



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:43 PM UTC

PDB ID : 3CDA / pdb_00003cda
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 : 2.07 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

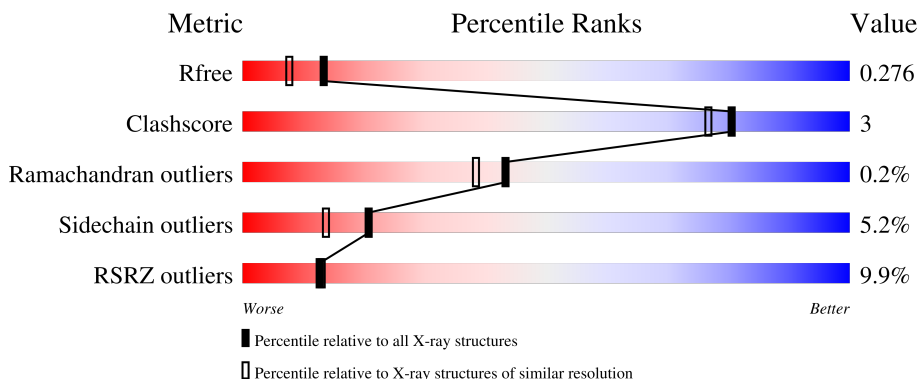
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	441	 11% 82% 12% 5% 5%
1	B	441	 5% 87% 8% 5% 5%
1	C	441	 12% 88% 5% 5% 5%
1	D	441	 10% 83% 6% 10% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12971 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	422	3141	1957	552	602	30	0	0	0
1	B	421	3133	1951	551	601	30	0	0	0
1	C	417	3096	1929	542	595	30	0	0	0
1	D	395	2928	1824	515	560	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

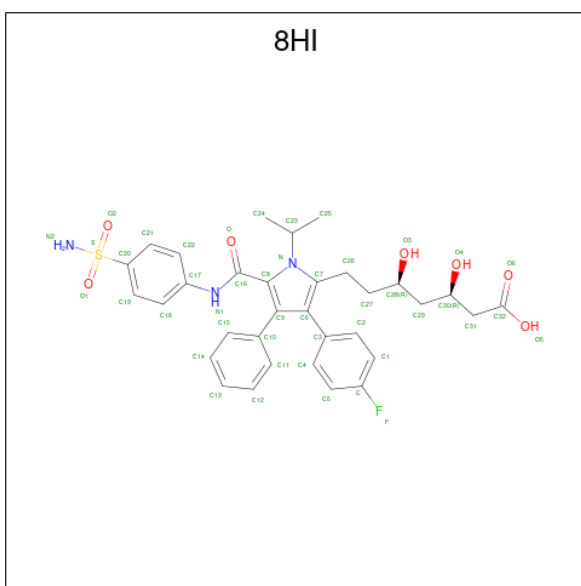
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered 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-fluorophenyl)-1-(1-methylethyl)-4-phenyl-5-[(4-sulfamoylphenyl)carbamoyl]-1H-pyrrol-2-yl}-3,5-dihydroxyheptanoic acid (CCD ID: 8HI) (formula: C₃₃H₃₆FN₃O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	Total	C	F	N	O	S	0	0
			45	33	1	3	7	1		
2	B	1	Total	C	F	N	O	S	0	0
			45	33	1	3	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			45	33	1	3	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			45	33	1	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		

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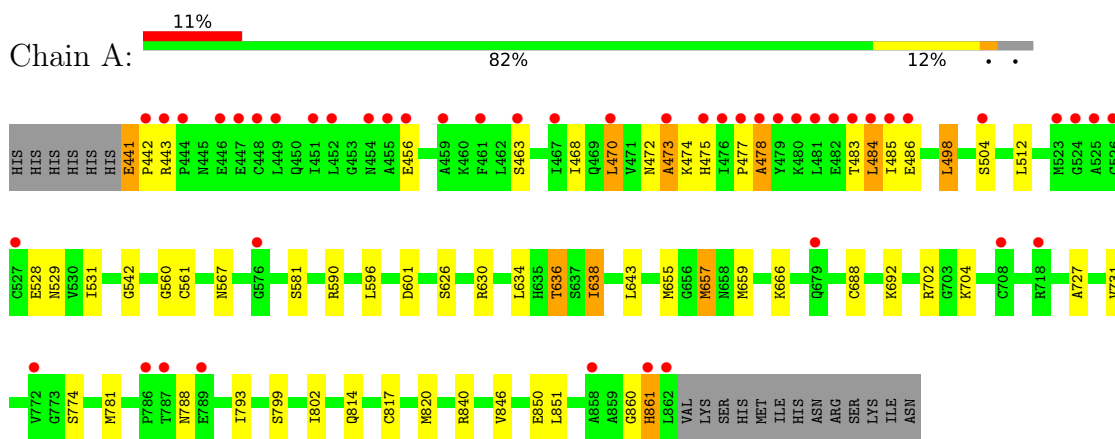
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	134	Total 134	O 134	0	0
3	C	98	Total 98	O 98	0	0
3	D	132	Total 132	O 132	0	0

