



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:33 AM UTC

PDB ID : 3CCZ / pdb_00003ccz
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 : 1.70 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

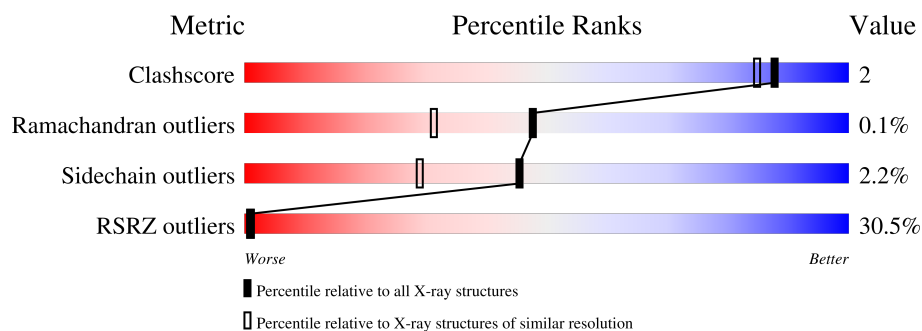
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

There are 4 unique types of molecules in this entry. The entry contains 13469 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
1	A	420	Total	C	N	O	S	0	3	0
			3128	1946	549	601	32			
1	B	405	Total	C	N	O	S	0	3	0
			3014	1874	529	580	31			
1	C	404	Total	C	N	O	S	0	3	0
			2997	1862	524	579	32			
1	D	394	Total	C	N	O	S	0	4	0
			2922	1815	512	565	30			

There are 28 discrepancies between the modelled and reference sequences:

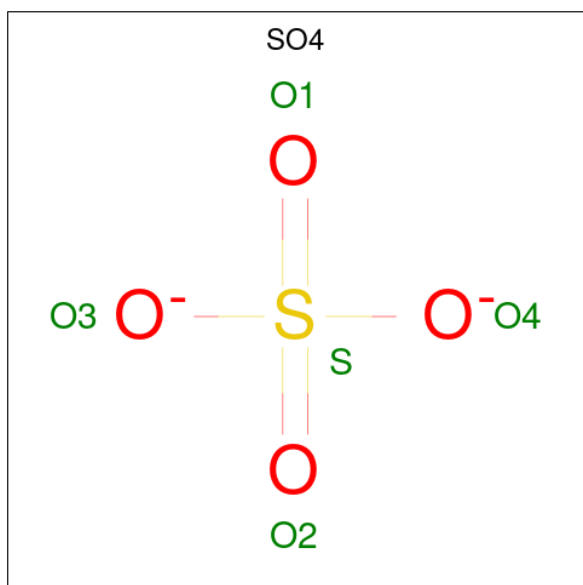
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered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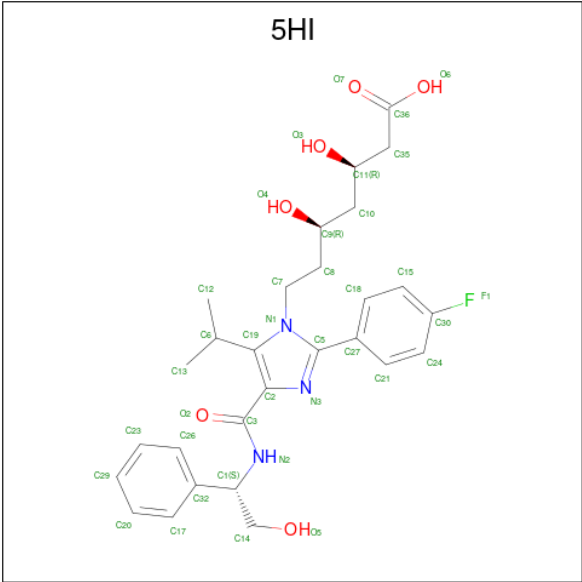
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

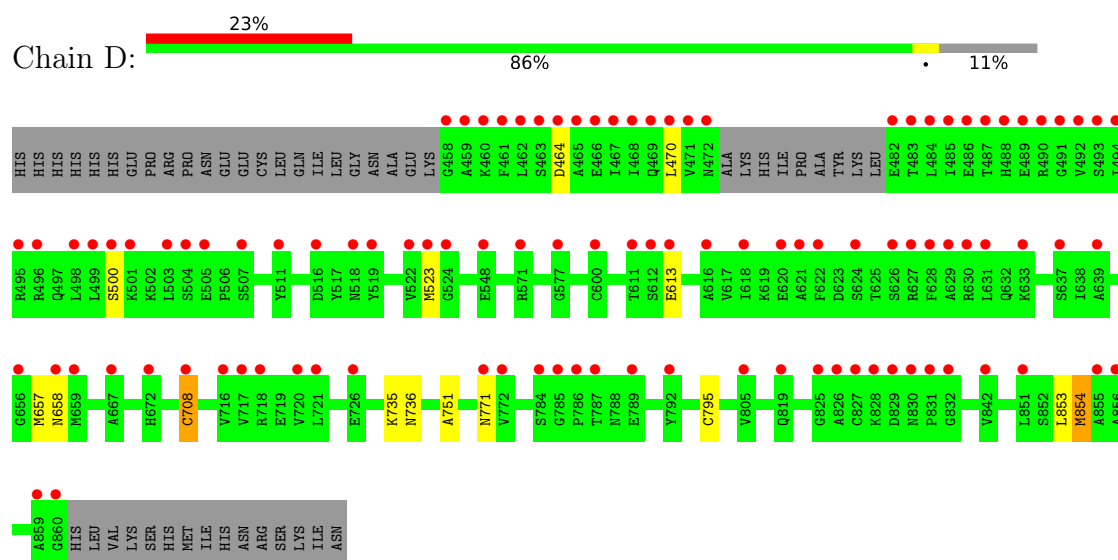
- Molecule 3 is (3R,5R)-7-[2-(4-fluorophenyl)-4-{[(1S)-2-hydroxy-1-phenylethyl]carbamoyl}-5-(1-methylethyl)-1H-imidazol-1-yl]-3,5-dihydroxyheptanoic acid (CCD ID: 5HI) (formula: C₂₈H₃₄FN₃O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	B	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	C	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	D	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total	O	0	0
			335	335		
4	B	316	Total	O	0	0
			316	316		
4	C	293	Total	O	0	0
			293	293		
4	D	292	Total	O	0	0
			292	292		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.86Å 135.66Å 83.15Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-1.70) 91.1 (50.00-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.72 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.257 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13469	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: 5HI, SO4

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	0.40	0/3188	0.75	0/4310
1	B	0.40	0/3069	0.74	0/4146
1	C	0.39	0/3051	0.74	0/4121
1	D	0.42	1/2981 (0.0%)	0.75	0/4028
All	All	0.40	1/12289 (0.0%)	0.74	0/16605

