



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:57 PM UTC

PDB ID : 3CCT / pdb_00003cct
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 : 2.12 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

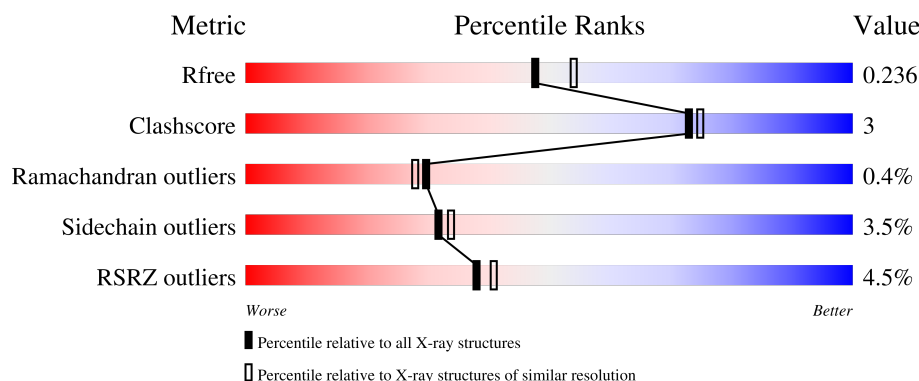
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	5% 84% 9% • 5%
1	B	441	3% 87% 7% • 5%
1	C	441	6% 87% 7% • 5%
1	D	441	3% 83% 6% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12845 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	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	B	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	C	417	Total	C	N	O	S	0	0	0
			3096	1929	542	595	30			
1	D	394	Total	C	N	O	S	0	0	0
			2920	1818	514	559	29			

There are 28 discrepancies between the modelled and reference sequences:

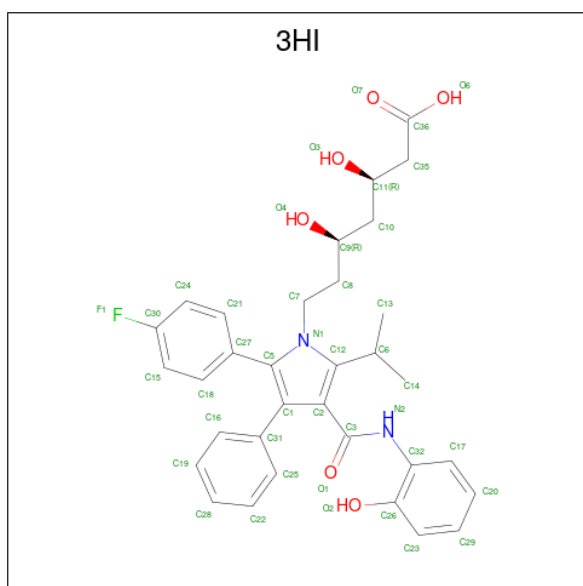
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered 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-[2-(4-fluorophenyl)-4-[(2-hydroxyphenyl)carbamoyl]-5-(1-methylethyl)-3-phenyl-1H-pyrrol-1-yl]-3,5-dihydroxyheptanoic acid (CCD ID: 3HI) (formula: $C_{33}H_{35}FN_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			42	33	1	2	6		
2	B	1	Total	C	F	N	O	0	0
			42	33	1	2	6		
2	C	1	Total	C	F	N	O	0	0
			42	33	1	2	6		
2	D	1	Total	C	F	N	O	0	0
			42	33	1	2	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		

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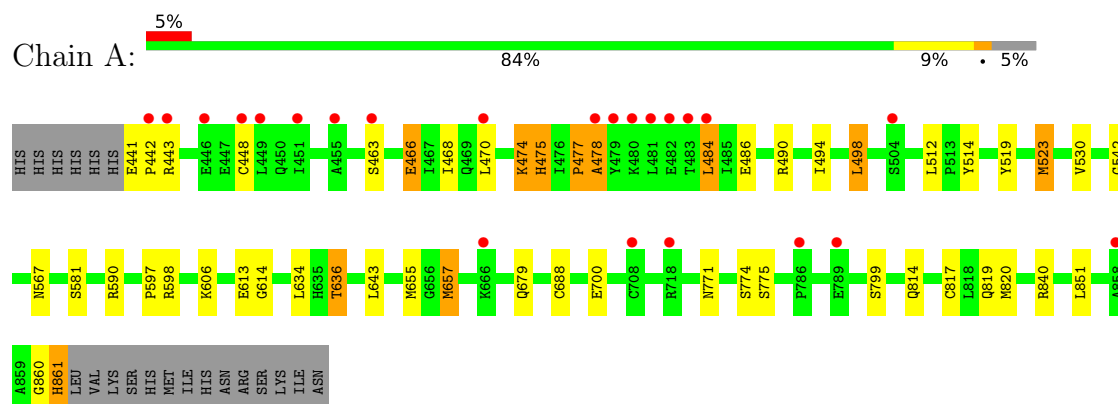
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	83	Total 83	O 83	0	0
3	D	103	Total 103	O 103	0	0

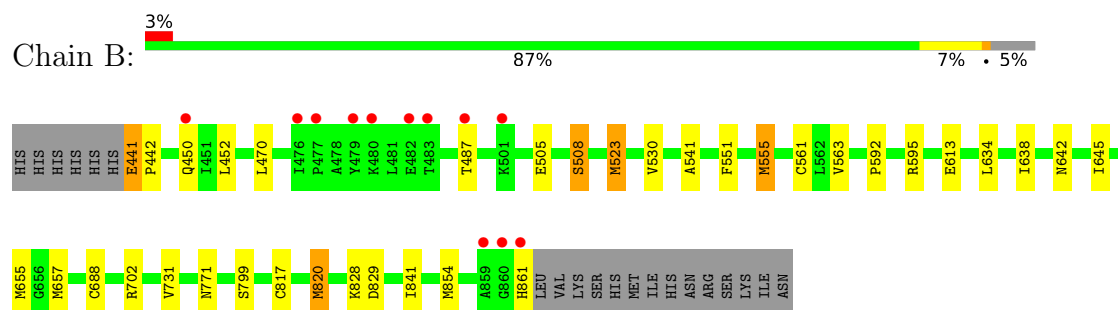
3 Residue-property plots [i](#)

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.