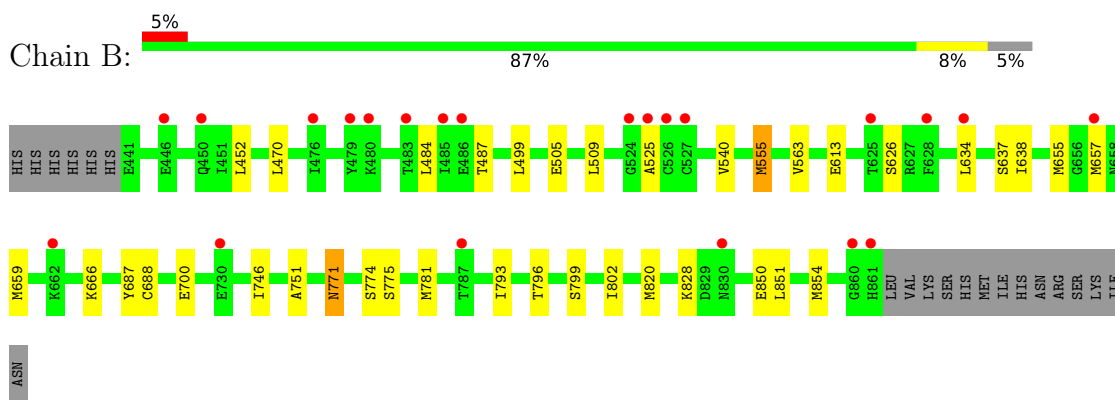
3 Residue-property plots [i](#)

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.

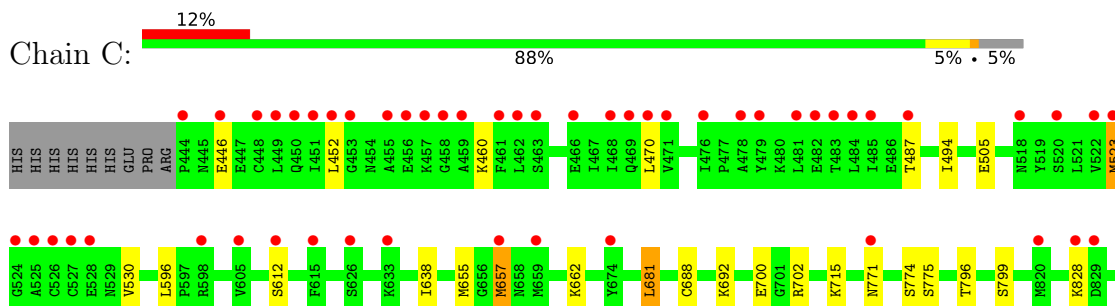
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



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



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



G860
 HIS
 LEU
 VAL
 LYS
 SER
 HIS
 MET
 ILE
 HIS
 ASN
 ASN
 ARG
 SER
 LYS
 ILE
 ASN

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

Chain D: 10% 83% 6% 10%

HIS
 HIS
 HIS
 HIS
 HIS
 HIS
 GLU
 PRO
 ARG
 PRO
 ASN
 ASN
 GLU
 GLU
 CYS
 LEU
 GLN
 ILE
 LEU
 LEU
 GLY
 ASN
 ALA
 ALA
 GLU
 LYS
 G458
 A459
 K460
 F461
 L462
 S463
 D464
 A465
 E466
 I467
 I468
 Q469
 L470
 L471
 M472
 A473
 K474
 H475
 I476
 PRO
 ALA
 TYR
 LYS
 LEU
 GLU
 THR
 L484
 I485
 E486
 T487
 H488
 H495
 E505
 N518

Y519
 S520
 L521
 V522
 M523
 G524
 A525
 C526
 C527
 E528
 N529
 C545
 T589
 R595
 G614
 V617
 S626
 R627
 R630
 K633
 S637
 N642
 F647
 M657
 M658
 M659
 I660
 K666
 V731
 A751
 P786
 T787
 N788
 L791
 T796
 I802
 K828
 P831
 G832

A856
 A859
 GLY
 HIS
 LEU
 VAL
 LYS
 SER
 HIS
 HIS
 MET
 ILE
 HIS
 ASN
 ARG
 SER
 SER
 LYS
 ILE
 ASN

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.61Å 172.25Å 75.62Å 90.00° 118.04° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.07) 90.7 (50.00-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.06Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.257 (Not available) , 0.276	Depositor DCC
R_{free} test set	2066 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtrriage
Anisotropy	0.862	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12971	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	1/3187 (0.0%)	0.80	0/4309
1	B	0.54	1/3179 (0.0%)	0.78	0/4298
1	C	0.52	0/3140	0.78	0/4244
1	D	0.52	0/2968	0.80	0/4010
All	All	0.53	2/12474 (0.0%)	0.79	0/16861

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-9.09	1.56	1.79
1	A	657	MET	SD-CE	-5.14	1.66	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	3141	0	3178	29	0
1	B	3133	0	3167	19	0
1	C	3096	0	3135	11	0
1	D	2928	0	2968	12	0
2	A	45	0	35	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	45	0	35	0	0
2	C	45	0	35	1	0
2	D	45	0	35	1	0
3	A	129	0	0	0	0
3	B	134	0	0	2	0
3	C	98	0	0	1	0
3	D	132	0	0	1	0
All	All	12971	0	12588	64	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 3.

