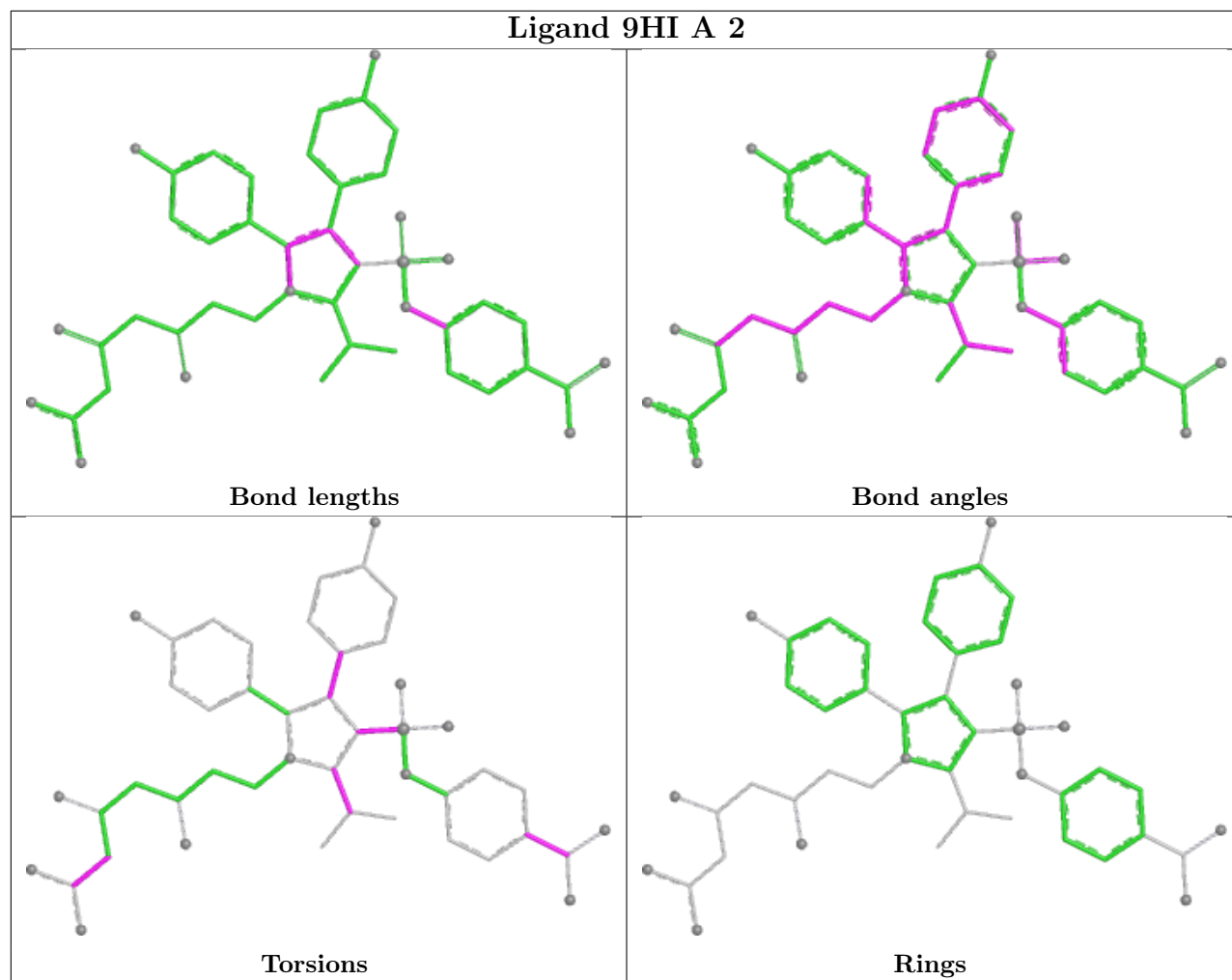
Mol	Chain	Res	Type	Atoms
2	C	4	9HI	C11-C35-C36-O6
2	D	3	9HI	C1-C2-S1-O2
2	A	2	9HI	C2-C1-C31-C25
2	A	1	9HI	C26-C32-N2-S1
