



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:50 AM EDT

PDB ID : 3CCW
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 : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

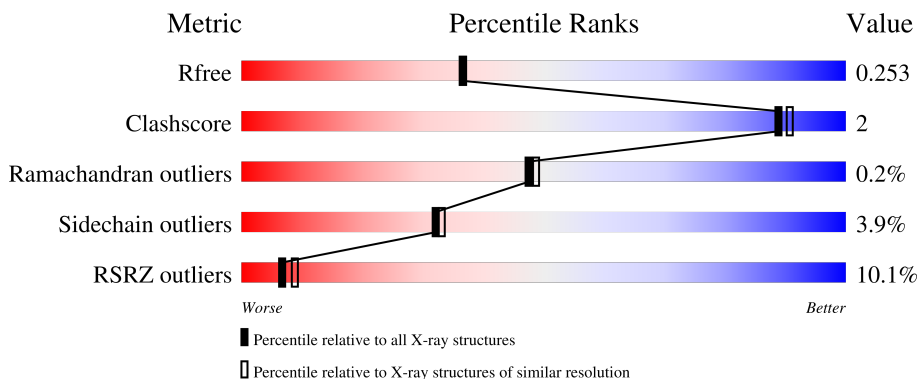
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
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 12823 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	3133	1951	551	601	30	0	0	0
1	C	414	3073	1915	538	590	30	0	0	0
1	D	394	2920	1818	514	559	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

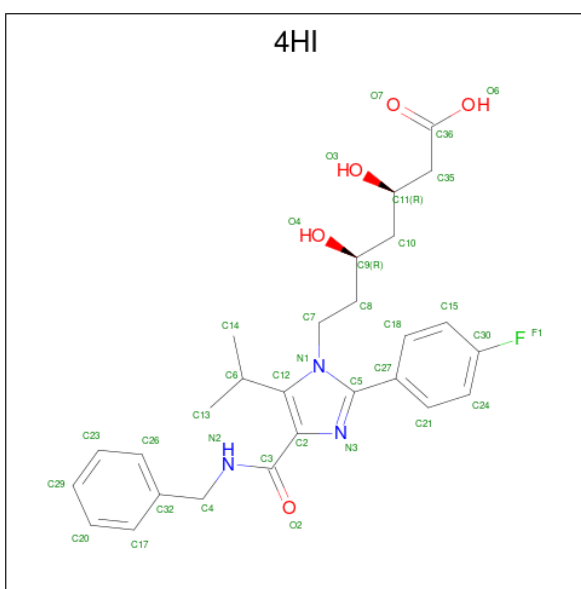
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered 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-[4-(benzylcarbamoyl)-2-(4-fluorophenyl)-5-(1-methylethyl)-1H-imidazol-1-yl]-3,5-dihydroxyheptanoic acid (three-letter code: 4HI) (formula: C₂₇H₃₂FN₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	C	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	D	1	Total	C	F	N	O	0	0
			36	27	1	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		

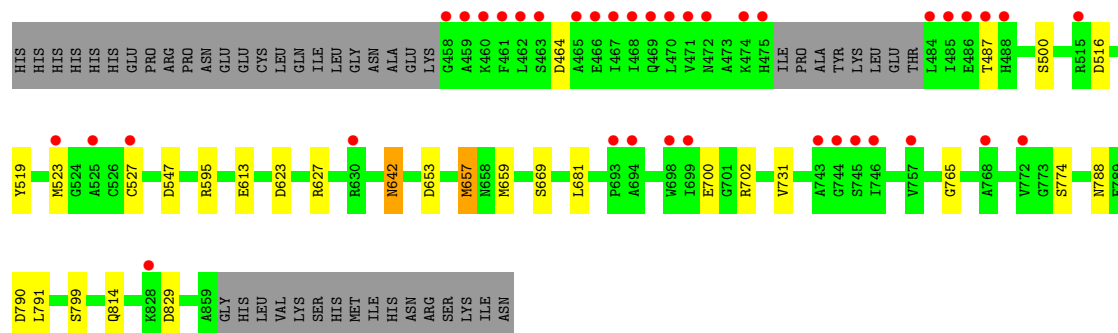
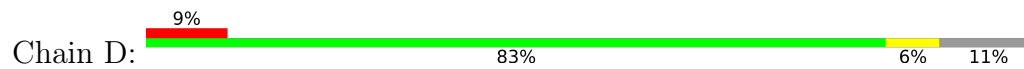
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	89	Total 89	O 89	0	0
3	D	109	Total 109	O 109	0	0

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

- 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, α , β , γ	73.93Å 174.38Å 76.08Å 90.00° 118.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (50.00-2.10) 88.4 (38.16-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.252 0.220 , 0.253	Depositor DCC
R_{free} test set	2647 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.027 for h,-k,-h-l 0.027 for -h-l,-k,l 0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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:
4HI

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	0.37	0/3179	0.63	4/4298 (0.1%)
1	B	0.37	0/3179	0.63	5/4298 (0.1%)
1	C	0.34	0/3116	0.60	4/4211 (0.1%)
1	D	0.36	0/2960	0.64	7/3999 (0.2%)
All	All	0.36	0/12434	0.62	20/16806 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	547	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	547	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	653	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	653	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	464	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	623	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	829	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	767	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	516	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	790	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	829	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	464	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	623	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	516	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	547	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	829	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	547	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	829	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	516	ASP	CB-CG-OD2	5.00	122.80	118.30