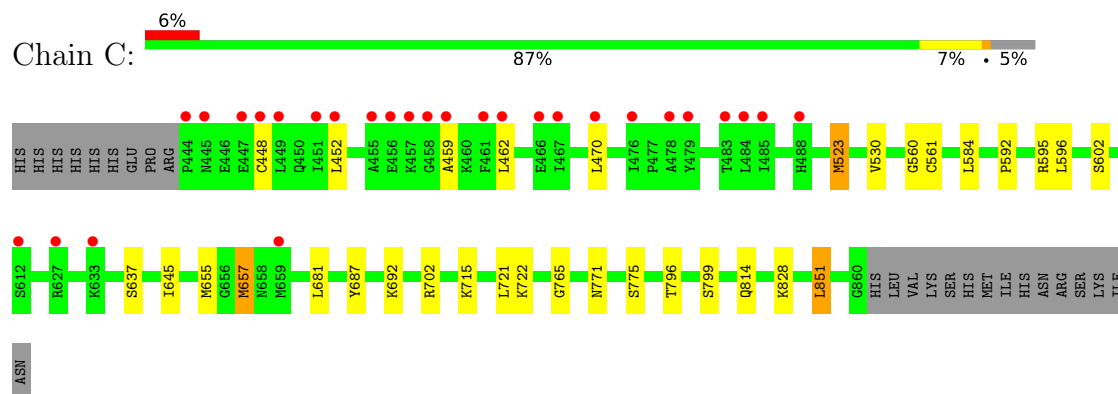
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



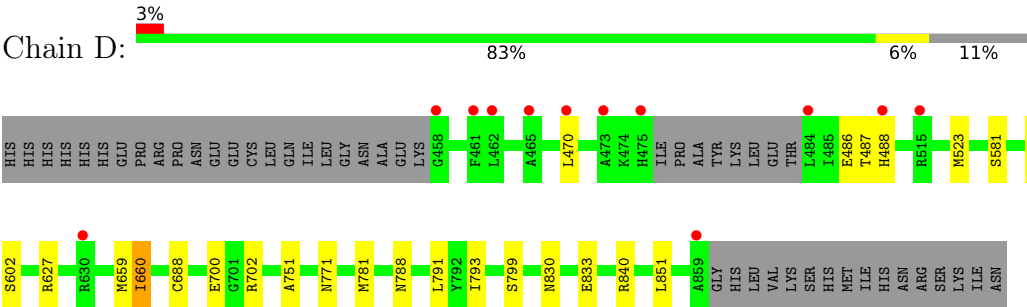
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.94Å 173.51Å 76.40Å 90.00° 119.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.12 30.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	88.7 (30.00-2.12) 88.8 (30.00-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.236 0.200 , 0.236	Depositor DCC
R_{free} test set	8708 reflections (9.17%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.025 for h,-k,-h-l 0.025 for l,-k,h 0.023 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12845	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: 3HI

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	0.63	2/3179 (0.1%)	0.86	0/4298
1	B	0.64	2/3179 (0.1%)	0.81	0/4298
1	C	0.59	0/3140	0.81	0/4244
1	D	0.59	0/2960	0.82	0/3999
All	All	0.61	4/12458 (0.0%)	0.83	0/16839

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-9.38	1.56	1.79
1	A	657	MET	SD-CE	-5.91	1.64	1.79
1	A	523	MET	SD-CE	-5.38	1.66	1.79
1	B	820	MET	SD-CE	-5.03	1.67	1.79

There are no bond angle outliers.

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	28	0
1	B	3133	0	3167	19	0
1	C	3096	0	3135	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2920	0	2957	12	0
2	B	84	0	66	4	0
2	C	42	0	33	0	0
2	D	42	0	33	0	0
3	A	96	0	0	1	0
3	B	113	0	0	0	0
3	C	83	0	0	2	0
3	D	103	0	0	1	0
All	All	12845	0	12558	79	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.