2	A	2	9HI	C11-C35-C36-O7
2	D	3	9HI	C32-N2-S1-C2
2	C	4	9HI	C2-C1-C31-C25
2	A	1	9HI	C17-C32-N2-S1

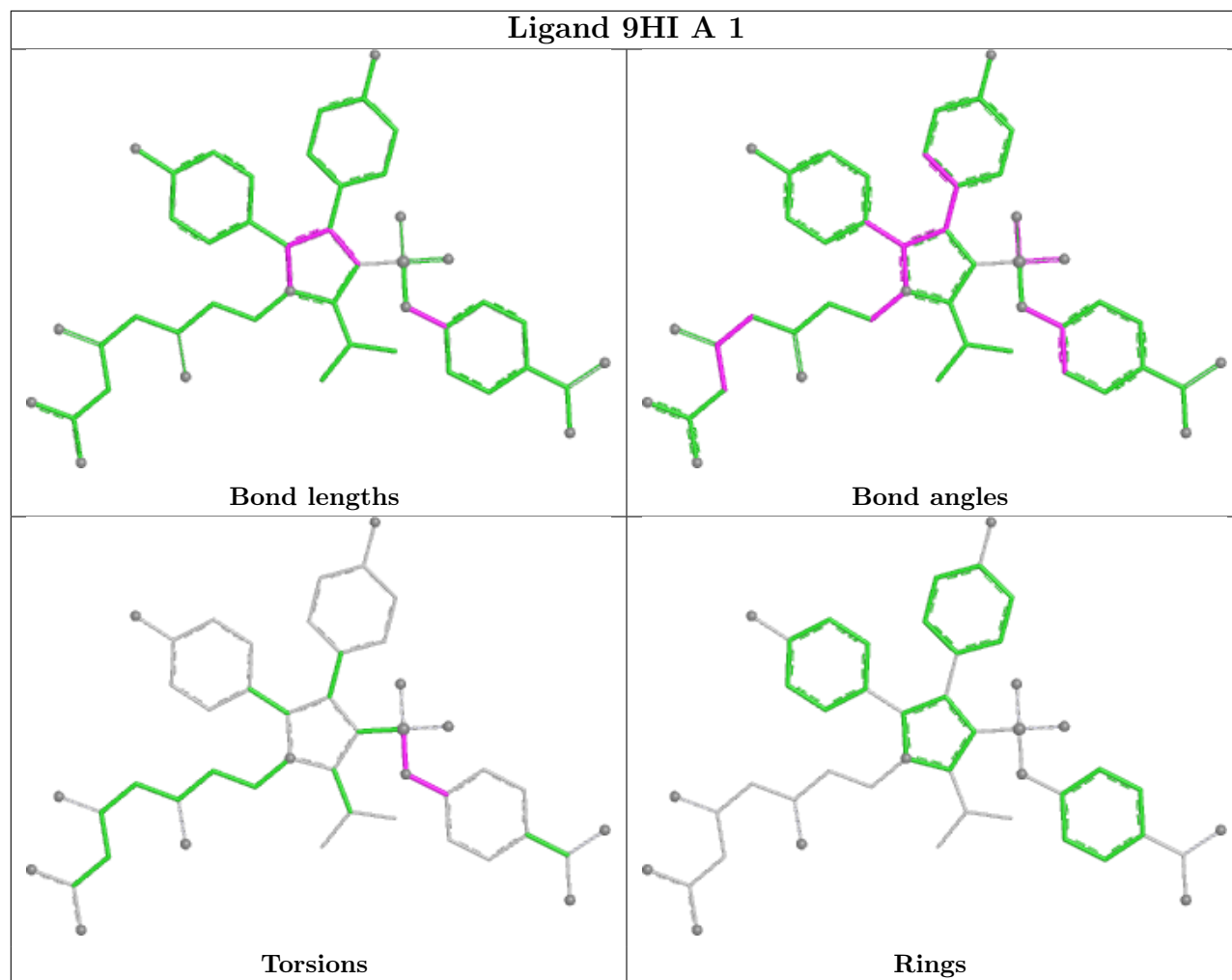
There are no ring outliers.