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	3133	0	3167	15	0
1	B	3133	0	3167	14	0
1	C	3073	0	3110	8	0
1	D	2920	0	2957	10	0
2	B	72	0	62	3	0
2	C	36	0	31	0	0
2	D	36	0	31	0	0
3	A	109	0	0	0	0
3	B	113	0	0	0	0
3	C	89	0	0	1	0
3	D	109	0	0	2	0
All	All	12823	0	12525	46	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 (46) 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:470:LEU:O	1:A:474:LYS:O	2.07	0.72
1:C:771:ASN:OD1	1:C:775:SER:OG	2.11	0.67
1:B:555:MET:HE1	1:B:563:VAL:HA	1.81	0.60
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.83	0.60
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.86	0.57
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.86	0.57
1:A:860:GLY:O	1:A:861:HIS:HB2	2.05	0.57
1:D:642:ASN:HD22	1:D:642:ASN:N	2.01	0.57
2:B:2:4HI:H7	2:B:2:4HI:H13B	1.87	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.08	0.54
1:B:555:MET:CE	1:B:563:VAL:HA	2.38	0.54
1:D:657:MET:HG3	3:D:197:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ASN:OD1	1:A:775:SER:OG	2.27	0.53
1:A:472:ASN:O	1:A:473:ALA:CB	2.57	0.52
2:B:2:4HI:H8A	2:B:2:4HI:H14B	1.92	0.52
1:A:441:GLU:N	1:A:442:PRO:CD	2.72	0.52
1:A:474:LYS:O	1:A:475:HIS:HB2	2.09	0.52
1:B:449:LEU:HD11	1:B:475:HIS:ND1	2.26	0.50
1:A:477:PRO:O	1:A:478:ALA:CB	2.59	0.49
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.29	0.49
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.95	0.48
1:B:450:GLN:HG3	1:B:451:ILE:N	2.29	0.48
1:A:702:ARG:O	1:A:799:SER:HA	2.14	0.48
1:C:529:ASN:ND2	3:C:252:HOH:O	2.48	0.46
1:C:470:LEU:O	1:C:473:ALA:O	2.34	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.16	0.46
1:B:555:MET:CE	1:B:563:VAL:HG22	2.46	0.46
1:B:638:ILE:O	1:C:796:THR:HG21	2.16	0.45
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.45
2:B:1:4HI:H7	2:B:1:4HI:H13B	1.98	0.45
1:B:592:PRO:HD2	1:B:645:ILE:O	2.17	0.45
1:D:519:TYR:O	1:D:523:MET:HG2	2.17	0.45
1:A:846:VAL:O	1:A:850:GLU:HG2	2.17	0.45
1:A:471:VAL:HG11	1:A:498:LEU:CD2	2.45	0.44
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.52	0.44
1:D:700:GLU:OE1	3:D:369:HOH:O	2.21	0.44
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.43
1:A:449:LEU:HD11	1:A:475:HIS:ND1	2.34	0.43
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.53	0.43
1:B:656:GLY:O	1:B:660:ILE:HG12	2.19	0.42
1:D:702:ARG:O	1:D:799:SER:HA	2.20	0.42
1:B:596:LEU:HB3	1:B:601:ASP:HB2	2.02	0.41
1:D:765:GLY:HA2	1:D:814:GLN:HG2	2.03	0.41
1:B:441:GLU:N	1:B:442:PRO:CD	2.85	0.40
1:B:555:MET:HE2	1:B:563:VAL:HG22	2.03	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%)	398 (95%)	18 (4%)	3 (1%)	22	18
1	B	419/441 (95%)	406 (97%)	12 (3%)	1 (0%)	47	49
1	C	410/441 (93%)	397 (97%)	13 (3%)	0	100	100
1	D	390/441 (88%)	377 (97%)	13 (3%)	0	100	100
All	All	1638/1764 (93%)	1578 (96%)	56 (3%)	4 (0%)	47	49

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	335/355 (94%)	321 (96%)	14 (4%)	30	30
1	B	335/355 (94%)	319 (95%)	16 (5%)	25	24
1	C	329/355 (93%)	319 (97%)	10 (3%)	41	44
1	D	312/355 (88%)	301 (96%)	11 (4%)	36	38
All	All	1311/1420 (92%)	1260 (96%)	51 (4%)	32	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	456	GLU
1	A	470	LEU
1	A	474	LYS
1	A	484	LEU
1	A	486	GLU
1	A	512	LEU
1	A	598	ARG
1	A	630	ARG
1	A	634	LEU
1	A	788	ASN
1	A	814	GLN
1	A	861	HIS
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	489	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	637	SER
1	B	649	SER
1	B	669	SER
1	B	752	HIS
1	B	828	LYS
1	B	829	ASP
1	C	446	GLU
1	C	470	LEU
1	C	476	ILE
1	C	505	GLU
1	C	523	MET
1	C	657	MET
1	C	670	LYS
1	C	681	LEU
1	C	688	CYS
1	C	782	GLU
1	D	487	THR
1	D	500	SER

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Mol	Chain	Res	Type
1	D	527	CYS
1	D	613	GLU
1	D	627	ARG
1	D	642	ASN
1	D	657	MET
1	D	659	MET
1	D	669	SER
1	D	788	ASN
1	D	791	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	A	672	HIS
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	632	GLN
1	C	469	GLN
1	C	472	ASN
1	C	672	HIS
1	C	679	GLN
1	C	824	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	788	ASN