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	854	MET	SD-CE	-6.93	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	3128	0	3164	22	0
1	B	3014	0	3050	21	0
1	C	2997	0	3026	15	0
1	D	2922	0	2953	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	38	0	33	0	0
3	B	38	0	33	1	0
3	C	38	0	33	1	0
3	D	38	0	33	0	0
4	A	335	0	0	0	0
4	B	316	0	0	0	0
4	C	293	0	0	0	0
4	D	292	0	0	0	0
All	All	13469	0	12325	48	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 (48) 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:C:771[B]:ASN:HD21	1:D:771[B]:ASN:CG	1.44	1.26
1:A:771[B]:ASN:OD1	1:B:771[B]:ASN:ND2	1.69	1.25
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:OD1	1.75	1.17
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:OD1	1.76	1.16
1:A:771[B]:ASN:CG	1:B:771[B]:ASN:HD21	1.68	1.00
1:A:771[B]:ASN:HD21	1:B:771[B]:ASN:CG	1.72	0.97
1:C:771[B]:ASN:CG	1:D:771[B]:ASN:HD21	1.72	0.96
1:C:771[B]:ASN:HD21	1:D:771[B]:ASN:ND2	1.64	0.95
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:CG	2.26	0.89
1:D:751:ALA:HB2	1:D:854:MET:HE2	1.56	0.86
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:ND2	2.24	0.85
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:ND2	2.09	0.84
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:HD21	1.76	0.84
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:OD1	2.03	0.77
1:A:771[A]:ASN:HD21	1:B:771[A]:ASN:CG	1.95	0.74
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:CG	2.32	0.73
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:HD21	1.97	0.72
1:D:751:ALA:HB2	1:D:854:MET:CE	2.20	0.71
1:D:736:ASN:HD21	1:D:854:MET:HE3	1.57	0.69
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:OD1	2.13	0.67
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:ND2	2.46	0.64
1:C:771[B]:ASN:OD1	1:D:771[B]:ASN:ND2	2.28	0.59
1:A:771[A]:ASN:HD21	1:B:771[A]:ASN:ND2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:OD1	2.35	0.59
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:ND2	2.36	0.57
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:HD21	2.01	0.57
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:OD1	2.49	0.56
1:A:771[B]:ASN:CG	1:B:771[B]:ASN:ND2	2.44	0.55
1:C:708[B]:CYS:SG	1:C:795:CYS:HB2	2.47	0.54
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:ND2	2.64	0.54
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:CG	2.63	0.54
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:CG	2.50	0.54
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:CG	2.47	0.52
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:OD1	2.43	0.52
1:D:708[B]:CYS:SG	1:D:795:CYS:HB2	2.49	0.52
1:C:771[A]:ASN:CG	1:D:771[A]:ASN:OD1	2.53	0.51
1:A:635:HIS:HB3	1:A:646:ARG:HB3	1.95	0.47
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:ND2	2.62	0.47
1:D:735:LYS:HD3	1:D:854:MET:HE1	1.96	0.47
3:B:876:5HI:H13A	3:B:876:5HI:O2	2.15	0.47
1:D:751:ALA:HB1	1:D:853:LEU:HD23	1.96	0.46
1:D:736:ASN:ND2	1:D:854:MET:HE3	2.27	0.45
1:A:708[B]:CYS:SG	1:A:795:CYS:HB2	2.57	0.44
1:C:702:ARG:O	1:C:799:SER:HA	2.18	0.44
3:C:876:5HI:H12A	3:C:876:5HI:O2	2.17	0.43
1:A:581:SER:HB3	1:A:708[A]:CYS:SG	2.58	0.43
1:B:441:GLU:N	1:B:442:PRO:CD	2.83	0.42

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	421/441 (96%)	405 (96%)	16 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	402/441 (91%)	390 (97%)	11 (3%)	1 (0%)	43	28
1	C	401/441 (91%)	387 (96%)	14 (4%)	0	100	100
1	D	394/441 (89%)	382 (97%)	12 (3%)	0	100	100
All	All	1618/1764 (92%)	1564 (97%)	53 (3%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	525	ALA

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	337/355 (95%)	330 (98%)	7 (2%)	47	30
1	B	326/355 (92%)	319 (98%)	7 (2%)	47	30
1	C	324/355 (91%)	316 (98%)	8 (2%)	42	24
1	D	316/355 (89%)	306 (97%)	10 (3%)	34	17
All	All	1303/1420 (92%)	1271 (98%)	32 (2%)	45	24

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	A	523	MET
1	A	630	ARG
1	A	657	MET
1	A	688	CYS
1	A	708[A]	CYS
1	A	708[B]	CYS
1	B	452	LEU
1	B	486	GLU
1	B	505	GLU

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Mol	Chain	Res	Type
1	B	595	ARG
1	B	613	GLU
1	B	630	ARG
1	B	657	MET
1	C	482	GLU
1	C	486	GLU
1	C	494	ILE
1	C	505	GLU
1	C	523	MET
1	C	627	ARG
1	C	630	ARG
1	C	657	MET
1	D	464	ASP
1	D	470	LEU
1	D	500[A]	SER
1	D	500[B]	SER
1	D	523	MET
1	D	613	GLU
1	D	657	MET
1	D	658	ASN
1	D	708[A]	CYS
1	D	708[B]	CYS

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	469	GLN
1	A	510	GLN
1	A	567	ASN
1	A	679	GLN
1	A	770	GLN
1	A	819	GLN
1	B	472	ASN
1	B	567	ASN
1	B	648	GLN
1	B	770	GLN
1	B	819	GLN
1	C	445	ASN
1	C	510	GLN
1	C	770	GLN
1	C	819	GLN
1	D	472	ASN

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Mol	Chain	Res	Type
1	D	567	ASN
1	D	632	GLN
1	D	736	ASN
1	D	770	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](#)