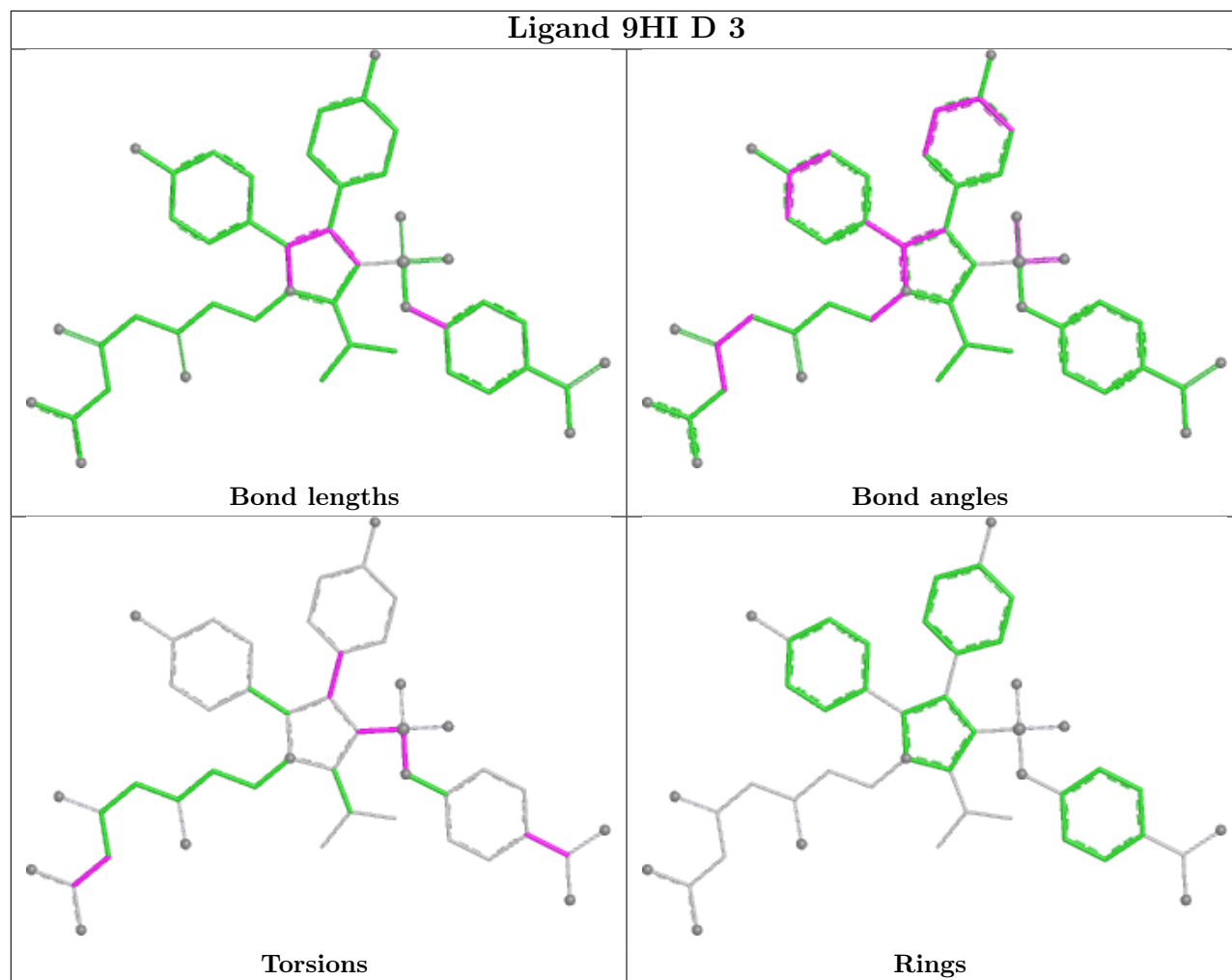
4 monomers are involved in 14 short contacts:

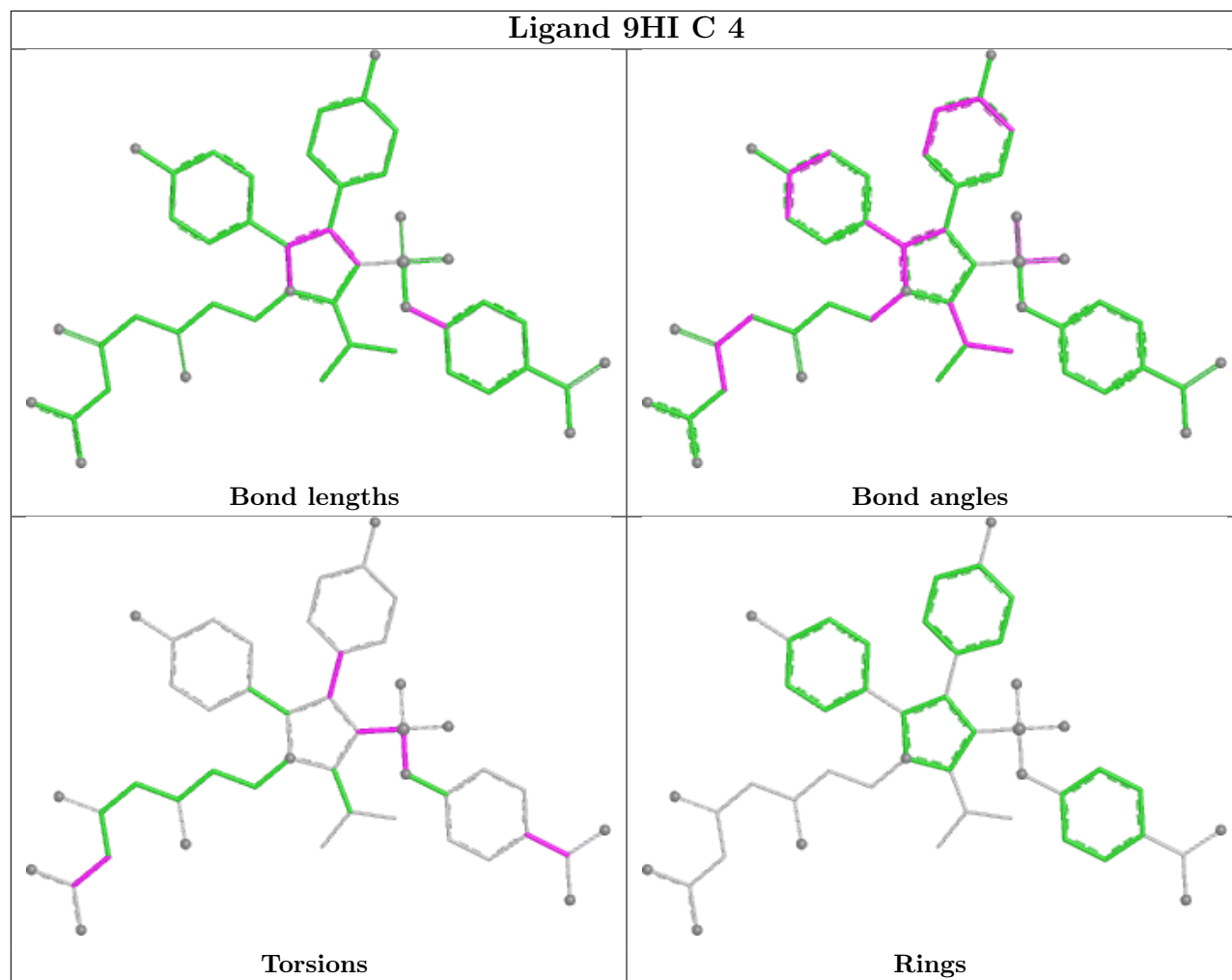
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	9HI	2	0
2	A	1	9HI	6	0
2	D	3	9HI	3	0
2	C	4	9HI	3	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	421/441 (95%)	0.32	28 (6%) 24 26	20, 32, 58, 65	0
1	B	421/441 (95%)	0.21	9 (2%) 63 65	20, 32, 44, 53	2 (0%)
1	C	415/441 (94%)	0.46	34 (8%) 17 19	19, 34, 69, 91	1 (0%)
1	D	396/441 (89%)	0.33	30 (7%) 20 21	20, 31, 68, 95	0
All	All	1653/1764 (93%)	0.33	101 (6%) 27 29	19, 32, 58, 95	3 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	HIS	6.8
1	B	861	HIS	5.4
1	D	861	HIS	5.1
1	A	483	THR	4.9
1	C	461	PHE	4.7