5.3.3 RNA

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 monosaccharides 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	4HI	B	2	-	30,38,38	0.56	0	40,52,52	1.41	4 (10%)
2	4HI	B	1	-	30,38,38	0.60	0	40,52,52	1.37	5 (12%)
2	4HI	D	3	-	30,38,38	0.53	0	40,52,52	1.36	4 (10%)
2	4HI	C	4	-	30,38,38	0.53	0	40,52,52	1.44	3 (7%)

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	4HI	B	2	-	-	3/25/30/30	0/3/3/3
2	4HI	B	1	-	-	5/25/30/30	0/3/3/3
2	4HI	D	3	-	-	5/25/30/30	0/3/3/3
2	4HI	C	4	-	-	5/25/30/30	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	4HI	C12-C2-C3	-4.46	122.62	131.18
2	C	4	4HI	C12-C2-C3	-3.99	123.53	131.18
2	D	3	4HI	C12-C2-C3	-3.86	123.77	131.18
2	B	1	4HI	C12-C2-C3	-3.67	124.14	131.18
2	C	4	4HI	C2-C12-C6	-3.66	123.89	129.87
2	B	2	4HI	C2-C12-C6	-3.57	124.05	129.87
2	D	3	4HI	C2-C12-C6	-3.56	124.06	129.87
2	B	1	4HI	C2-C12-C6	-2.95	125.06	129.87
2	D	3	4HI	C4-N2-C3	2.59	127.94	121.81
2	B	2	4HI	C4-N2-C3	2.40	127.49	121.81
2	B	2	4HI	N3-C5-N1	-2.20	109.58	115.11
2	C	4	4HI	C4-N2-C3	2.20	127.02	121.81
2	B	1	4HI	C24-C30-C15	-2.15	119.97	122.83
2	B	1	4HI	C4-N2-C3	2.13	126.86	121.81
2	D	3	4HI	N3-C5-N1	-2.12	109.80	115.11
2	B	1	4HI	N3-C5-N1	-2.07	109.91	115.11

There are no chirality outliers.

All (18) torsion outliers are listed below:

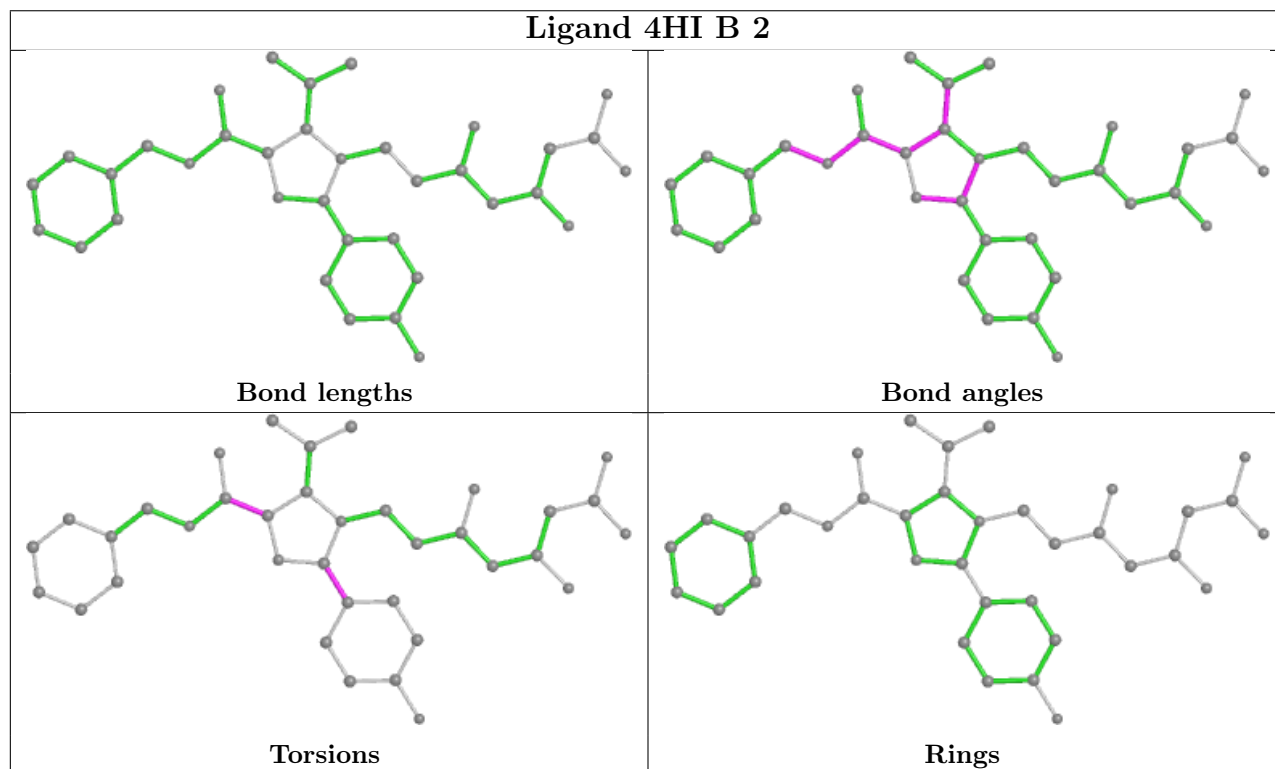
Mol	Chain	Res	Type	Atoms
2	B	1	4HI	C12-C2-C3-O2
2	B	2	4HI	C12-C2-C3-O2
2	C	4	4HI	C21-C27-C5-N1
2	C	4	4HI	C12-C2-C3-O2
2	D	3	4HI	C21-C27-C5-N1
2	D	3	4HI	C18-C27-C5-N1
2	D	3	4HI	C12-C2-C3-O2
2	D	3	4HI	C18-C27-C5-N3
2	C	4	4HI	C18-C27-C5-N3
2	D	3	4HI	C21-C27-C5-N3
2	B	1	4HI	C21-C27-C5-N3
2	C	4	4HI	C21-C27-C5-N3
2	B	1	4HI	C18-C27-C5-N3
2	B	1	4HI	C21-C27-C5-N1
2	B	1	4HI	C18-C27-C5-N1
2	C	4	4HI	C18-C27-C5-N1
2	B	2	4HI	C18-C27-C5-N3
2	B	2	4HI	C21-C27-C5-N3