The worst 5 of 64 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:SD	1:A:657:MET:HG2	2.14	0.87
1:C:771:ASN:OD1	1:C:775:SER:OG	1.96	0.83
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.66	0.77
1:B:775:SER:OG	3:B:993:HOH:O	2.02	0.76
1:B:771:ASN:HB2	3:B:993:HOH:O	1.92	0.69

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	420/441 (95%)	398 (95%)	19 (4%)	3 (1%)	18 10
1	B	419/441 (95%)	404 (96%)	14 (3%)	1 (0%)	43 38
1	C	415/441 (94%)	399 (96%)	16 (4%)	0	100 100
1	D	391/441 (89%)	376 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1645/1764 (93%)	1577 (96%)	64 (4%)	4 (0%)	43 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	478	ALA
1	A	484	LEU
1	B	525	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/355 (95%)	310 (92%)	26 (8%)	12 5
1	B	335/355 (94%)	321 (96%)	14 (4%)	26 20
1	C	331/355 (93%)	315 (95%)	16 (5%)	23 16
1	D	313/355 (88%)	301 (96%)	12 (4%)	29 23
All	All	1315/1420 (93%)	1247 (95%)	68 (5%)	21 14

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	486	GLU
1	D	527	CYS
1	D	788	ASN
1	A	814	GLN
1	A	802	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	819	GLN

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Mol	Chain	Res	Type
1	D	819	GLN
1	C	679	GLN
1	D	770	GLN
1	C	497	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](#)

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	8HI	C	4	-	48,48,48	1.81	5 (10%)	59,69,69	1.69	9 (15%)
2	8HI	A	2	-	48,48,48	1.85	6 (12%)	59,69,69	1.74	9 (15%)
2	8HI	B	1	-	48,48,48	1.78	4 (8%)	59,69,69	1.91	11 (18%)
2	8HI	D	3	-	48,48,48	1.77	5 (10%)	59,69,69	1.66	7 (11%)

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	8HI	C	4	-	-	4/39/39/39	0/4/4/4
2	8HI	A	2	-	-	6/39/39/39	0/4/4/4
2	8HI	B	1	-	-	5/39/39/39	0/4/4/4
2	8HI	D	3	-	-	6/39/39/39	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	8HI	C20-S	-10.67	1.60	1.77
2	C	4	8HI	C20-S	-10.47	1.61	1.77
2	D	3	8HI	C20-S	-10.09	1.61	1.77
2	B	1	8HI	C20-S	-10.03	1.61	1.77
2	D	3	8HI	O6-C32	3.47	1.33	1.22

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	8HI	O2-S-O1	-7.57	107.16	118.80
2	C	4	8HI	O2-S-O1	-6.50	108.81	118.80
2	B	1	8HI	C16-C8-N	6.13	129.10	122.33
2	A	2	8HI	O2-S-O1	-5.99	109.59	118.80
2	D	3	8HI	O2-S-O1	-5.62	110.15	118.80

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	8HI	N1-C16-C8-N
2	B	1	8HI	N1-C16-C8-N
2	C	4	8HI	N1-C16-C8-N
2	D	3	8HI	N1-C16-C8-N
2	B	1	8HI	C26-C27-C28-O3