1	C	444	PRO	4.7
1	D	465	ALA	4.7
1	D	484	LEU	4.3
1	D	475	HIS	4.2
1	C	861	HIS	4.2
1	A	479	TYR	4.1
1	D	462	LEU	4.1
1	D	463	SER	4.0
1	C	451	ILE	4.0
1	C	454	ASN	3.9
1	C	448	CYS	3.7
1	D	468	ILE	3.7
1	D	471	VAL	3.7
1	D	461	PHE	3.7
1	B	860	GLY	3.7
1	B	524	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	525	ALA	3.5
1	A	452	LEU	3.5
1	D	458	GLY	3.4
1	C	473	ALA	3.4
1	C	452	LEU	3.4
1	A	860	GLY	3.4
1	A	482	GLU	3.4
1	A	451	ILE	3.3
1	A	456	GLU	3.3
1	A	477	PRO	3.3
1	D	473	ALA	3.2
1	C	462	LEU	3.2
1	C	449	LEU	3.2
1	D	470	LEU	3.2
1	C	524	GLY	3.2
1	D	860	GLY	3.1
1	C	450	GLN	3.1
1	A	480	LYS	3.1
1	C	487	THR	3.0
1	D	527	CYS	3.0
1	C	460	LYS	3.0
1	A	787	THR	3.0
1	C	446	GLU	3.0
1	B	450	GLN	3.0