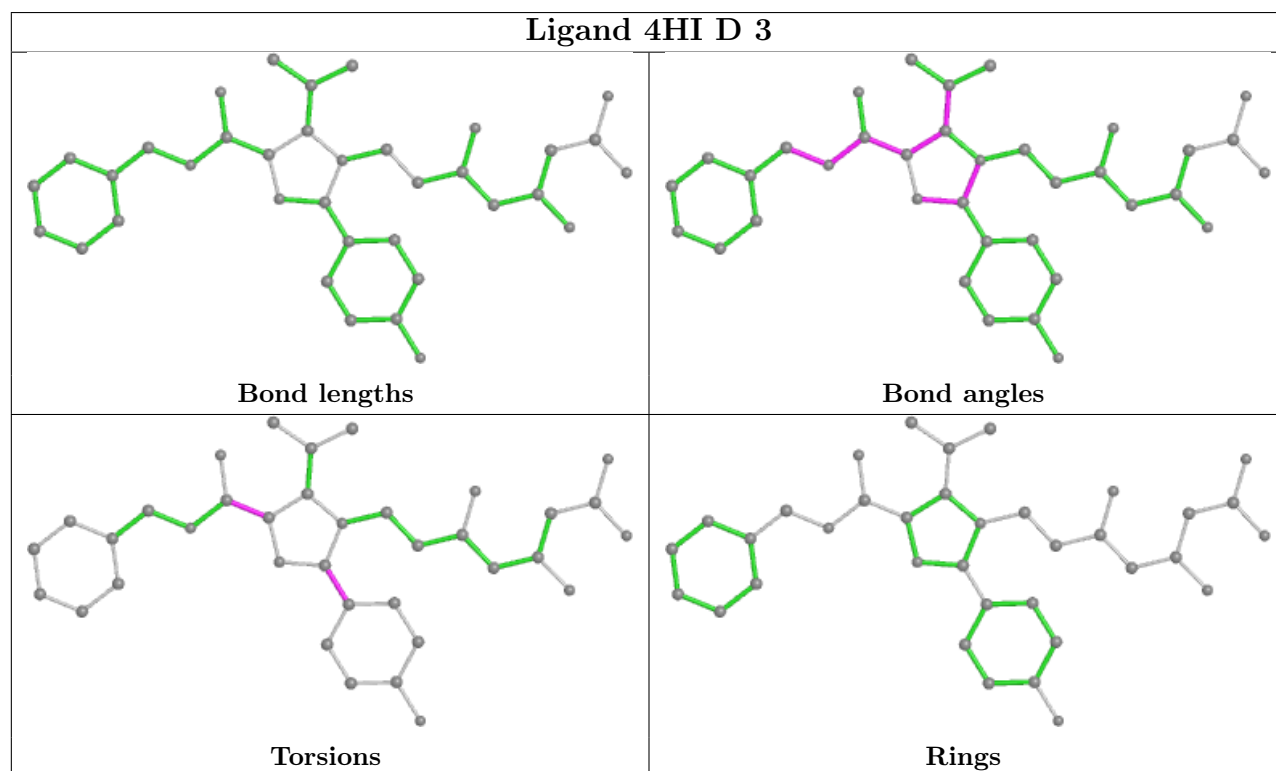
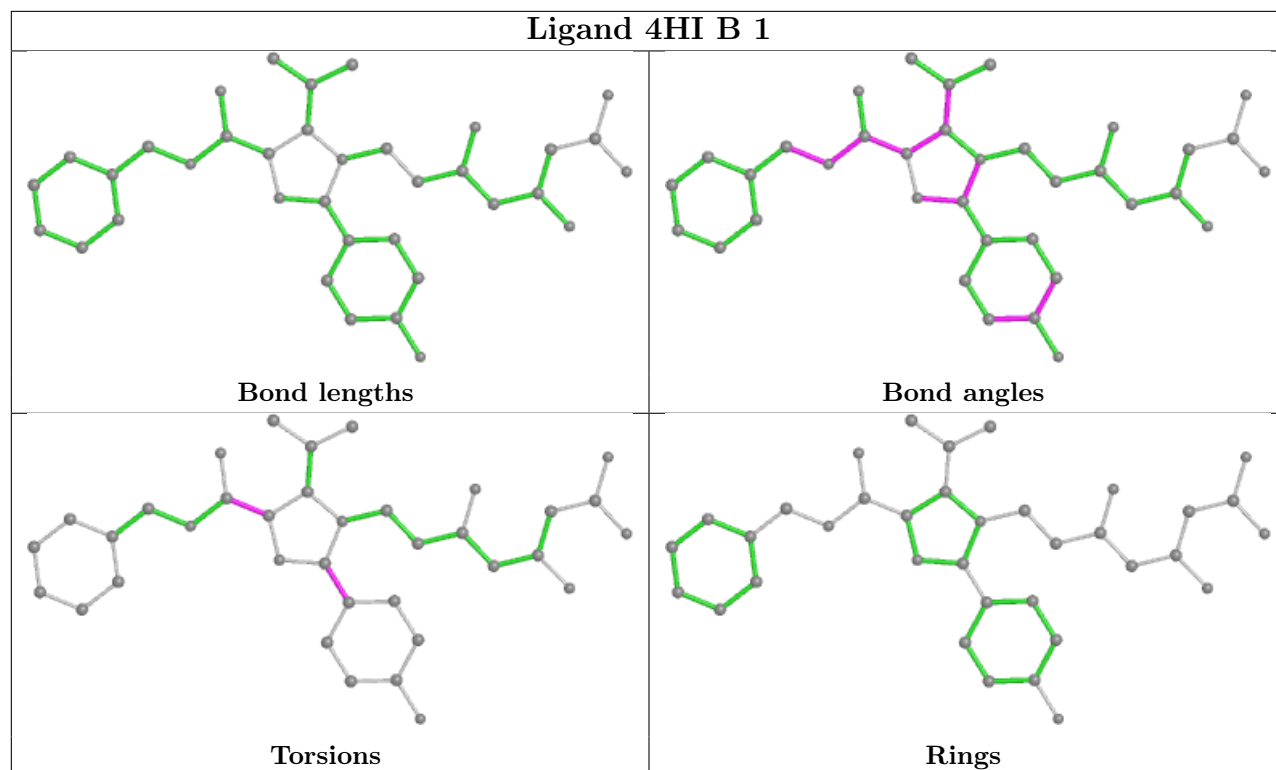
There are no ring outliers.