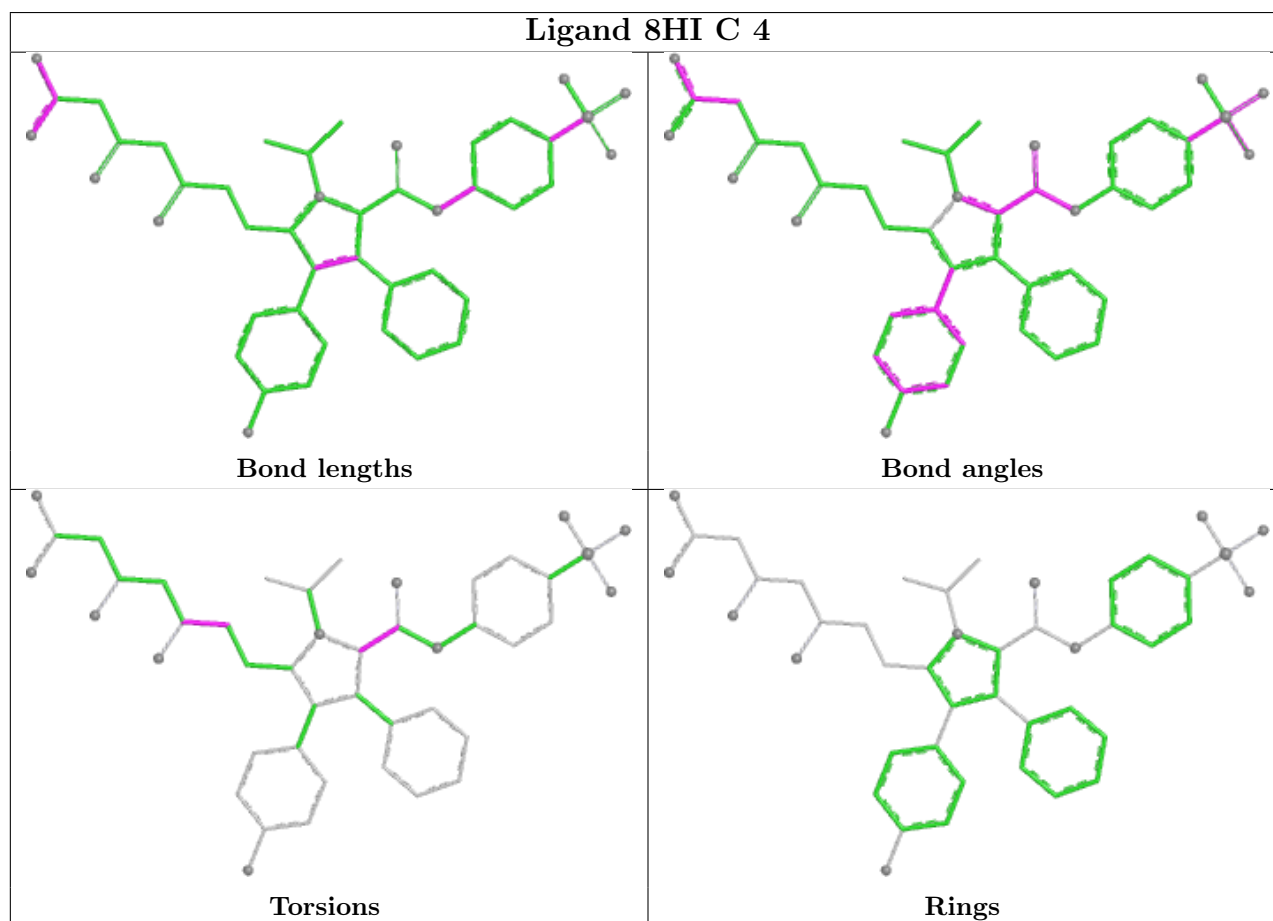
There are no ring outliers.

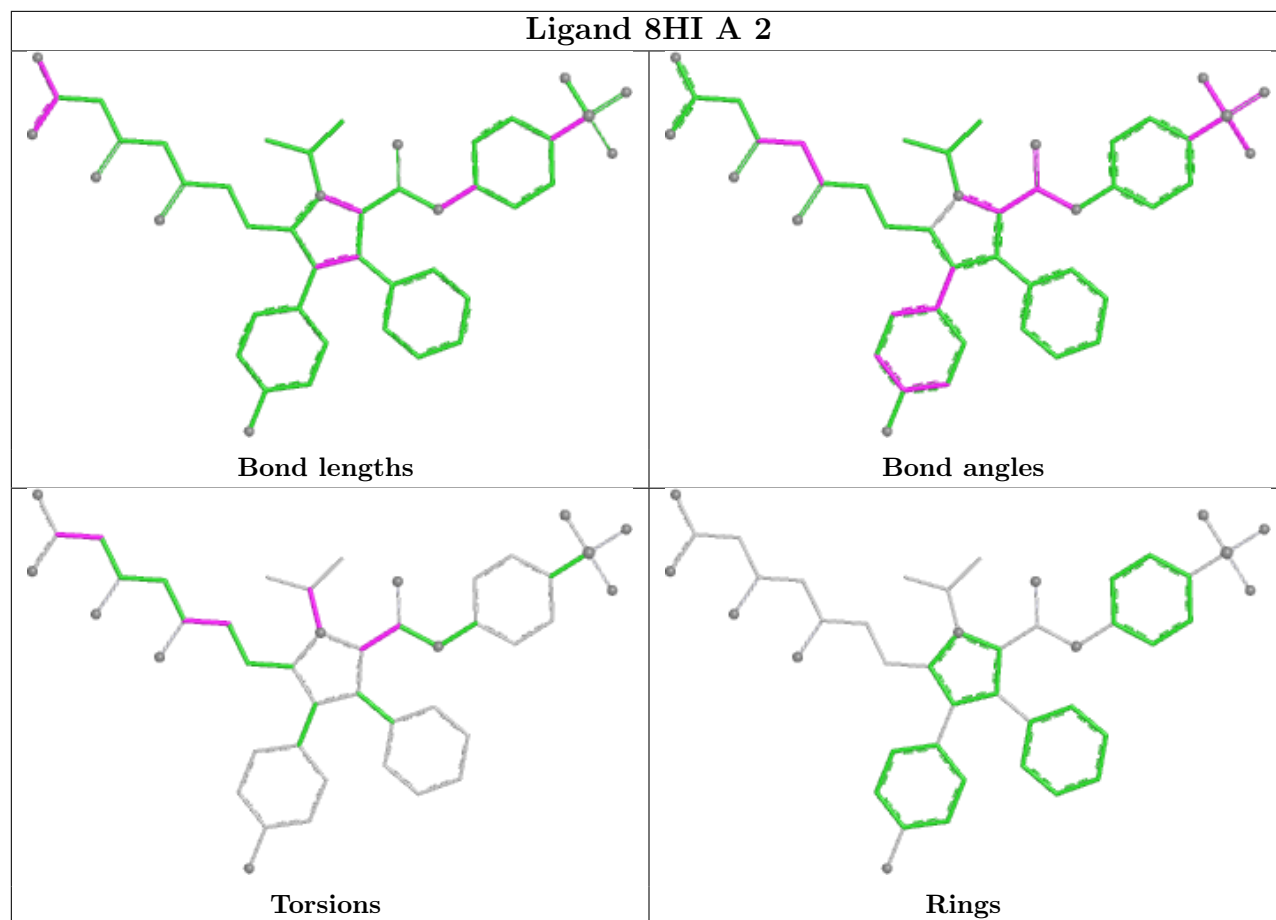
2 monomers are involved in 2 short contacts:

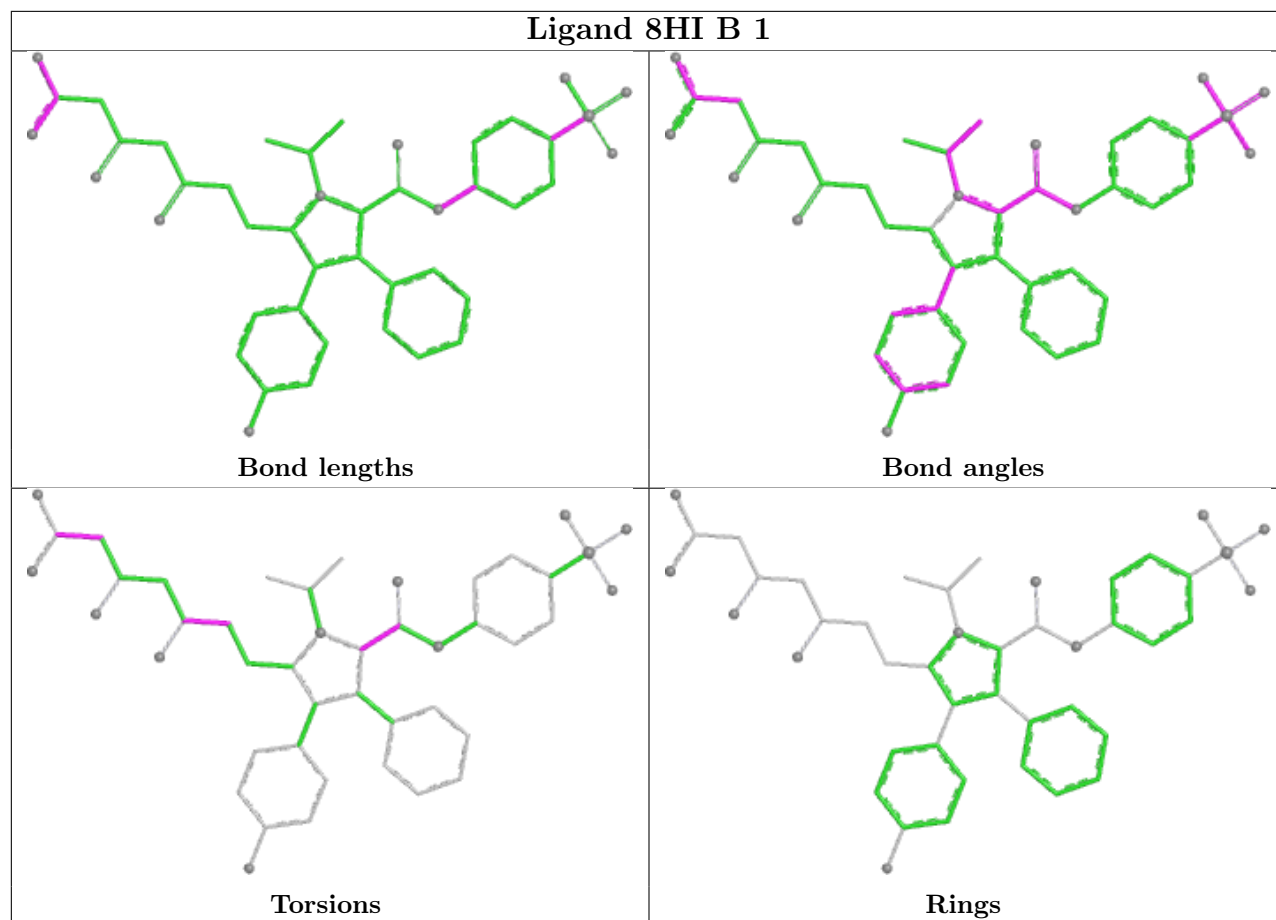
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	8HI	1	0
2	D	3	8HI	1	0