1	A	525	ALA	2.9
1	D	472	ASN	2.9
1	D	469	GLN	2.9
1	C	458	GLY	2.8
1	C	447	GLU	2.8
1	B	657[A]	MET	2.8
1	C	523	MET	2.7
1	A	484	LEU	2.7
1	C	612	SER	2.6
1	A	455	ALA	2.6
1	C	860	GLY	2.6
1	C	488	HIS	2.6
1	C	657[A]	MET	2.5
1	D	464	ASP	2.5
1	A	453	GLY	2.5
1	C	771	ASN	2.5
1	D	459	ALA	2.5
1	D	829	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLY	2.5
1	D	504	SER	2.5
1	A	478	ALA	2.5
1	C	459	ALA	2.5
1	A	444	PRO	2.5
1	A	450	GLN	2.5
1	D	474	LYS	2.4
1	B	631	LEU	2.4
1	C	453	GLY	2.4
1	A	457	LYS	2.4
1	C	468	ILE	2.4
1	D	485	ILE	2.3
1	A	504	SER	2.3
1	C	463	SER	2.3
1	A	789	GLU	2.3
1	D	486	GLU	2.3
1	D	487	THR	2.3
1	C	477	PRO	2.2
1	B	479	TYR	2.2
1	B	525	ALA	2.2
1	A	449	LEU	2.2
1	D	501	LYS	2.2