8 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	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.07	0
3	5HI	B	876	-	39,40,40	0.86	1 (2%)	53,55,55	1.43	9 (16%)
3	5HI	A	876	-	39,40,40	0.87	1 (2%)	53,55,55	1.35	7 (13%)
2	SO4	A	1	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	3	-	4,4,4	0.23	0	6,6,6	0.10	0
3	5HI	D	876	-	39,40,40	0.88	1 (2%)	53,55,55	1.45	8 (15%)
3	5HI	C	876	-	39,40,40	0.88	1 (2%)	53,55,55	1.42	8 (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
3	5HI	A	876	-	-	8/35/35/35	0/3/3/3
3	5HI	B	876	-	-	11/35/35/35	0/3/3/3
3	5HI	D	876	-	-	8/35/35/35	0/3/3/3
3	5HI	C	876	-	-	9/35/35/35	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	876	5HI	C32-C1	-2.24	1.49	1.52
3	B	876	5HI	C32-C1	-2.15	1.49	1.52
3	C	876	5HI	C32-C1	-2.13	1.49	1.52
3	A	876	5HI	C32-C1	-2.07	1.49	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	876	5HI	C14-C1-N2	-3.94	103.66	109.01
3	B	876	5HI	C19-C2-N3	-3.90	107.94	111.12
3	D	876	5HI	C19-C2-N3	-3.82	108.01	111.12
3	C	876	5HI	C19-C2-N3	-3.77	108.05	111.12
3	A	876	5HI	C19-C2-N3	-3.65	108.15	111.12
3	B	876	5HI	N1-C5-N3	-3.24	109.12	111.42
3	C	876	5HI	N1-C5-N3	-3.23	109.13	111.42
3	D	876	5HI	N1-C5-N3	-3.20	109.15	111.42
3	A	876	5HI	N1-C5-N3	-3.09	109.23	111.42
3	C	876	5HI	C14-C1-N2	-2.86	105.13	109.01
3	B	876	5HI	C14-C1-N2	-2.84	105.15	109.01
3	B	876	5HI	C2-C3-N2	2.79	118.67	114.27
3	B	876	5HI	C7-N1-C5	-2.70	123.82	127.65
3	A	876	5HI	C32-C1-N2	2.63	116.55	112.07
3	B	876	5HI	C8-C7-N1	-2.54	107.72	112.16
3	D	876	5HI	C32-C1-N2	2.50	116.34	112.07
3	D	876	5HI	C8-C7-N1	-2.48	107.82	112.16
3	C	876	5HI	C2-C3-N2	2.47	118.17	114.27
3	A	876	5HI	C1-N2-C3	2.44	125.63	122.21
3	C	876	5HI	C8-C7-N1	-2.43	107.91	112.16
3	C	876	5HI	C3-C2-N3	2.43	125.46	121.06
3	C	876	5HI	C32-C1-N2	2.42	116.19	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	876	5HI	C14-C1-N2	-2.36	105.81	109.01
3	B	876	5HI	C32-C1-N2	2.28	115.96	112.07
3	D	876	5HI	C3-C2-N3	2.22	125.09	121.06
3	C	876	5HI	C24-C30-C15	-2.19	119.93	122.80
3	B	876	5HI	C24-C30-C15	-2.18	119.95	122.80
3	D	876	5HI	C24-C30-C15	-2.13	120.00	122.80
3	B	876	5HI	C2-N3-C5	2.05	108.26	104.85
3	A	876	5HI	C24-C30-C15	-2.05	120.12	122.80
3	A	876	5HI	C3-C2-N3	2.04	124.76	121.06
3	D	876	5HI	C1-N2-C3	2.00	125.01	122.21

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	876	5HI	N3-C2-C3-O2
3	B	876	5HI	C2-C19-C6-C13
3	B	876	5HI	N3-C2-C3-O2
3	B	876	5HI	C19-C2-C3-O2
3	B	876	5HI	N3-C2-C3-N2
3	B	876	5HI	C19-C2-C3-N2
3	C	876	5HI	N3-C2-C3-O2
3	C	876	5HI	C19-C2-C3-O2
3	C	876	5HI	N3-C2-C3-N2
3	D	876	5HI	N3-C2-C3-O2
3	A	876	5HI	C18-C27-C5-N3
3	D	876	5HI	C18-C27-C5-N3
3	A	876	5HI	N3-C2-C3-N2
3	D	876	5HI	N3-C2-C3-N2
3	A	876	5HI	C18-C27-C5-N1
3	D	876	5HI	C21-C27-C5-N3
3	A	876	5HI	C19-C2-C3-O2
3	D	876	5HI	C19-C2-C3-O2
3	A	876	5HI	C21-C27-C5-N3
3	A	876	5HI	C21-C27-C5-N1
3	D	876	5HI	C18-C27-C5-N1
3	B	876	5HI	C18-C27-C5-N3
3	B	876	5HI	C21-C27-C5-N1
3	D	876	5HI	C21-C27-C5-N1
3	B	876	5HI	N1-C19-C6-C13
3	B	876	5HI	C18-C27-C5-N1
3	B	876	5HI	C21-C27-C5-N3

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Mol	Chain	Res	Type	Atoms
3	C	876	5HI	C18-C27-C5-N3
3	C	876	5HI	C19-C2-C3-N2
3	D	876	5HI	C19-C2-C3-N2
3	C	876	5HI	C21-C27-C5-N1
3	C	876	5HI	C21-C27-C5-N3
3	C	876	5HI	C18-C27-C5-N1
3	A	876	5HI	C19-C2-C3-N2
3	B	876	5HI	C7-C8-C9-O4
3	C	876	5HI	C7-C8-C9-O4

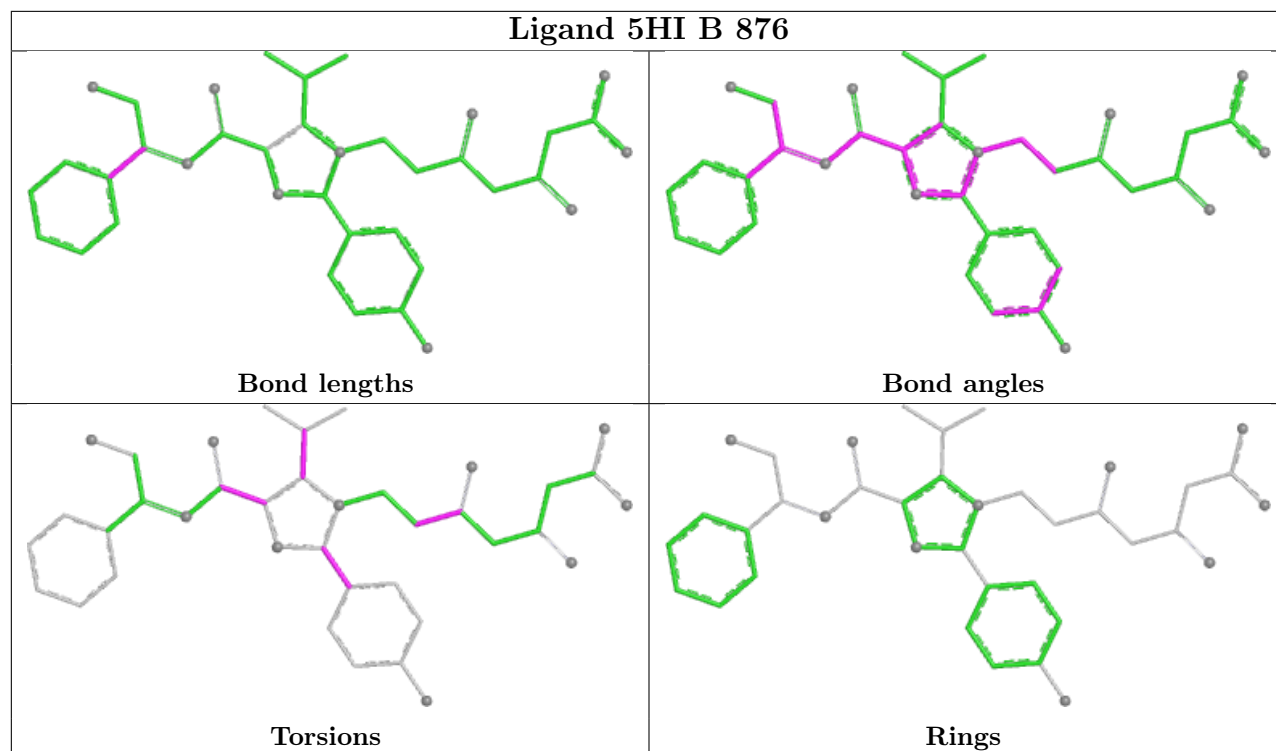
There are no ring outliers.