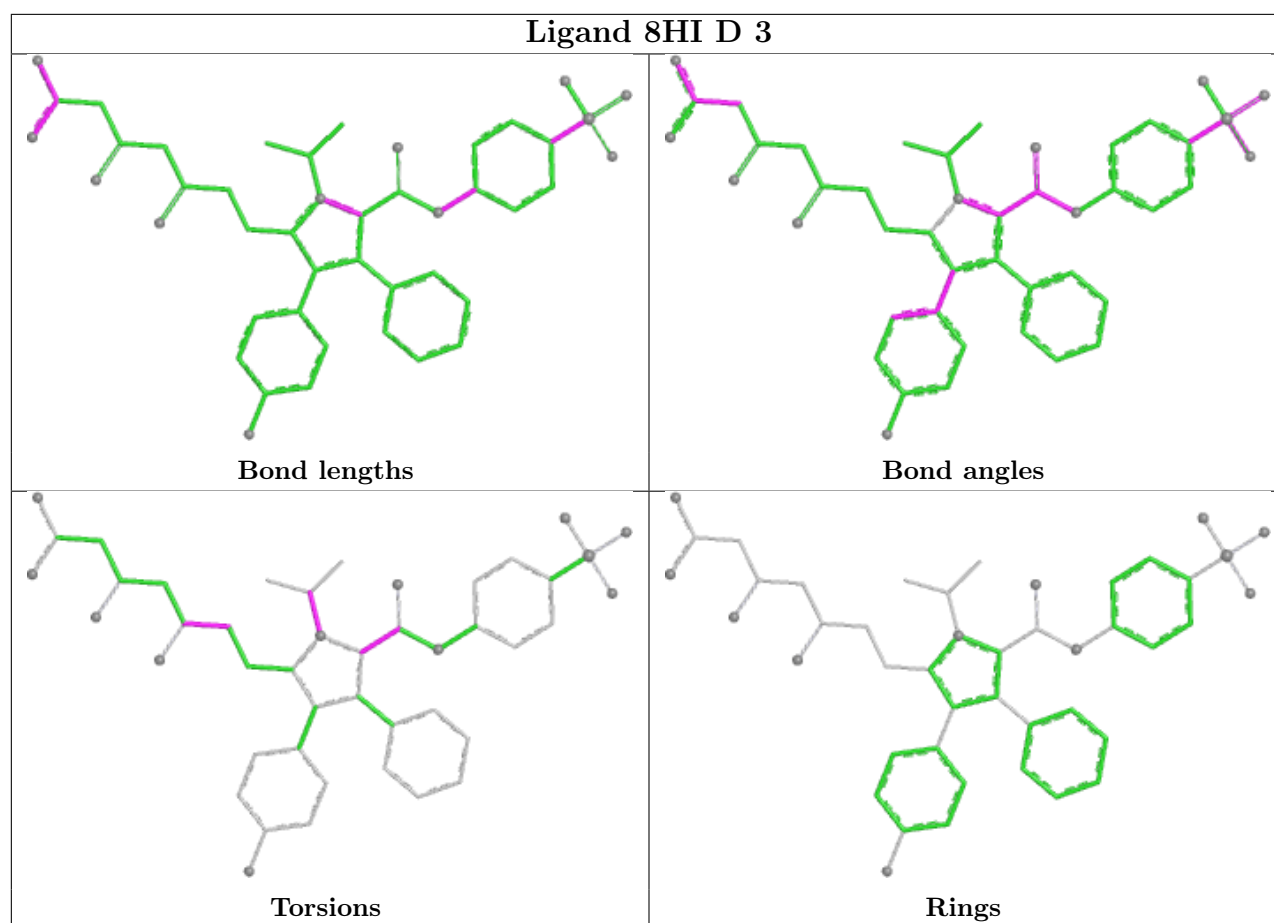
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 [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, 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	422/441 (95%)	0.78	47 (11%) 10 10	24, 35, 56, 63	0
1	B	421/441 (95%)	0.70	22 (5%) 33 32	25, 35, 48, 57	0
1	C	417/441 (94%)	0.87	53 (12%) 8 7	23, 36, 59, 65	0
1	D	395/441 (89%)	0.86	42 (10%) 11 11	24, 35, 59, 64	0
All	All	1655/1764 (93%)	0.80	164 (9%) 13 13	23, 35, 56, 65	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	CYS	9.3
1	D	525	ALA	9.2
1	C	525	ALA	7.7
1	A	527	CYS	7.7
1	B	861	HIS	6.6

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](#)