1	A	473	ALA	2.2
1	C	445	ASN	2.2
1	A	786	PRO	2.2
1	B	482	GLU	2.2
1	C	483	THR	2.2
1	A	454	ASN	2.1
1	A	461	PHE	2.1
1	C	479	TYR	2.1
1	C	474	LYS	2.1
1	C	485	ILE	2.1
1	D	460	LYS	2.1
1	D	466	GLU	2.1
1	A	463	SER	2.1
1	D	828	LYS	2.1
1	D	786	PRO	2.0
1	D	488	HIS	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

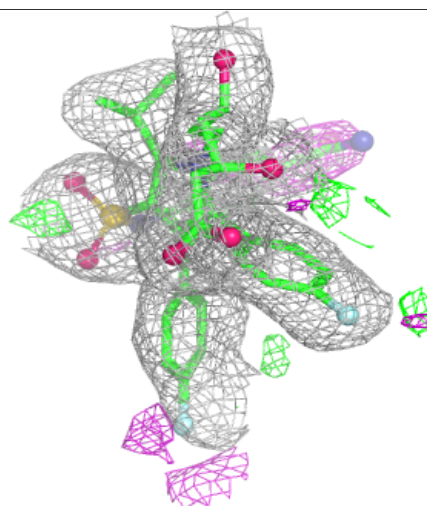
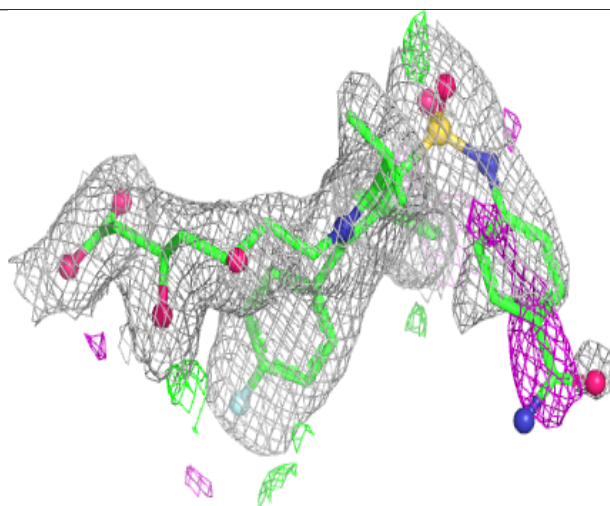
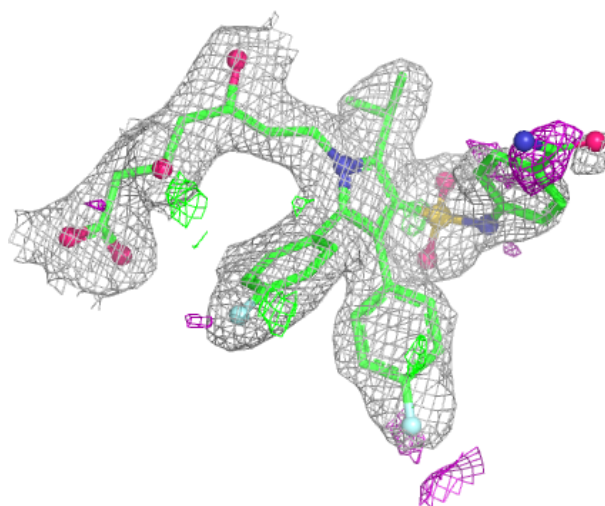
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	9HI	A	1	46/46	0.90	0.13	27,44,53,55	0
2	9HI	C	4	46/46	0.91	0.12	29,45,53,53	0
2	9HI	D	3	46/46	0.91	0.12	25,44,52,54	0
2	9HI	A	2	46/46	0.92	0.11	29,44,50,52	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.