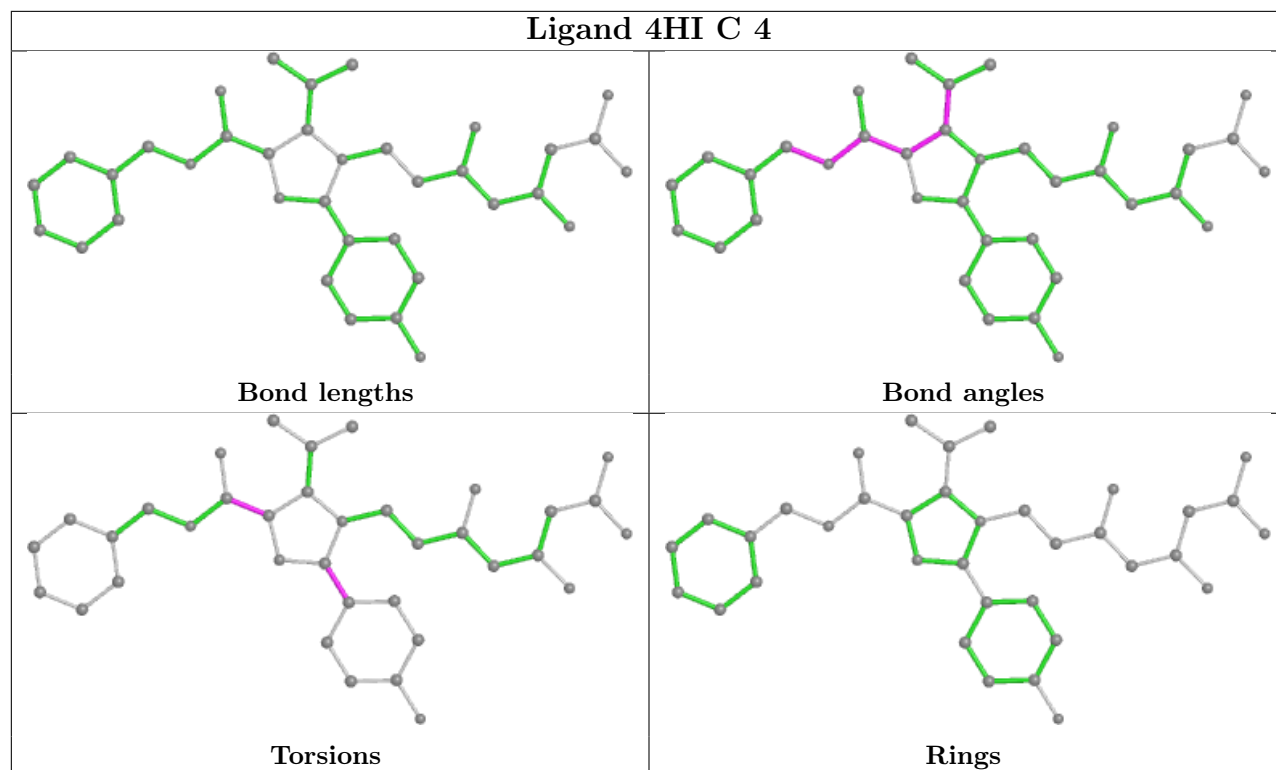
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	4HI	2	0
2	B	1	4HI	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	421/441 (95%)	0.55	60 (14%) 2 3	29, 42, 62, 69	0
1	B	421/441 (95%)	0.32	29 (6%) 16 21	29, 43, 56, 72	0
1	C	414/441 (93%)	0.57	40 (9%) 7 10	30, 46, 83, 103	0
1	D	394/441 (89%)	0.42	38 (9%) 8 10	29, 43, 82, 108	0
All	All	1650/1764 (93%)	0.46	167 (10%) 7 9	29, 43, 66, 108	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	GLY	11.5
1	D	461	PHE	7.9
1	D	470	LEU	7.6
1	C	452	LEU	7.5
1	B	861	HIS	6.9
1	D	475	HIS	6.7
1	C	525	ALA	6.6
1	D	459	ALA	6.6
1	C	453	GLY	6.4
1	C	524	GLY	6.4
1	A	479	TYR	6.2
1	A	452	LEU	6.2
1	C	481	LEU	6.0
1	D	527	CYS	5.9
1	D	485	ILE	5.9
1	D	484	LEU	5.6
1	D	486	GLU	5.6
1	C	484	LEU	5.6
1	C	483	THR	5.4
1	A	861	HIS	5.2
1	A	446	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	461	PHE	5.2
1	D	471	VAL	5.1
1	D	474	LYS	5.0
1	A	448	CYS	4.8
1	D	460	LYS	4.7
1	A	462	LEU	4.7
1	A	476	ILE	4.6
1	A	475	HIS	4.6
1	C	523	MET	4.5
1	A	467	ILE	4.5
1	A	455	ALA	4.5
1	C	527	CYS	4.4
1	A	445	ASN	4.3
1	C	461	PHE	4.3
1	D	469	GLN	4.3
1	C	451	ILE	4.2
1	B	828	LYS	4.1
1	A	473	ALA	4.0
1	A	450	GLN	3.9
1	A	470	LEU	3.9
1	A	447	GLU	3.9
1	C	450	GLN	3.9
1	C	487	THR	3.8
1	D	523	MET	3.8
1	C	746	ILE	3.7
1	C	748	GLY	3.6
1	A	444	PRO	3.6
1	C	454	ASN	3.5
1	B	772	VAL	3.5
1	B	829	ASP	3.5
1	C	485	ILE	3.5
1	A	477	PRO	3.5
1	A	449	LEU	3.5
1	D	462	LEU	3.5
1	A	474	LYS	3.5
1	A	746	ILE	3.5
1	C	449	LEU	3.4
1	A	828	LYS	3.4
1	A	463	SER	3.3
1	A	481	LEU	3.3
1	A	471	VAL	3.3
1	C	486	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	488	HIS	3.3
1	D	525	ALA	3.3
1	A	772	VAL	3.2
1	B	446	GLU	3.2
1	B	699	ILE	3.2
1	D	746	ILE	3.2
1	A	457	LYS	3.2
1	A	451	ILE	3.2
1	C	458	GLY	3.2
1	C	628	PHE	3.1
1	A	689	THR	3.1
1	B	527	CYS	3.1
1	A	773	GLY	3.1
1	D	463	SER	3.1
1	C	772	VAL	3.1
1	A	443	ARG	3.0
1	A	741	ALA	3.0
1	A	458	GLY	3.0
1	A	469	GLN	3.0
1	D	772	VAL	3.0
1	A	483	THR	3.0
1	D	744	GLY	3.0
1	A	442	PRO	3.0
1	A	456	GLU	2.9
1	A	480	LYS	2.8
1	C	479	TYR	2.8
1	B	698	TRP	2.8
1	A	484	LEU	2.7
1	A	696	ILE	2.7
1	C	778	ILE	2.7
1	C	627	ARG	2.7
1	A	775	SER	2.7
1	B	746	ILE	2.7
1	A	460	LYS	2.7
1	A	693	PRO	2.7
1	D	693	PRO	2.7
1	B	482	GLU	2.6
1	A	769	ALA	2.6
1	D	745	SER	2.6
1	D	768	ALA	2.6
1	D	828	LYS	2.5
1	D	472	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	699	ILE	2.5
1	A	694	ALA	2.5
1	B	757	VAL	2.5
1	A	441	GLU	2.5
1	B	479	TYR	2.5
1	C	662	LYS	2.5
1	C	520	SER	2.5
1	B	481	LEU	2.5
1	C	469	GLN	2.5
1	B	741	ALA	2.5
1	D	515	ARG	2.4
1	A	698	TRP	2.4
1	C	626	SER	2.4
1	C	771	ASN	2.4
1	B	743	ALA	2.4
1	D	465	ALA	2.4
1	C	624	SER	2.4
1	A	761	TYR	2.4
1	A	695	ALA	2.4
1	B	693	PRO	2.4
1	D	694	ALA	2.4
1	D	467	ILE	2.4
1	C	699	ILE	2.3
1	A	789	GLU	2.3
1	A	635	HIS	2.3
1	B	777	CYS	2.3
1	A	482	GLU	2.3
1	B	860	GLY	2.3
1	C	741	ALA	2.3
1	B	739	GLY	2.3
1	A	453	GLY	2.2
1	D	698	TRP	2.2
1	A	829	ASP	2.2
1	B	483	THR	2.2
1	B	754	ALA	2.2
1	D	488	HIS	2.2
1	D	757	VAL	2.2
1	A	466	GLU	2.2
1	B	450	GLN	2.2
1	A	749	TYR	2.2
1	A	768	ALA	2.1
1	D	468	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	749	TYR	2.1
1	C	769	ALA	2.1
1	D	630	ARG	2.1
1	A	762	ILE	2.1
1	B	773	GLY	2.1
1	B	745	SER	2.1
1	B	694	ALA	2.1
1	C	744	GLY	2.1
1	B	469	GLN	2.1
1	B	753	ALA	2.1
1	D	743	ALA	2.1
1	C	673	GLU	2.0
1	D	466	GLU	2.0
1	D	699	ILE	2.0
1	C	459	ALA	2.0
1	A	472	ASN	2.0
1	B	737	LEU	2.0
1	C	695	ALA	2.0
1	D	487	THR	2.0
1	C	860	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