2 monomers are involved in 2 short contacts:

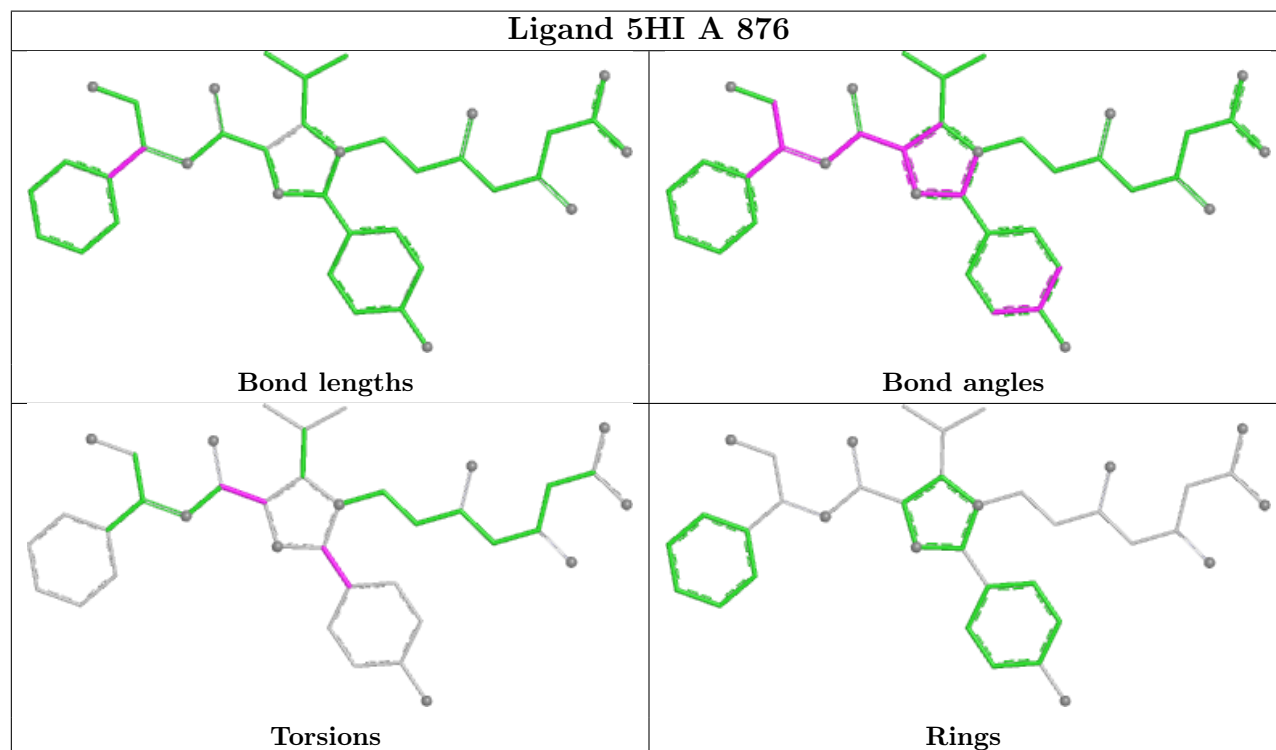
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	876	5HI	1	0
3	C	876	5HI	1	0

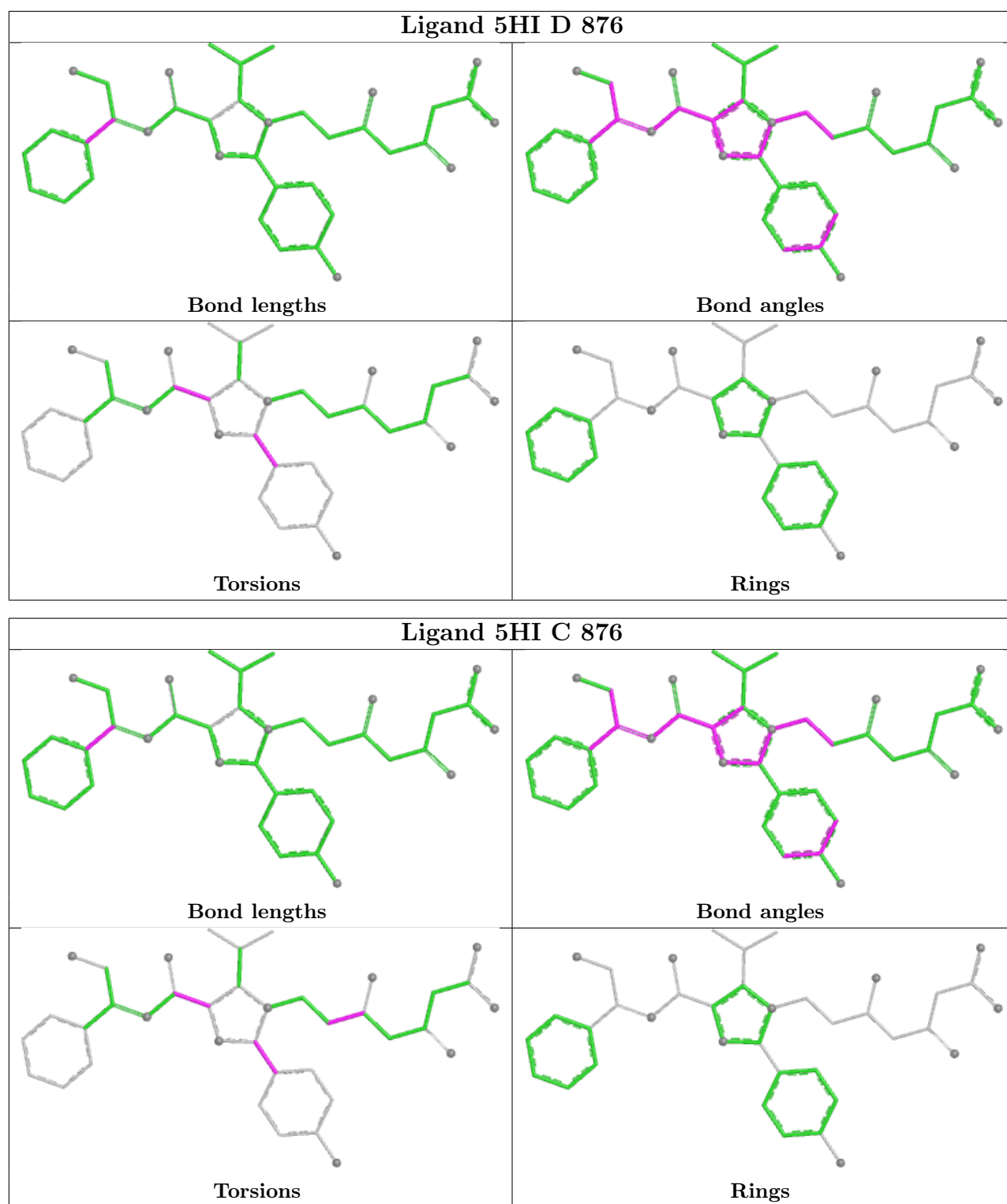
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 5HI B 876