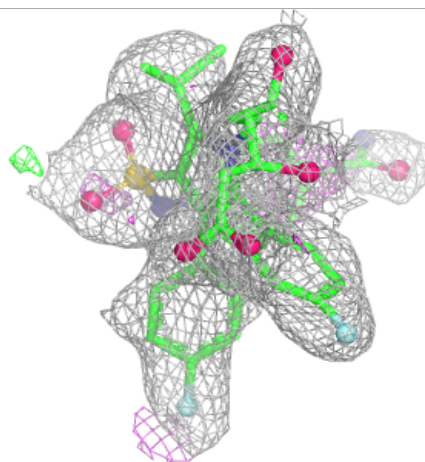
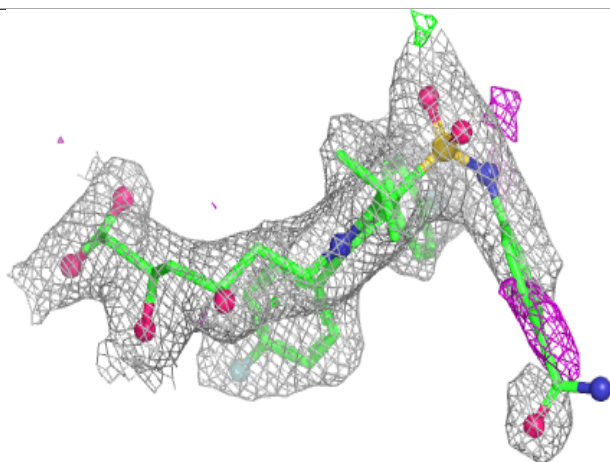
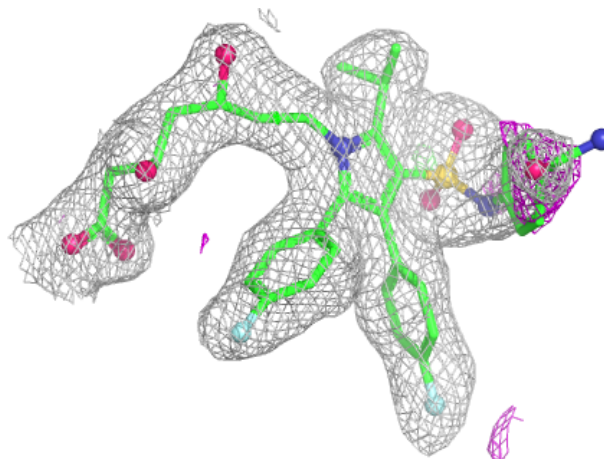
**Electron density around 9HI A 1:**

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



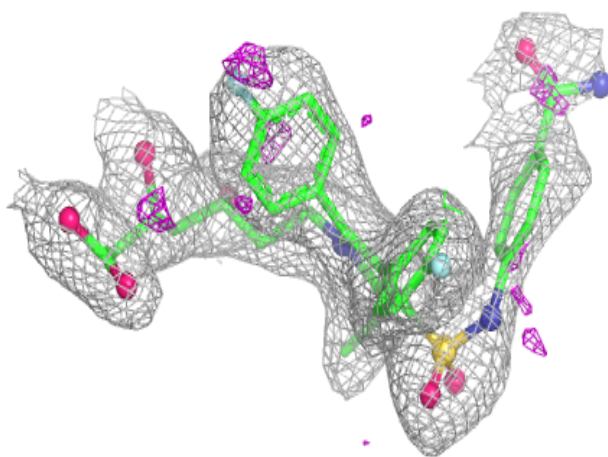