All (79) 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	2.19	0.83
1:C:771:ASN:OD1	1:C:775:SER:OG	2.03	0.74
1:A:817:CYS:HA	1:A:820:MET:HE3	1.71	0.71
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.10	0.69
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.75	0.69
1:A:679:GLN:NE2	3:A:343:HOH:O	2.27	0.68
1:C:523:MET:HE1	1:C:530:VAL:HG21	1.76	0.67
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.26	0.65
1:B:523:MET:HE1	1:B:530:VAL:HB	1.79	0.63
2:B:1:3HI:H7	2:B:1:3HI:H13B	1.81	0.61
1:A:860:GLY:O	1:A:861:HIS:HB2	2.00	0.61
1:D:596:LEU:HD13	1:D:602:SER:HA	1.83	0.59
1:C:655:MET:SD	1:C:657:MET:HG2	2.43	0.58
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.85	0.58
1:B:655:MET:HE1	1:B:657:MET:HG3	1.86	0.57
1:C:655:MET:HE1	1:C:657:MET:HG3	1.87	0.56
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.87	0.56
1:B:655:MET:SD	1:B:657:MET:HG2	2.46	0.55
1:D:627:ARG:HG3	3:D:111:HOH:O	2.06	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.07	0.54
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.38	0.54
1:B:441:GLU:N	1:B:442:PRO:CD	2.71	0.54
1:A:590:ARG:NH2	1:A:657:MET:HE3	2.22	0.54
1:B:655:MET:HE1	1:B:657:MET:CG	2.38	0.54
1:B:541:ALA:HB2	1:B:555:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:HG12	1:A:498:LEU:HD11	1.91	0.52
1:A:771:ASN:OD1	1:A:775:SER:OG	2.28	0.52
1:A:819:GLN:HB3	1:B:508:SER:HB3	1.91	0.52
1:B:817:CYS:HA	1:B:820:MET:HE3	1.92	0.52
1:C:523:MET:HA	1:C:523:MET:HE3	1.93	0.51
1:A:774:SER:HA	1:A:799:SER:O	2.11	0.51
1:C:596:LEU:HD13	1:C:602:SER:HA	1.91	0.51
1:A:542:GLY:H	1:A:567:ASN:ND2	2.09	0.51
1:C:523:MET:HE2	3:C:199:HOH:O	2.11	0.51
2:B:1:3HI:H14B	2:B:1:3HI:H8A	1.94	0.50
1:B:592:PRO:HD2	1:B:645:ILE:O	2.13	0.48
1:D:702:ARG:O	1:D:799:SER:HA	2.13	0.48
1:A:490:ARG:O	1:A:494:ILE:HG12	2.13	0.48
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.42	0.47
1:B:731:VAL:HG12	1:B:854:MET:HE1	1.96	0.47
1:C:702:ARG:O	1:C:799:SER:HA	2.15	0.47
1:B:555:MET:HE1	1:B:563:VAL:HA	1.95	0.47
1:A:474:LYS:O	1:A:475:HIS:CB	2.63	0.47
1:D:781:MET:HE2	1:D:793:ILE:HD12	1.96	0.47
1:A:441:GLU:N	1:A:442:PRO:CD	2.78	0.47
1:B:702:ARG:O	1:B:799:SER:HA	2.14	0.46
1:A:606:LYS:HG3	1:A:636:THR:HG21	1.98	0.46
1:D:791:LEU:HD23	1:D:791:LEU:C	2.42	0.45
1:A:474:LYS:O	1:A:475:HIS:CG	2.69	0.45
1:C:692:LYS:NZ	1:D:751:ALA:O	2.50	0.45
1:C:637:SER:OG	1:C:687:TYR:OH	2.30	0.45
1:D:581:SER:OG	1:D:840:ARG:HD2	2.17	0.44
1:A:477:PRO:O	1:A:478:ALA:CB	2.65	0.44
1:C:452:LEU:HD21	1:C:459:ALA:HB2	1.99	0.44
1:A:448:CYS:SG	1:A:466:GLU:HG2	2.58	0.44
1:A:519:TYR:HB3	1:A:523:MET:HE3	2.00	0.44
1:A:581:SER:OG	1:A:840:ARG:HD2	2.19	0.43
1:C:592:PRO:HD2	1:C:645:ILE:O	2.19	0.43
2:B:2:3HI:O1	2:B:2:3HI:H13B	2.17	0.43
1:B:541:ALA:HB2	1:B:555:MET:CE	2.49	0.43
1:B:561:CYS:HB3	2:B:2:3HI:O2	2.18	0.43
1:C:722:LYS:NZ	3:C:192:HOH:O	2.51	0.43
1:C:721:LEU:CD1	1:C:851:LEU:HD22	2.49	0.43
1:A:597:PRO:O	1:A:598:ARG:HD3	2.19	0.43
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.85	0.43
1:B:638:ILE:HD12	1:C:584:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:ILE:O	1:C:796:THR:HG21	2.19	0.42
1:C:765:GLY:CA	1:C:814:GLN:HG2	2.49	0.42
1:B:551:PHE:CE2	1:B:841:ILE:HD11	2.55	0.42
1:C:765:GLY:HA2	1:C:814:GLN:HG2	2.02	0.42
1:D:590:ARG:HB2	1:D:660:ILE:HG22	2.02	0.41
1:B:595:ARG:HD2	1:B:642:ASN:OD1	2.20	0.41
1:C:448:CYS:SG	1:C:462:LEU:HD22	2.60	0.41
1:A:613:GLU:HG2	1:A:614:GLY:N	2.35	0.41
1:D:488:HIS:HD2	1:D:523:MET:HG3	1.85	0.41
1:C:771:ASN:HB3	1:D:771:ASN:HD21	1.86	0.41
1:D:830:ASN:O	1:D:833:GLU:HB2	2.21	0.40
1:C:560:GLY:O	1:C:561:CYS:HB2	2.22	0.40
1:C:828:LYS:H	1:C:828:LYS:HG2	1.75	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%)	400 (96%)	13 (3%)	6 (1%)	9	5
1	B	419/441 (95%)	403 (96%)	16 (4%)	0	100	100
1	C	415/441 (94%)	395 (95%)	20 (5%)	0	100	100
1	D	390/441 (88%)	376 (96%)	14 (4%)	0	100	100
All	All	1643/1764 (93%)	1574 (96%)	63 (4%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	LEU
1	A	475	HIS

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Mol	Chain	Res	Type
1	A	478	ALA
1	A	474	LYS
1	A	477	PRO
1	A	514	TYR

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	335/355 (94%)	321 (96%)	14 (4%)	26	27
1	B	335/355 (94%)	320 (96%)	15 (4%)	24	24
1	C	331/355 (93%)	324 (98%)	7 (2%)	47	54
1	D	312/355 (88%)	302 (97%)	10 (3%)	34	37
All	All	1313/1420 (92%)	1267 (96%)	46 (4%)	32	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	463	SER
1	A	466	GLU
1	A	470	LEU
1	A	484	LEU
1	A	486	GLU
1	A	498	LEU
1	A	512	LEU
1	A	634	LEU
1	A	636	THR
1	A	688	CYS
1	A	814	GLN
1	A	851	LEU
1	A	861	HIS
1	B	441	GLU
1	B	450	GLN
1	B	452	LEU