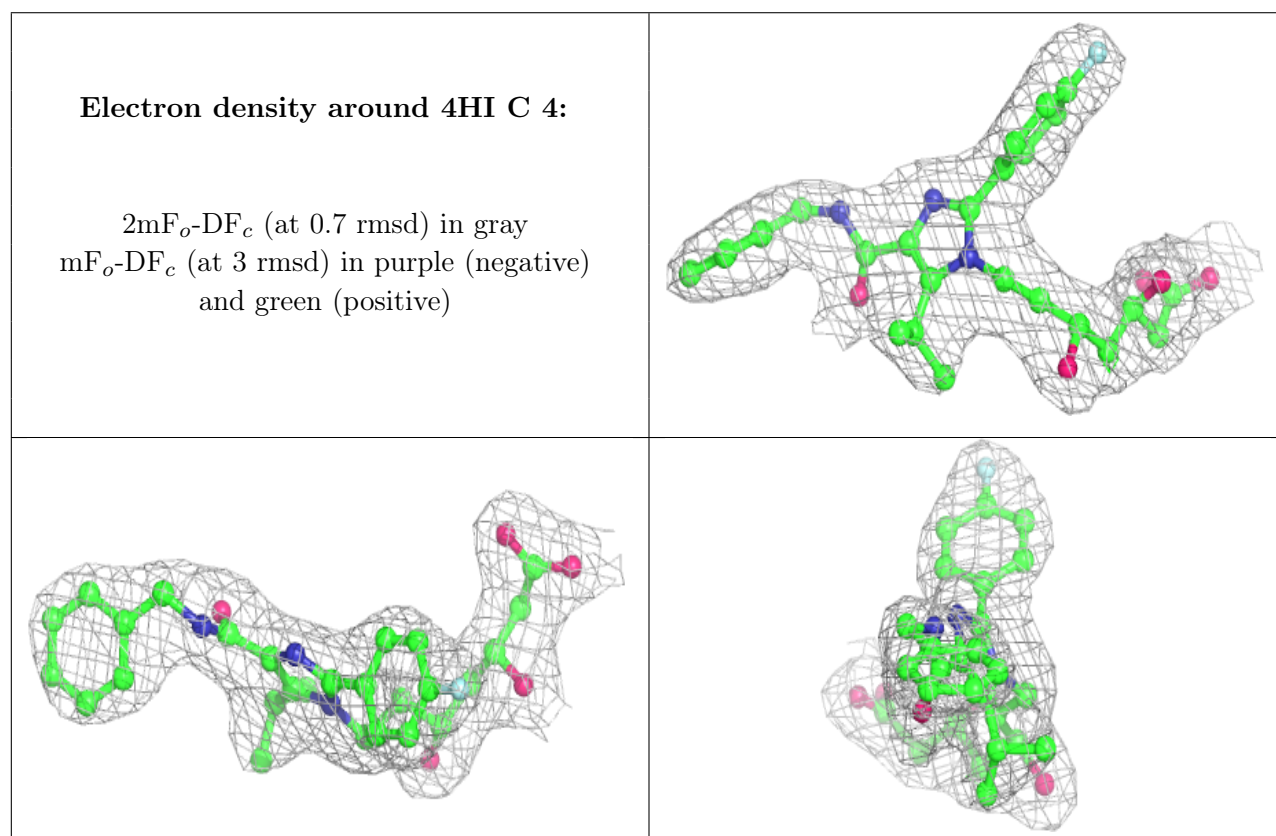
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4HI	C	4	36/36	0.87	0.15	33,45,47,51	0
2	4HI	D	3	36/36	0.89	0.14	31,41,44,47	0
2	4HI	B	1	36/36	0.94	0.11	32,41,42,44	0