Ligand 5HI A 876





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	420/441 (95%)	1.66	140 (33%) 1 1	13, 24, 54, 79	3 (0%)
1	B	405/441 (91%)	1.70	130 (32%) 1 1	14, 24, 80, 99	3 (0%)
1	C	404/441 (91%)	1.66	122 (30%) 1 1	13, 23, 80, 96	3 (0%)
1	D	394/441 (89%)	1.57	103 (26%) 1 1	13, 24, 59, 93	4 (1%)
All	All	1623/1764 (92%)	1.65	495 (30%) 1 1	13, 23, 69, 99	13 (0%)

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	471	VAL	10.8
1	D	467	ILE	9.8
1	D	470	LEU	9.5
1	A	453	GLY	9.4
1	C	444	PRO	9.3
1	C	449	LEU	9.3
1	B	462	LEU	8.8
1	C	467	ILE	8.6
1	B	442	PRO	8.6
1	B	452	LEU	8.4
1	B	451	ILE	8.3
1	B	444	PRO	8.2
1	B	465	ALA	8.1
1	C	462	LEU	8.1
1	B	461	PHE	7.9
1	C	471	VAL	7.9
1	D	462	LEU	7.7
1	D	487	THR	7.7
1	C	445	ASN	7.7
1	C	470	LEU	7.6
1	B	448	CYS	7.5