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Mol	Chain	Res	Type
1	B	470	LEU
1	B	487	THR
1	B	505	GLU
1	B	508	SER
1	B	523	MET
1	B	613	GLU
1	B	634	LEU
1	B	688	CYS
1	B	771	ASN
1	B	828	LYS
1	B	829	ASP
1	B	861	HIS
1	C	470	LEU
1	C	523	MET
1	C	595	ARG
1	C	657	MET
1	C	681	LEU
1	C	715	LYS
1	C	851	LEU
1	D	470	LEU
1	D	486	GLU
1	D	487	THR
1	D	595	ARG
1	D	596	LEU
1	D	659	MET
1	D	660	ILE
1	D	688	CYS
1	D	788	ASN
1	D	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	497	GLN
1	A	567	ASN
1	A	635	HIS
1	A	672	HIS
1	A	770	GLN
1	A	788	ASN
1	A	819	GLN
1	B	450	GLN

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Mol	Chain	Res	Type
1	B	469	GLN
1	B	472	ASN
1	B	648	GLN
1	B	679	GLN
1	B	819	GLN
1	C	472	ASN
1	C	475	HIS
1	C	497	GLN
1	C	510	GLN
1	C	632	GLN
1	C	679	GLN
1	D	488	HIS
1	D	497	GLN
1	D	518	ASN
1	D	642	ASN
1	D	788	ASN
1	D	819	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	3HI	B	1	-	45,45,45	1.11	3 (6%)	57,63,63	1.56	7 (12%)
2	3HI	C	4	-	45,45,45	1.18	3 (6%)	57,63,63	1.53	10 (17%)
2	3HI	B	2	-	45,45,45	1.17	3 (6%)	57,63,63	1.61	9 (15%)
2	3HI	D	3	-	45,45,45	1.29	3 (6%)	57,63,63	1.46	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	3HI	B	1	-	-	0/33/33/33	0/4/4/4
2	3HI	C	4	-	-	5/33/33/33	0/4/4/4
2	3HI	B	2	-	-	1/33/33/33	0/4/4/4
2	3HI	D	3	-	-	3/33/33/33	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	3HI	C1-C5	5.35	1.48	1.39
2	C	4	3HI	C1-C5	4.38	1.46	1.39
2	B	2	3HI	C1-C5	4.33	1.46	1.39
2	B	1	3HI	C1-C5	4.08	1.46	1.39
2	C	4	3HI	C5-N1	-3.76	1.33	1.39
2	D	3	3HI	C5-N1	-3.65	1.33	1.39
2	B	2	3HI	C5-N1	-3.55	1.33	1.39
2	B	1	3HI	C5-N1	-3.46	1.33	1.39
2	B	1	3HI	C1-C2	-3.02	1.37	1.44
2	B	2	3HI	C1-C2	-2.63	1.38	1.44
2	C	4	3HI	C1-C2	-2.39	1.38	1.44
2	D	3	3HI	C1-C2	-2.01	1.39	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	3HI	C27-C5-N1	6.00	134.26	122.89
2	B	1	3HI	C27-C5-C1	-4.74	118.22	128.66
2	C	4	3HI	C21-C27-C5	-4.35	114.00	120.56
2	B	2	3HI	C21-C27-C5	-4.34	114.01	120.56
2	D	3	3HI	O1-C3-C2	-4.22	115.20	121.53
2	B	2	3HI	C27-C5-N1	4.01	130.49	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	3HI	O1-C3-C2	-3.73	115.94	121.53
2	D	3	3HI	C2-C3-N2	3.67	122.09	115.81
2	B	2	3HI	C18-C27-C5	3.58	125.97	120.56
2	C	4	3HI	C27-C5-N1	3.46	129.45	122.89
2	C	4	3HI	O1-C3-C2	-3.42	116.41	121.53
2	C	4	3HI	C2-C3-N2	3.28	121.42	115.81
2	B	2	3HI	C27-C5-C1	-3.25	121.51	128.66
2	D	3	3HI	C27-C5-N1	3.20	128.96	122.89
2	C	4	3HI	C18-C27-C5	3.20	125.40	120.56
2	D	3	3HI	C23-C26-C32	2.90	122.00	119.67
2	B	1	3HI	C7-N1-C5	-2.82	121.48	126.72
2	B	1	3HI	C10-C11-C35	-2.78	107.29	112.96
2	B	2	3HI	C2-C3-N2	2.75	120.52	115.81
2	D	3	3HI	C21-C27-C5	-2.66	116.55	120.56
2	C	4	3HI	C27-C5-C1	-2.63	122.87	128.66
2	B	1	3HI	O1-C3-C2	-2.56	117.70	121.53
2	B	2	3HI	C10-C9-C8	-2.55	107.02	112.42
2	B	1	3HI	C2-C3-N2	2.41	119.94	115.81
2	B	2	3HI	C23-C26-C32	2.33	121.54	119.67
2	B	1	3HI	C21-C27-C5	-2.28	117.12	120.56
2	C	4	3HI	C10-C11-C35	-2.26	108.34	112.96
2	D	3	3HI	C7-C8-C9	-2.20	108.78	113.31
2	B	2	3HI	C7-N1-C5	-2.19	122.65	126.72
2	D	3	3HI	C27-C5-C1	-2.12	123.98	128.66
2	C	4	3HI	C7-N1-C5	-2.11	122.79	126.72
2	C	4	3HI	C14-C6-C12	-2.09	108.82	112.92
2	C	4	3HI	C31-C1-C5	-2.09	122.95	127.01
2	D	3	3HI	C10-C9-C8	-2.03	108.13	112.42
2	D	3	3HI	C18-C27-C5	2.02	123.61	120.56