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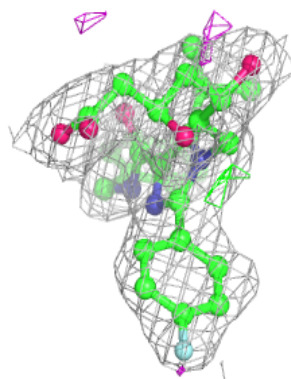
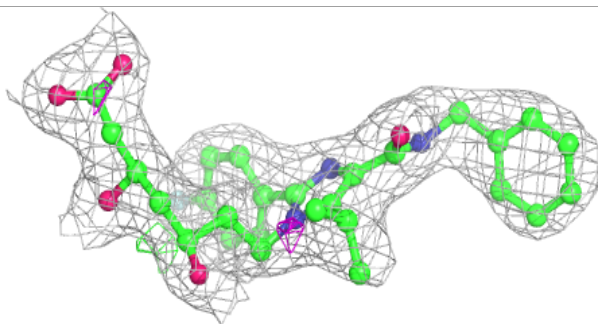
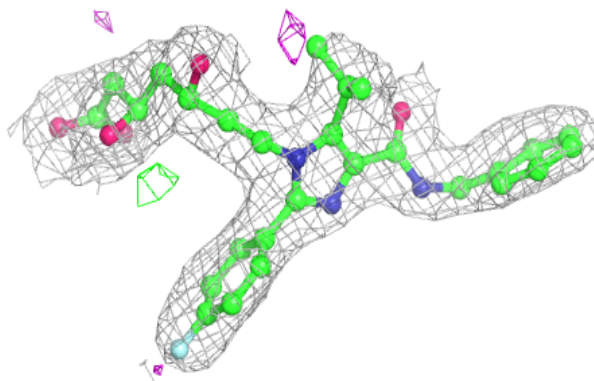
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4HI	B	2	36/36	0.94	0.13	29,37,43,46	0

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.