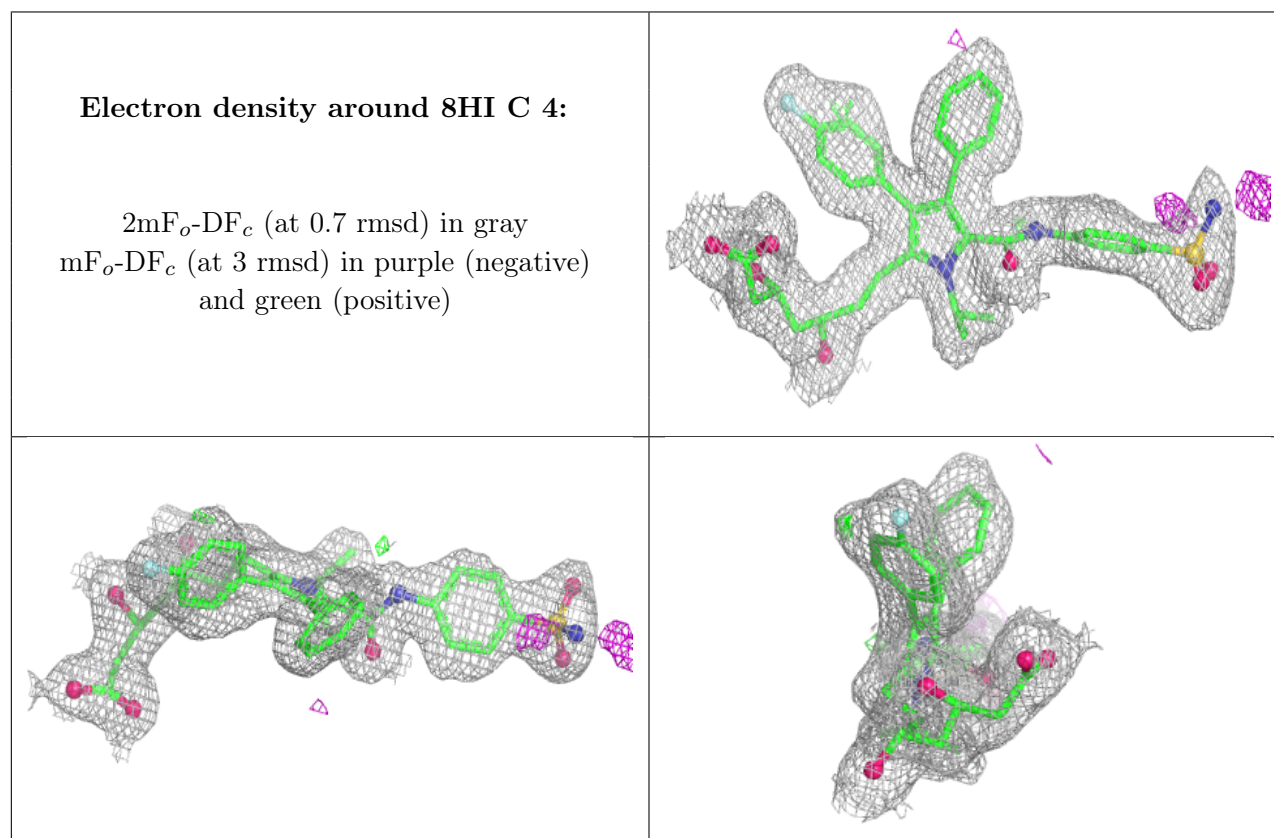
There are no oligosaccharides in this entry.

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, 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.

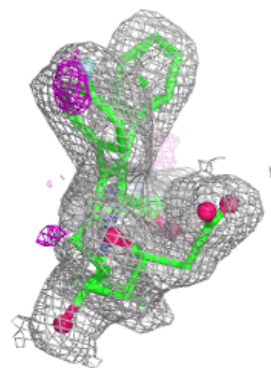
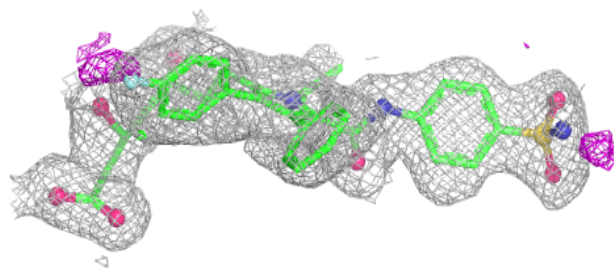
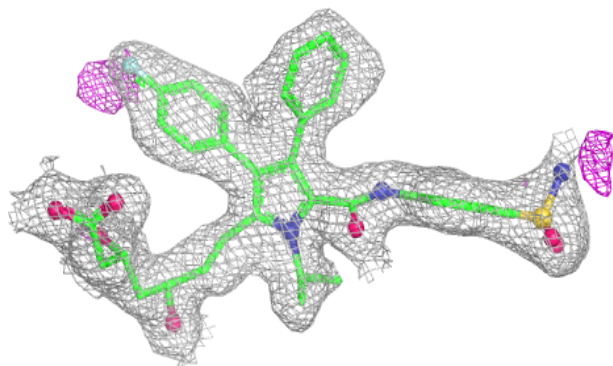
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	8HI	C	4	45/45	0.92	0.09	28,31,36,37	0
2	8HI	A	2	45/45	0.93	0.09	26,30,35,36	0
2	8HI	D	3	45/45	0.93	0.09	25,32,34,36	0
2	8HI	B	1	45/45	0.94	0.08	27,34,37,38	0

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.