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	3HI	C12-C2-C3-O1
2	D	3	3HI	C12-C2-C3-O1
2	D	3	3HI	C1-C2-C3-O1
2	D	3	3HI	C1-C2-C3-N2
2	C	4	3HI	C1-C2-C3-O1
2	C	4	3HI	C7-C8-C9-O4
2	C	4	3HI	O1-C3-N2-C32
2	C	4	3HI	C7-C8-C9-C10

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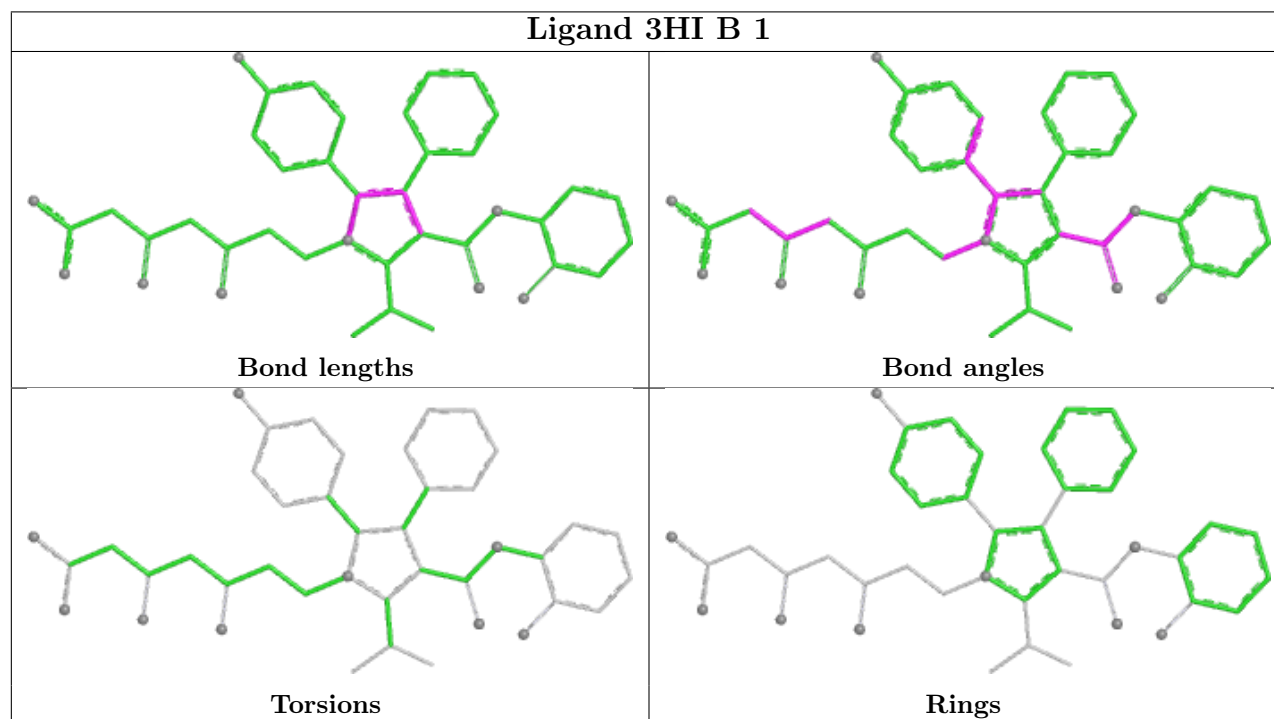
Mol	Chain	Res	Type	Atoms
2	B	2	3HI	C1-C2-C3-O1