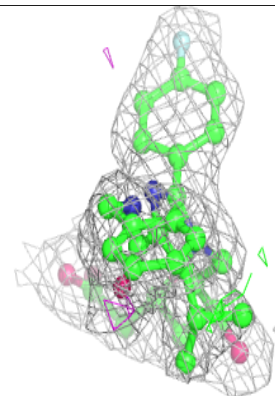
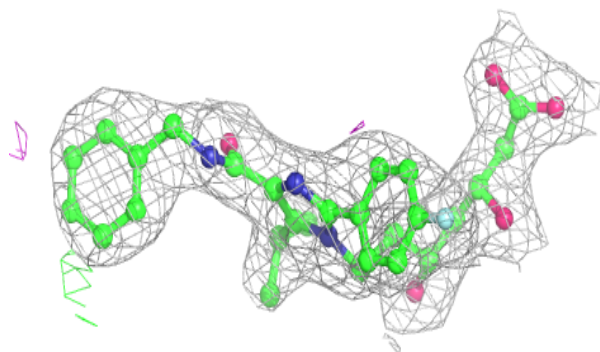
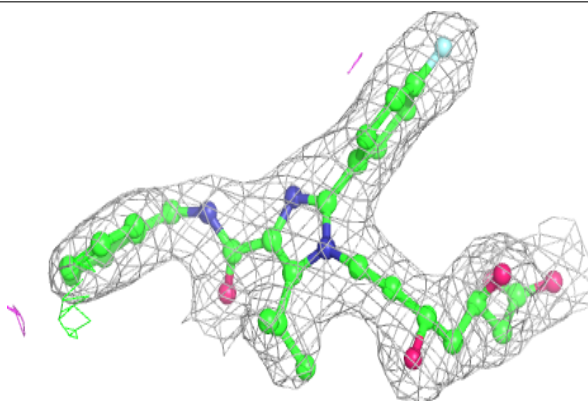


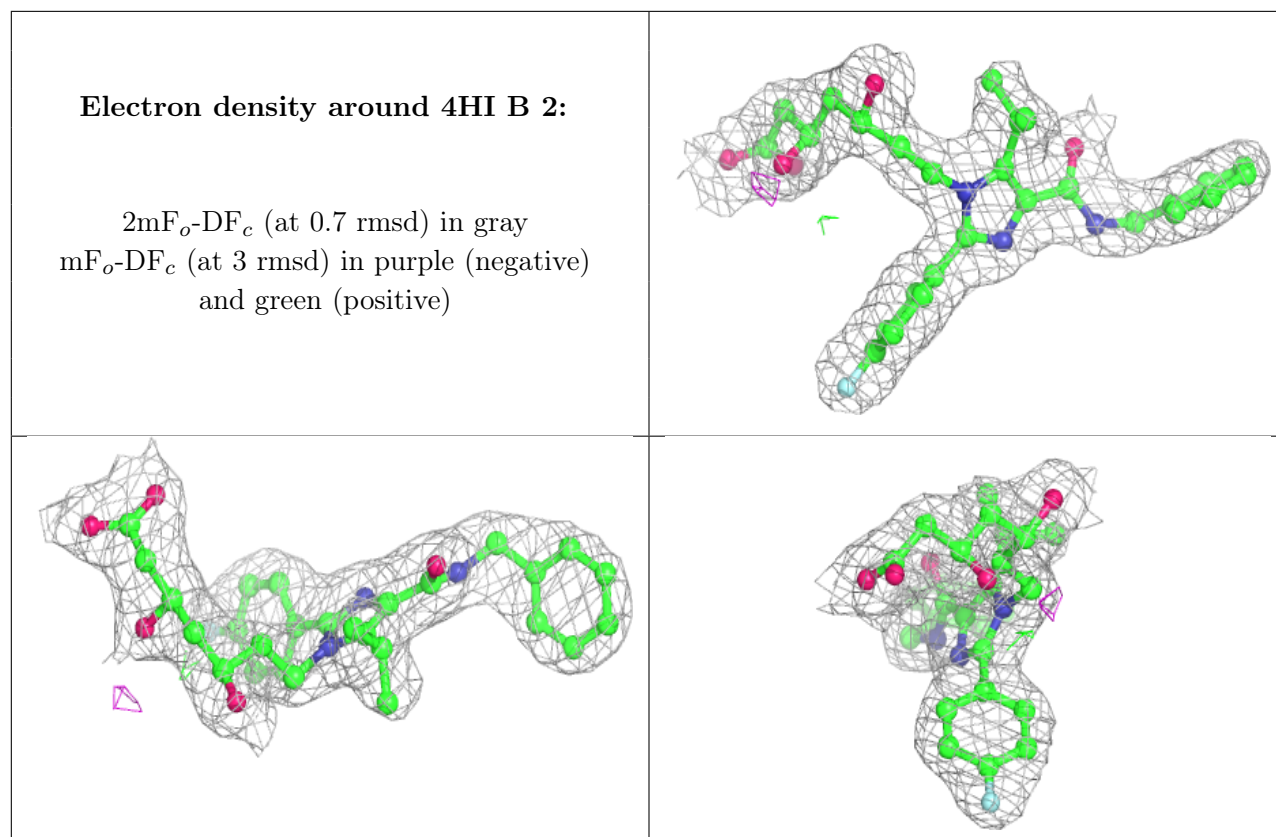
Electron density around 4HI D 3:

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

**Electron density around 4HI B 1:**

$2mF_o-DF_c$ (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.