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Mol	Chain	Res	Type	RSRZ
1	D	465	ALA	7.5
1	D	484	LEU	7.4
1	A	442	PRO	7.3
1	C	463	SER	7.2
1	D	468	ILE	7.1
1	A	450	GLN	7.1
1	D	463	SER	7.1
1	B	484	LEU	7.0
1	A	455	ALA	7.0
1	A	451	ILE	7.0
1	C	452	LEU	6.8
1	C	453	GLY	6.8
1	C	461	PHE	6.8
1	D	461	PHE	6.7
1	C	454	ASN	6.7
1	A	635	HIS	6.7
1	B	468	ILE	6.7
1	B	459	ALA	6.6
1	C	492	VAL	6.5
1	C	491	GLY	6.4
1	A	463	SER	6.4
1	B	492	VAL	6.4
1	A	462	LEU	6.4
1	D	458	GLY	6.3
1	C	483	THR	6.3
1	A	448	CYS	6.3
1	B	471	VAL	6.2
1	D	483	THR	6.2
1	D	472	ASN	6.1
1	C	487	THR	6.1
1	B	473	ALA	6.1
1	A	465	ALA	6.0
1	C	459	ALA	6.0
1	D	459	ALA	6.0
1	C	785	GLY	5.9
1	C	465	ALA	5.9
1	B	485	ILE	5.9
1	D	488	HIS	5.9
1	A	459	ALA	5.8
1	B	474	LYS	5.8
1	C	451	ILE	5.8
1	B	449	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	468	ILE	5.7
1	A	446	GLU	5.7
1	A	458	GLY	5.7
1	C	448	CYS	5.7
1	B	470	LEU	5.6
1	D	492	VAL	5.6
1	C	485	ILE	5.5
1	B	503	LEU	5.5
1	B	488	HIS	5.5
1	D	469	GLN	5.5
1	A	860	GLY	5.4
1	B	464	ASP	5.4
1	B	467	ILE	5.4
1	C	488	HIS	5.4
1	D	464	ASP	5.3
1	D	829	ASP	5.3
1	C	458	GLY	5.3
1	C	484	LEU	5.3
1	B	469	GLN	5.3
1	A	859	ALA	5.3
1	A	461	PHE	5.2
1	C	447	GLU	5.2
1	B	487	THR	5.1
1	A	444	PRO	5.1
1	A	471	VAL	5.0
1	C	469	GLN	5.0
1	A	468	ILE	5.0
1	A	509	LEU	5.0
1	C	486	GLU	4.9
1	C	490	ARG	4.9
1	A	452	LEU	4.9
1	A	464	ASP	4.9
1	C	482	GLU	4.9
1	A	443	ARG	4.9
1	B	463	SER	4.8
1	B	441	GLU	4.8
1	B	445	ASN	4.7
1	B	491	GLY	4.6
1	D	491	GLY	4.6
1	B	460	LYS	4.6
1	B	495	ARG	4.5
1	C	464	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	829	ASP	4.5
1	B	443	ARG	4.5
1	A	485	ILE	4.5
1	B	472	ASN	4.5
1	A	445	ASN	4.4
1	C	637	SER	4.4
1	B	829	ASP	4.4
1	C	787	THR	4.4
1	A	467	ILE	4.4
1	D	485	ILE	4.4
1	A	785	GLY	4.3
1	A	484	LEU	4.3
1	A	498	LEU	4.3
1	D	786	PRO	4.3
1	C	612	SER	4.3
1	B	498	LEU	4.3
1	A	456	GLU	4.3
1	D	482	GLU	4.3
1	D	460	LYS	4.2
1	D	708[A]	CYS	4.2
1	C	507	SER	4.1
1	B	486	GLU	4.1
1	B	447	GLU	4.1
1	D	489	GLU	4.1
1	A	483	THR	4.1
1	C	630	ARG	4.1
1	A	523	MET	4.0
1	B	490	ARG	4.0
1	B	596	LEU	4.0
1	C	503	LEU	4.0
1	C	635	HIS	4.0
1	C	611	THR	4.0
1	B	446	GLU	4.0
1	A	454	ASN	3.9
1	A	449	LEU	3.9
1	B	516	ASP	3.9
1	C	489	GLU	3.9
1	D	466	GLU	3.9
1	A	475	HIS	3.9
1	C	860	GLY	3.9
1	A	473	ALA	3.9
1	B	450	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	659	MET	3.8
1	A	787	THR	3.8
1	B	577	GLY	3.8
1	D	548	GLU	3.8
1	A	487	THR	3.8
1	C	826	ALA	3.8
1	B	501	LYS	3.7
1	D	494	ILE	3.7
1	C	446	GLU	3.7
1	C	499	LEU	3.7
1	C	674	TYR	3.7
1	C	616	ALA	3.7
1	A	658	ASN	3.7
1	D	490	ARG	3.6
1	B	628	PHE	3.6
1	A	488	HIS	3.6
1	A	492	VAL	3.6
1	D	830	ASN	3.6
1	A	612	SER	3.6
1	B	504	SER	3.6
1	B	828	LYS	3.6
1	A	495	ARG	3.6
1	B	517	TYR	3.6
1	C	450	GLN	3.5
1	B	506	PRO	3.5
1	A	460	LYS	3.5
1	B	859	ALA	3.5
1	A	772	VAL	3.5
1	B	496	ARG	3.5
1	A	486	GLU	3.4
1	C	830	ASN	3.4
1	C	615	PHE	3.4
1	C	493	SER	3.4
1	A	481	LEU	3.4
1	D	495	ARG	3.4
1	D	785	GLY	3.4
1	D	860	GLY	3.4
1	A	633	LYS	3.4
1	C	786	PRO	3.4
1	A	514	TYR	3.4
1	C	505	GLU	3.4
1	B	787	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	489	GLU	3.4
1	D	613	GLU	3.4
1	B	493	SER	3.4
1	D	507	SER	3.4
1	C	859	ALA	3.3
1	A	470	LEU	3.3
1	A	441	GLU	3.3
1	C	613	GLU	3.3
1	B	672	HIS	3.3
1	B	660	ILE	3.3
1	B	512	LEU	3.3
1	A	447	GLU	3.3
1	C	460	LYS	3.3
1	B	466	GLU	3.3
1	C	466	GLU	3.2
1	C	548	GLU	3.2
1	B	624	SER	3.2
1	B	494	ILE	3.2
1	B	499	LEU	3.2
1	D	486	GLU	3.2
1	A	659	MET	3.2
1	C	708[A]	CYS	3.2
1	A	501	LYS	3.2
1	A	828	LYS	3.2
1	B	666	LYS	3.2
1	A	516	ASP	3.2
1	C	659	MET	3.2
1	B	638	ILE	3.2
1	A	577	GLY	3.2
1	B	716	VAL	3.2
1	A	479	TYR	3.1
1	C	524	GLY	3.1
1	A	789	GLU	3.1
1	D	519	TYR	3.1
1	D	787	THR	3.1
1	A	650	ARG	3.1
1	A	829	ASP	3.1
1	C	509	LEU	3.1
1	C	521	LEU	3.1
1	C	828	LYS	3.1
1	C	515	ARG	3.0
1	D	496	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	3.0
1	C	494	ILE	3.0
1	A	457	LYS	3.0
1	A	826	ALA	3.0
1	A	507	SER	3.0
1	A	708[A]	CYS	3.0
1	D	523	MET	3.0
1	D	524	GLY	3.0
1	A	637	SER	3.0
1	B	631	LEU	3.0
1	C	496	ARG	3.0
1	C	498	LEU	3.0
1	B	772	VAL	2.9
1	B	595	ARG	2.9
1	B	548	GLU	2.9
1	B	502	LYS	2.9
1	A	613	GLU	2.9
1	D	717	VAL	2.9
1	A	525	ALA	2.9
1	D	826	ALA	2.9
1	A	671	LEU	2.9
1	D	827	CYS	2.9
1	A	786	PRO	2.9
1	B	523	MET	2.9
1	B	612	SER	2.9
1	A	472	ASN	2.9
1	D	859	ALA	2.9
1	A	521	LEU	2.9
1	B	509	LEU	2.9
1	A	500	SER	2.9
1	A	628	PHE	2.8
1	A	595	ARG	2.8
1	A	616	ALA	2.8
1	B	613	GLU	2.8
1	D	500[A]	SER	2.8
1	A	598	ARG	2.8
1	B	621	ALA	2.8
1	B	635	HIS	2.8
1	B	620	GLU	2.8
1	A	627	ARG	2.8
1	A	630	ARG	2.8
1	A	512	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	2.8
1	C	596	LEU	2.8
1	D	503	LEU	2.8
1	C	660	ILE	2.8
1	D	633	LYS	2.8
1	C	607	ALA	2.7
1	D	630	ARG	2.7
1	D	639	ALA	2.7
1	D	518	ASN	2.7
1	B	659	MET	2.7
1	C	511	TYR	2.7
1	B	618	ILE	2.7
1	B	500	SER	2.7
1	D	658	ASN	2.7
1	A	478	ALA	2.7
1	C	639	ALA	2.7
1	A	713	PRO	2.7
1	B	827	CYS	2.7
1	A	466	GLU	2.7
1	A	574	GLY	2.7
1	D	656	GLY	2.7
1	A	506	PRO	2.7
1	B	675	PHE	2.7
1	D	622	PHE	2.7
1	B	789	GLU	2.7
1	D	493	SER	2.7
1	B	785	GLY	2.7
1	B	633	LYS	2.7
1	B	630	ARG	2.6
1	A	482	GLU	2.6
1	B	637	SER	2.6
1	C	626	SER	2.6
1	A	631	LEU	2.6
1	B	668	LEU	2.6
1	B	708	CYS	2.6
1	C	577	GLY	2.6
1	C	519	TYR	2.6
1	C	495	ARG	2.6
1	C	621	ALA	2.6
1	D	667	ALA	2.6
1	B	524	GLY	2.6
1	B	833	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	516	ASP	2.6
1	A	476	ILE	2.6
1	A	638	ILE	2.6
1	D	618	ILE	2.6
1	A	856	ALA	2.6
1	B	825	GLY	2.6
1	C	665	GLU	2.6
1	D	499	LEU	2.6
1	D	772	VAL	2.6
1	C	504	SER	2.6
1	C	633	LYS	2.6
1	B	505	GLU	2.6
1	D	628	PHE	2.5
1	D	600	CYS	2.5
1	A	499	LEU	2.5
1	D	624	SER	2.5
1	C	805	VAL	2.5
1	A	660	ILE	2.5
1	A	491	GLY	2.5
1	D	825	GLY	2.5
1	D	612	SER	2.5
1	D	718	ARG	2.5
1	D	789	GLU	2.5
1	A	622	PHE	2.5
1	A	681	LEU	2.5
1	A	792	TYR	2.5
1	C	792	TYR	2.5
1	D	511	TYR	2.5
1	D	792	TYR	2.5
1	A	469	GLN	2.5
1	A	632	GLN	2.5
1	B	525	ALA	2.5
1	B	805	VAL	2.5
1	C	573	ILE	2.5
1	C	598	ARG	2.5
1	B	507	SER	2.5
1	C	631	LEU	2.5
1	A	831	PRO	2.5
1	C	725	THR	2.5
1	D	505	GLU	2.4
1	A	822	GLY	2.4
1	D	832	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	621	ALA	2.4
1	A	522	VAL	2.4
1	C	605	VAL	2.4
1	C	661	SER	2.4
1	C	810	ASN	2.4
1	B	665	GLU	2.4
1	A	515	ARG	2.4
1	B	598	ARG	2.4
1	C	628	PHE	2.4
1	C	675	PHE	2.4
1	B	616	ALA	2.4
1	C	500	SER	2.4
1	D	629	ALA	2.4
1	B	511	TYR	2.4
1	D	620	GLU	2.4
1	D	501	LYS	2.4
1	C	624	SER	2.4
1	D	504	SER	2.4
1	A	858	ALA	2.4
1	C	618	ILE	2.4
1	A	832	GLY	2.3
1	B	520	SER	2.3
1	C	587	GLY	2.3
1	C	658	ASN	2.3
1	A	477	PRO	2.3
1	C	512	LEU	2.3
1	C	718	ARG	2.3
1	D	851	LEU	2.3
1	A	617	VAL	2.3
1	C	617	VAL	2.3
1	D	522	VAL	2.3
1	B	515	ARG	2.3
1	D	571	ARG	2.3
1	D	616	ALA	2.3
1	B	671	LEU	2.3
1	D	721	LEU	2.3
1	A	511	TYR	2.3
1	B	514	TYR	2.3
1	B	860	GLY	2.3
1	B	831	PRO	2.3
1	A	827	CYS	2.3
1	A	679	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	826	ALA	2.3
1	A	503	LEU	2.3
1	D	498	LEU	2.3
1	B	830	ASN	2.3
1	A	669	SER	2.3
1	B	622	PHE	2.3
1	B	718	ARG	2.3
1	D	627	ARG	2.3
1	A	524	GLY	2.3
1	A	573	ILE	2.3
1	D	611	THR	2.2
1	A	561	CYS	2.2
1	D	855	ALA	2.2
1	A	634	LEU	2.2
1	D	631	LEU	2.2
1	A	480	LYS	2.2
1	A	615	PHE	2.2
1	D	577	GLY	2.2
1	A	717	VAL	2.2
1	B	530	VAL	2.2
1	D	720	VAL	2.2
1	D	842	VAL	2.2
1	C	518	ASN	2.2
1	C	654	ALA	2.2
1	C	827	CYS	2.2
1	D	828	LYS	2.2
1	C	825	GLY	2.2
1	A	494	ILE	2.2
1	A	513	PRO	2.2
1	A	720	VAL	2.2
1	C	501	LYS	2.2
1	C	772	VAL	2.2
1	A	504	SER	2.2
1	C	726	GLU	2.2
1	D	726	GLU	2.2
1	B	656	GLY	2.2
1	A	718	ARG	2.2
1	C	650	ARG	2.2
1	A	502	LYS	2.2
1	C	788	ASN	2.2
1	D	771[A]	ASN	2.2
1	C	517	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	664	THR	2.2
1	C	676	PRO	2.2
1	D	831	PRO	2.2
1	A	580	SER	2.2
1	D	637	SER	2.2
1	B	522	VAL	2.1
1	D	716	VAL	2.1
1	C	629	ALA	2.1
1	B	650	ARG	2.1
1	A	675	PHE	2.1
1	A	620	GLU	2.1
1	A	665	GLU	2.1
1	B	676	PRO	2.1
1	B	519	TYR	2.1
1	B	563	VAL	2.1
1	B	717	VAL	2.1
1	B	783	ALA	2.1
1	A	672	HIS	2.1
1	C	576	GLY	2.1
1	A	546	LEU	2.1
1	D	784	SER	2.1
1	C	622	PHE	2.1
1	A	666	LYS	2.1
1	B	807	GLY	2.1
1	B	617	VAL	2.1
1	B	658	ASN	2.1
1	B	819	GLN	2.1
1	D	819	GLN	2.1
1	B	669	SER	2.1
1	A	840	ARG	2.1
1	B	634	LEU	2.1
1	B	664	THR	2.1
1	D	672	HIS	2.1
1	A	517	TYR	2.1
1	C	699	ILE	2.1
1	A	629	ALA	2.0
1	C	677	GLU	2.0
1	B	510	GLN	2.0
1	C	679	GLN	2.0
1	A	530	VAL	2.0
1	C	623	ASP	2.0
1	D	626	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	805	VAL	2.0
1	A	857	LEU	2.0
1	C	681	LEU	2.0
1	B	597	PRO	2.0
1	A	576	GLY	2.0
1	A	496	ARG	2.0
1	A	541	ALA	2.0
1	A	607	ALA	2.0
1	B	667	ALA	2.0
1	B	835	ALA	2.0
1	D	856	ALA	2.0
1	C	662	LYS	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, 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.