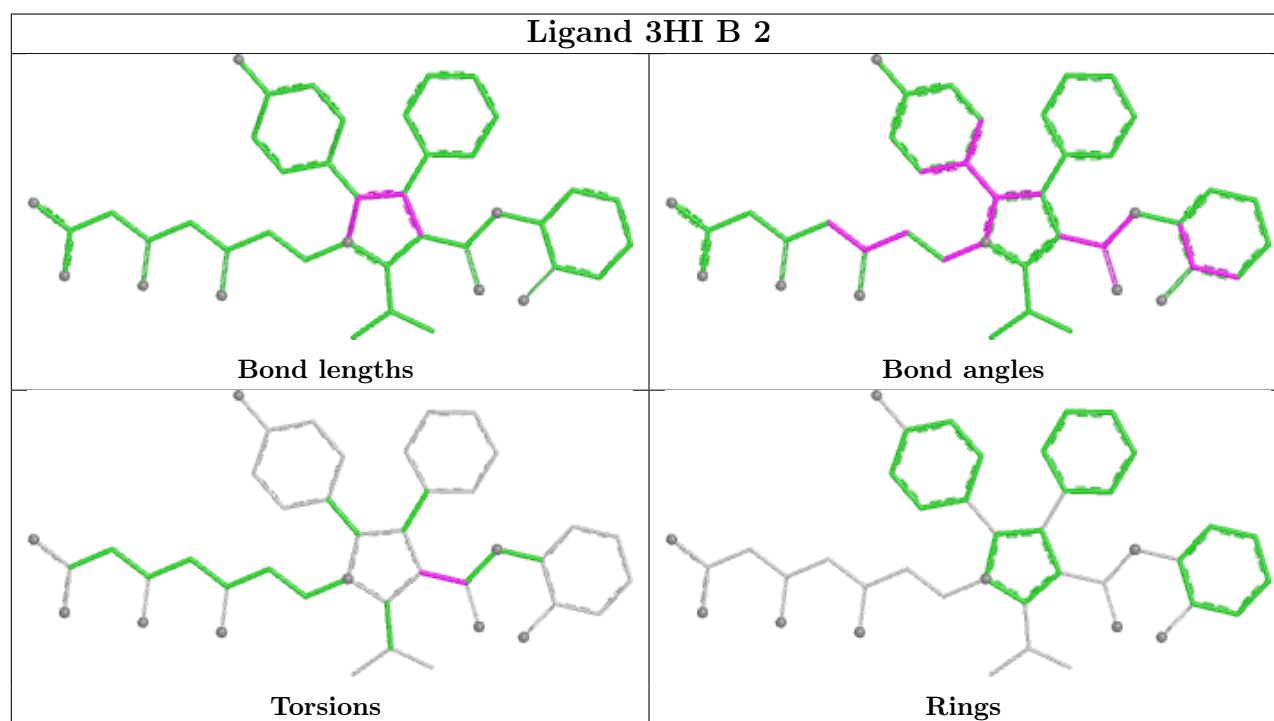
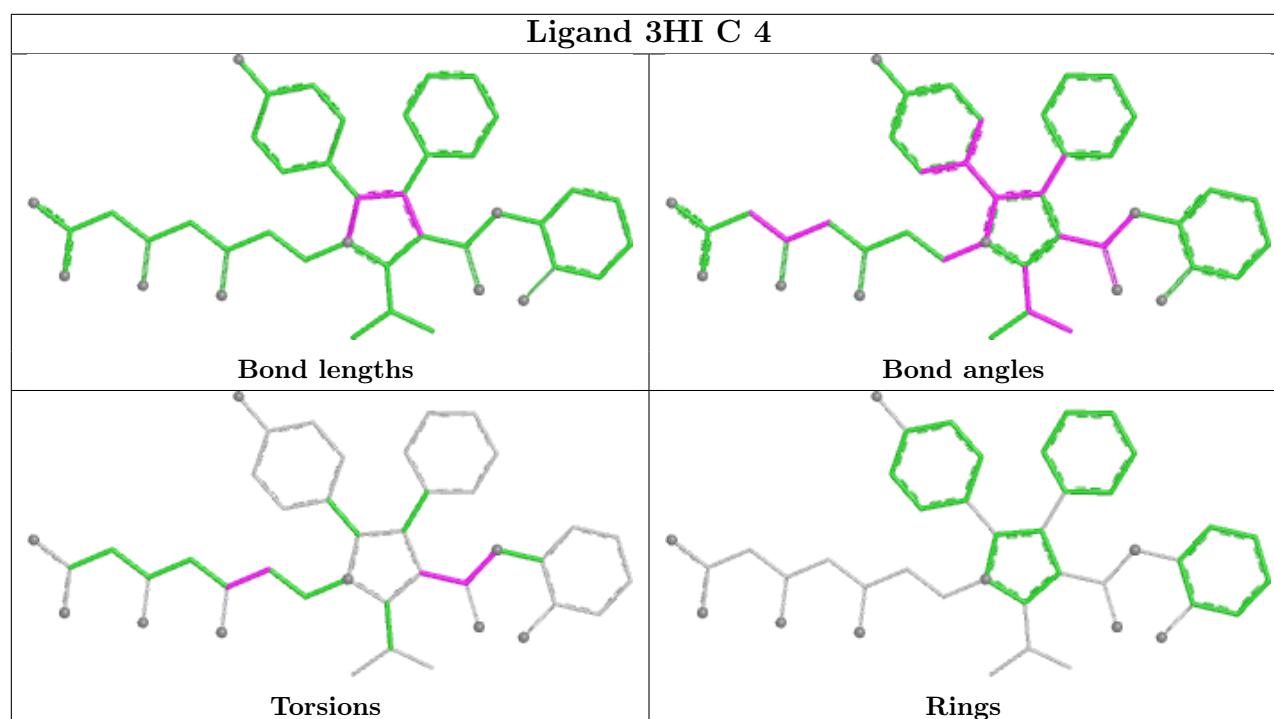
There are no ring outliers.