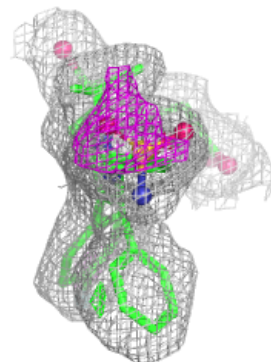
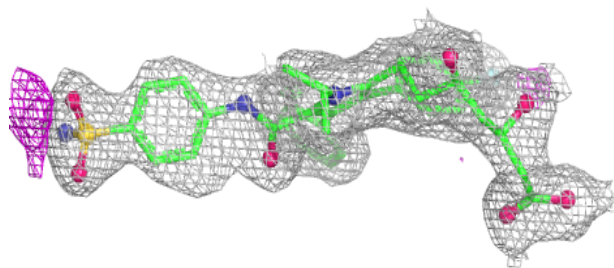
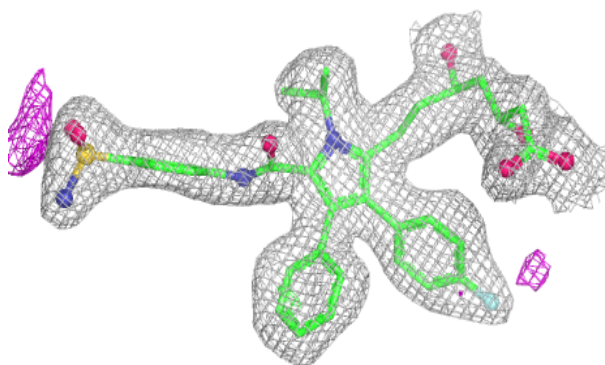


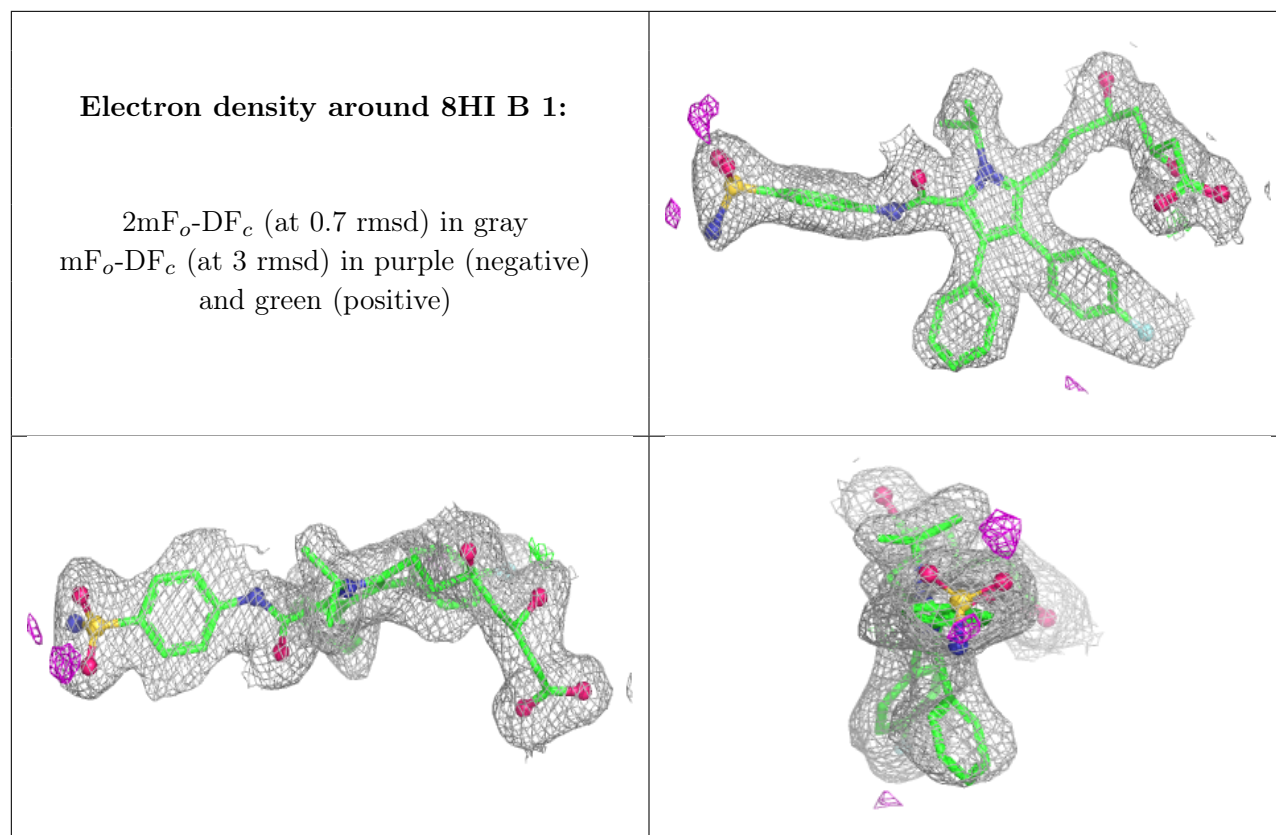
Electron density around 8HI A 2:

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

**Electron density around 8HI 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.