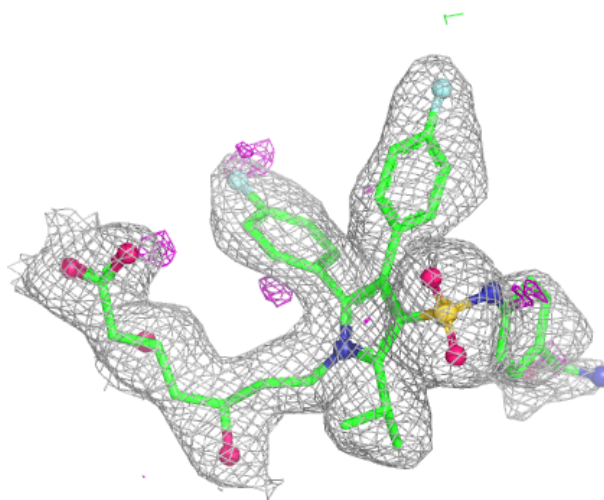
**Electron density around 9HI C 4:**

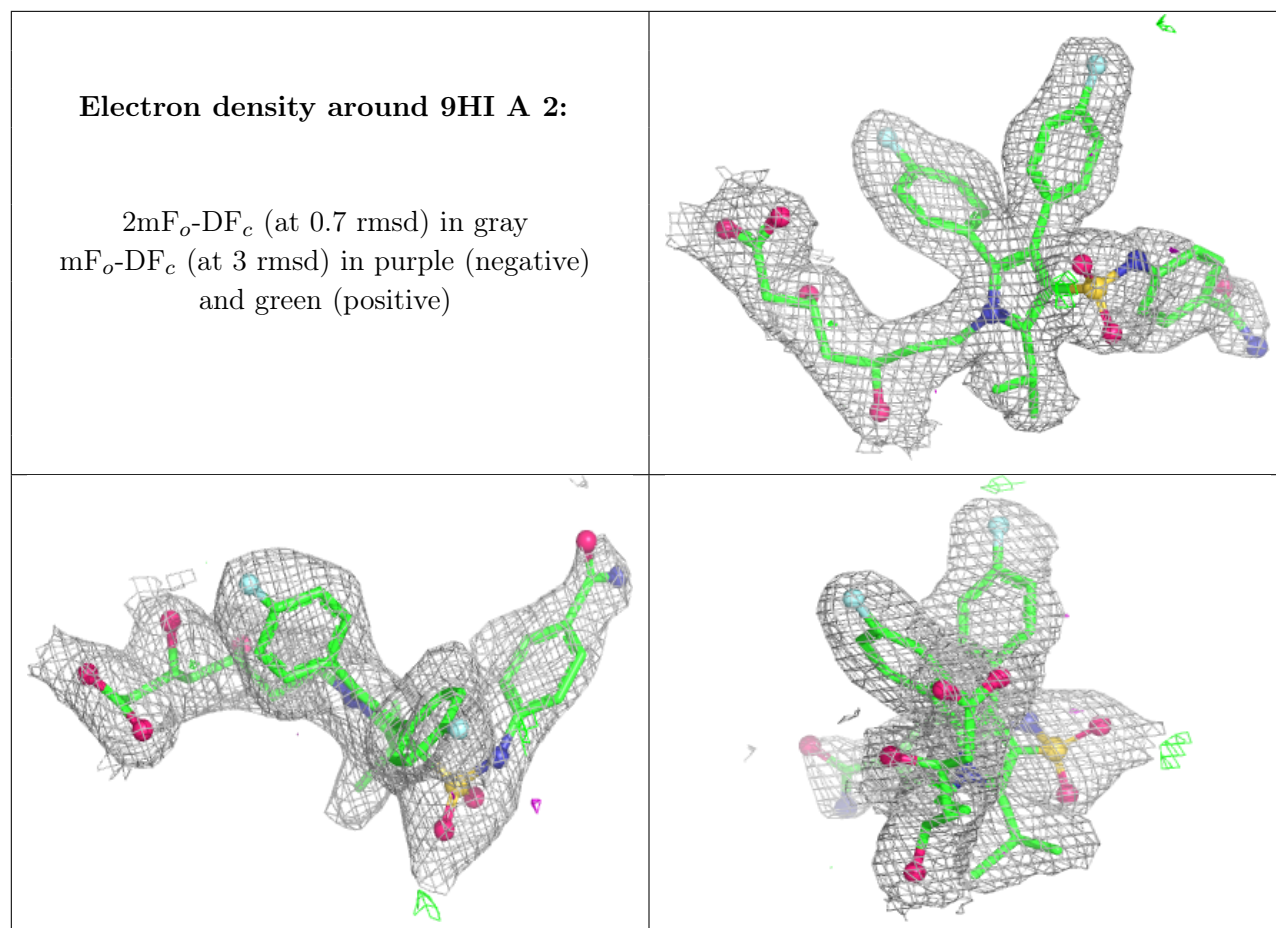
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 9HI D 3:**

$2mF_o-DF_c$  (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.