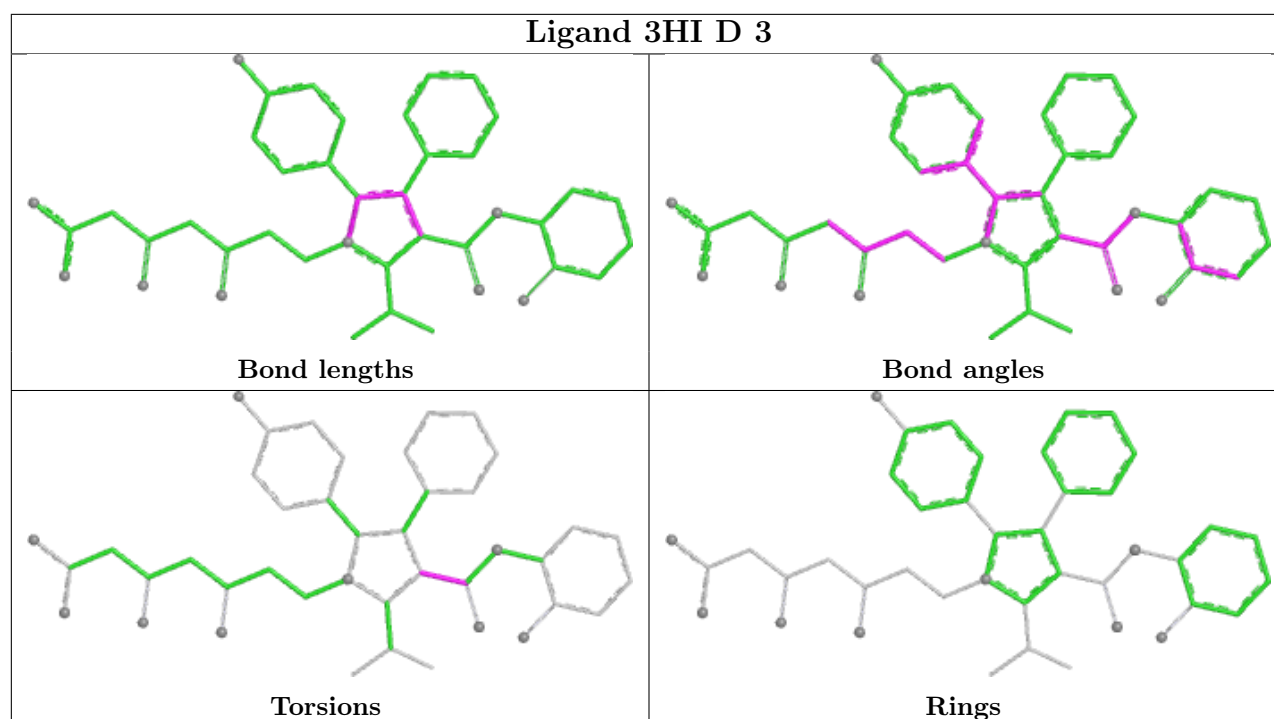
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	3HI	2	0
2	B	2	3HI	2	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%)	0.21	23 (5%) 30 33	20, 33, 74, 98	0
1	B	421/441 (95%)	0.16	12 (2%) 53 56	20, 33, 51, 84	0
1	C	417/441 (94%)	0.40	28 (6%) 24 26	20, 37, 83, 95	0
1	D	394/441 (89%)	0.16	12 (3%) 52 55	19, 32, 72, 99	0
All	All	1653/1764 (93%)	0.24	75 (4%) 38 41	19, 33, 72, 99	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	444	PRO	5.0
1	D	484	LEU	4.4
1	A	482	GLU	4.3
1	A	479	TYR	4.2
1	C	451	ILE	4.1
1	A	484	LEU	4.0
1	A	478	ALA	3.9
1	D	475	HIS	3.6
1	A	443	ARG	3.5
1	D	461	PHE	3.5
1	D	488	HIS	3.5
1	B	479	TYR	3.5
1	C	452	LEU	3.3
1	A	481	LEU	3.3
1	C	484	LEU	3.3
1	B	861	HIS	3.2
1	C	449	LEU	3.2
1	C	461	PHE	3.2
1	A	483	THR	3.2
1	A	448	CYS	3.2
1	A	442	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	479	TYR	3.0
1	D	859	ALA	2.9
1	A	463	SER	2.9
1	C	462	LEU	2.8
1	A	666	LYS	2.8
1	B	450	GLN	2.8
1	D	462	LEU	2.8
1	C	457	LYS	2.8
1	C	485	ILE	2.8
1	A	449	LEU	2.8
1	A	470	LEU	2.7
1	B	482	GLU	2.7
1	B	476	ILE	2.7
1	C	448	CYS	2.7
1	A	718	ARG	2.7
1	D	465	ALA	2.6
1	C	488	HIS	2.6
1	B	860	GLY	2.5
1	B	480	LYS	2.5
1	A	786	PRO	2.5
1	C	483	THR	2.5
1	A	480	LYS	2.5
1	C	445	ASN	2.5
1	B	477	PRO	2.4
1	A	708	CYS	2.4
1	C	627	ARG	2.4
1	D	470	LEU	2.4
1	C	467	ILE	2.3
1	A	446	GLU	2.3
1	B	487	THR	2.3
1	C	459	ALA	2.3
1	C	466	GLU	2.3
1	C	447	GLU	2.2
1	D	515	ARG	2.2
1	C	478	ALA	2.2
1	B	859	ALA	2.1
1	C	470	LEU	2.1
1	A	504	SER	2.1
1	C	659	MET	2.1
1	B	483	THR	2.1
1	A	451	ILE	2.1
1	C	458	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	630	ARG	2.1
1	A	789	GLU	2.1
1	C	456	GLU	2.1
1	C	633	LYS	2.1
1	D	473	ALA	2.1
1	C	476	ILE	2.1
1	A	455	ALA	2.1
1	C	455	ALA	2.1
1	C	612	SER	2.1
1	B	501	LYS	2.0
1	D	458	GLY	2.0
1	A	858	ALA	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](#)

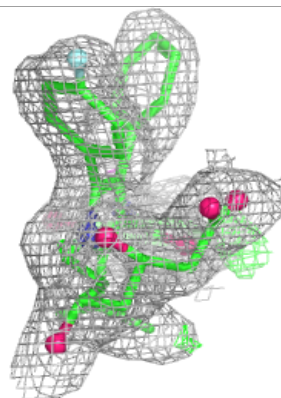
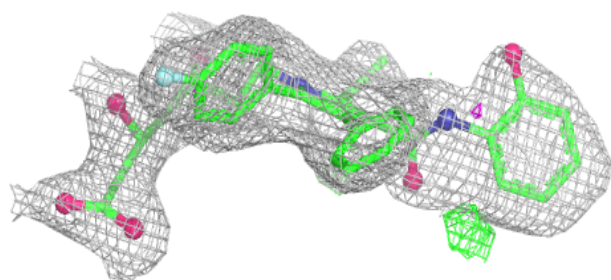
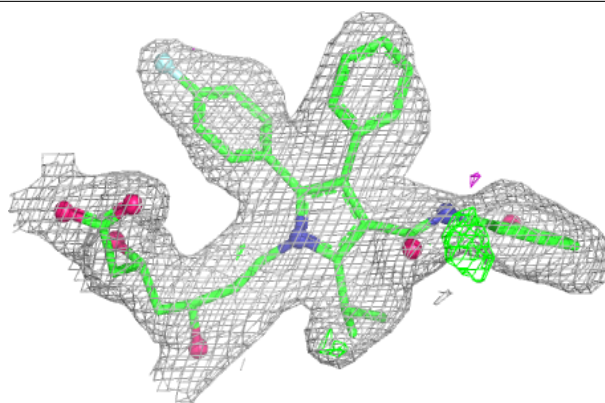
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3HI	C	4	42/42	0.89	0.11	23,40,42,44	0
2	3HI	B	1	42/42	0.90	0.11	22,39,52,53	0
2	3HI	B	2	42/42	0.93	0.09	23,33,53,54	0
2	3HI	D	3	42/42	0.93	0.09	21,34,41,43	0