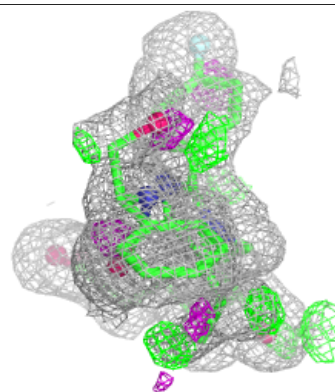
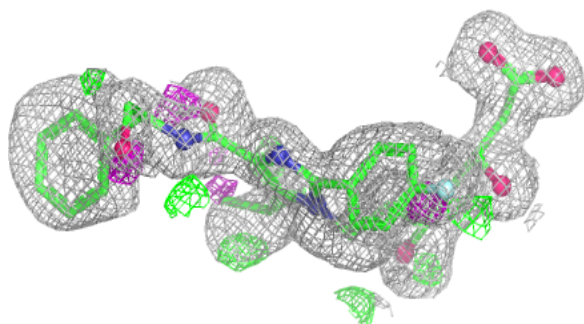
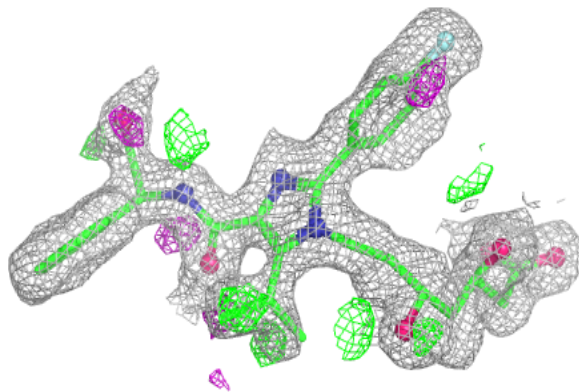
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	2	5/5	0.53	0.26	81,81,81,81	0
2	SO4	D	4	5/5	0.68	0.30	69,69,69,69	0
2	SO4	A	1	5/5	0.69	0.23	77,77,77,77	0
2	SO4	C	3	5/5	0.71	0.28	70,70,70,70	0
3	5HI	B	876	38/38	0.85	0.13	21,29,30,30	0
3	5HI	A	876	38/38	0.87	0.12	19,25,27,29	0
3	5HI	C	876	38/38	0.87	0.12	20,27,29,30	0
3	5HI	D	876	38/38	0.87	0.12	21,27,28,29	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.

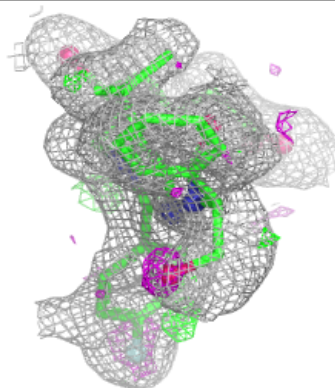
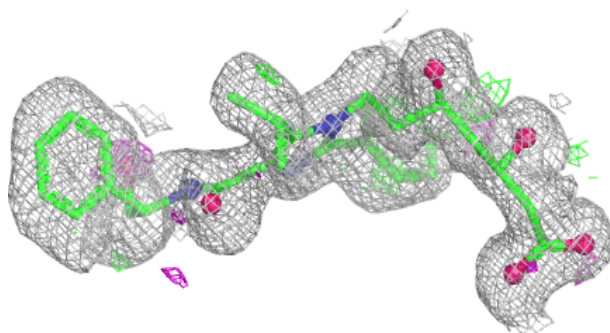
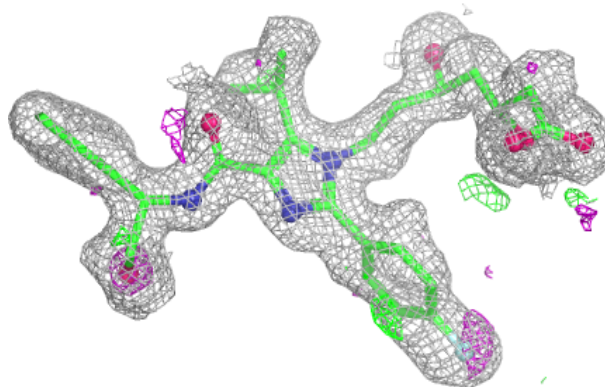
Electron density around 5HI B 876:

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



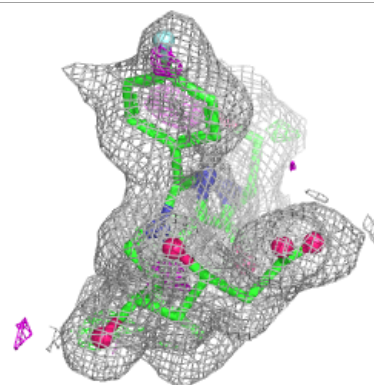
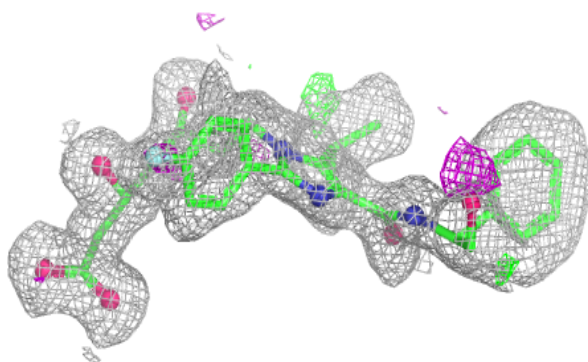
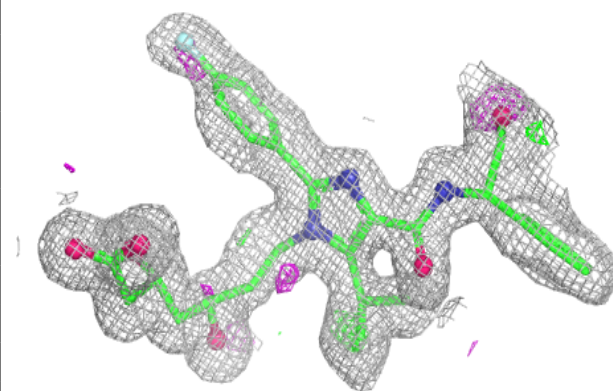
Electron density around 5HI A 876:

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

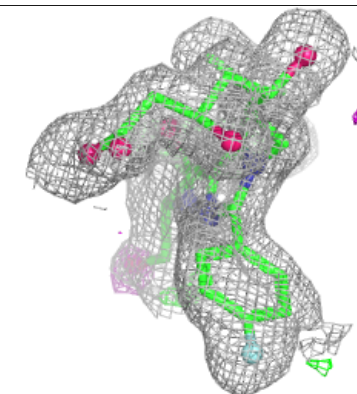
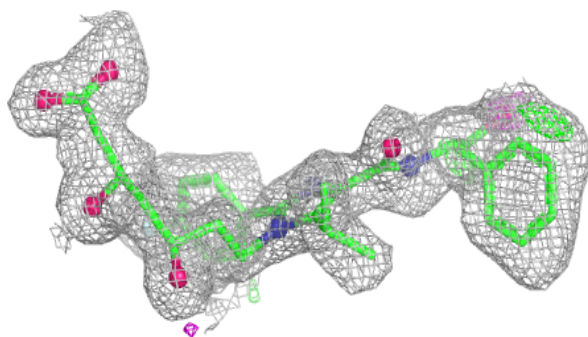
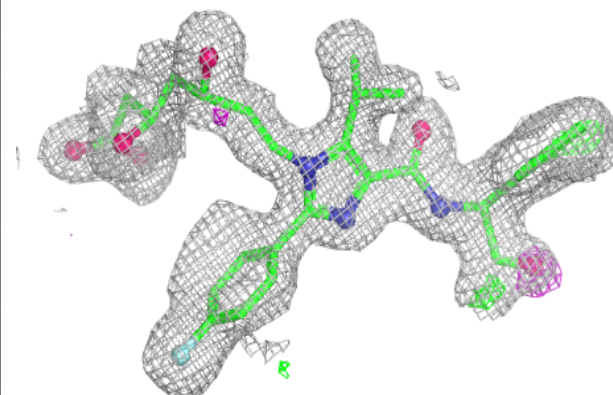


Electron density around 5HI C 876:

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

**Electron density around 5HI D 876:**

$2mF_o-DF_c$ (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.