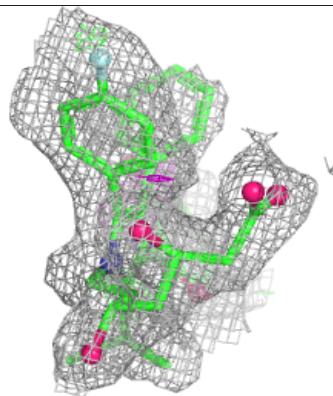
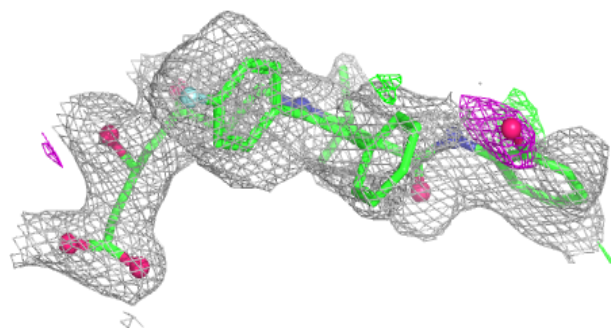
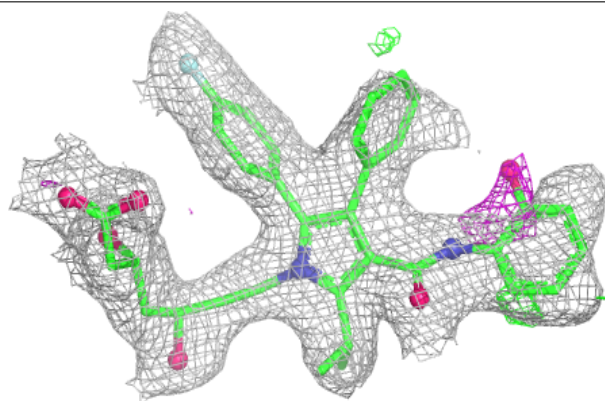
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3HI 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)

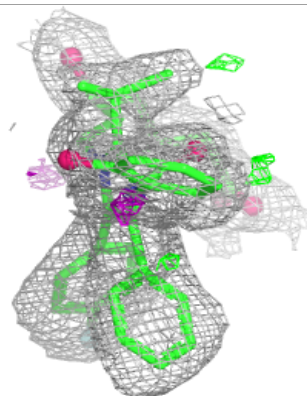
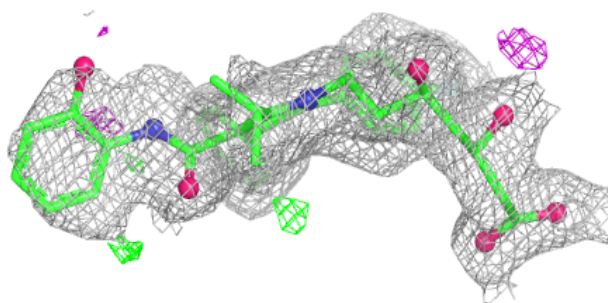
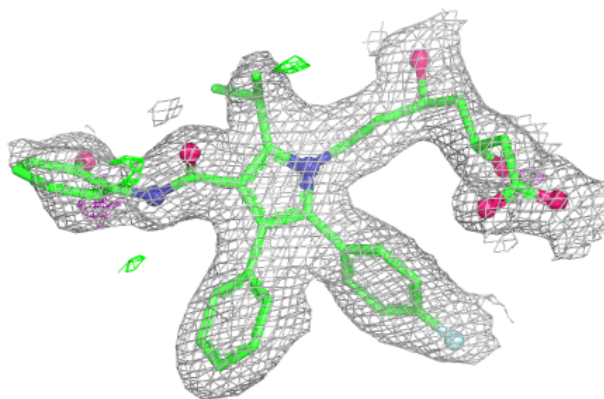
**Electron density around 3HI B 1:**

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

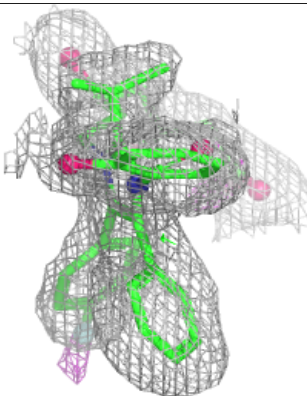
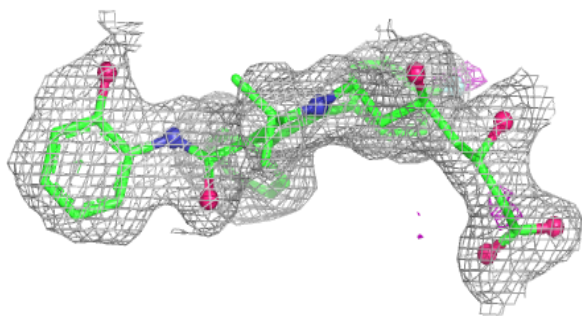
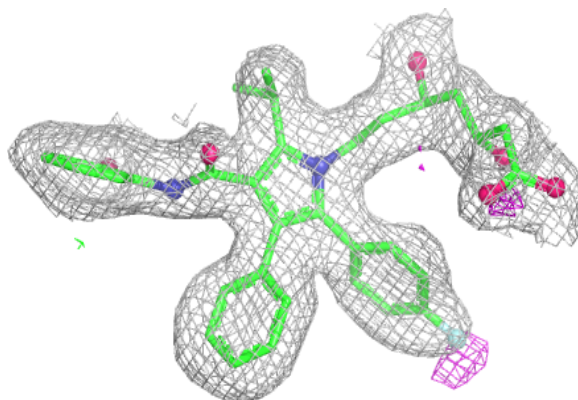


Electron density around 3HI B 2:

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

**Electron density around 3HI 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.