



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:59 PM UTC

PDB ID : 3CD0 / pdb_00003cd0
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 : 2.40 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

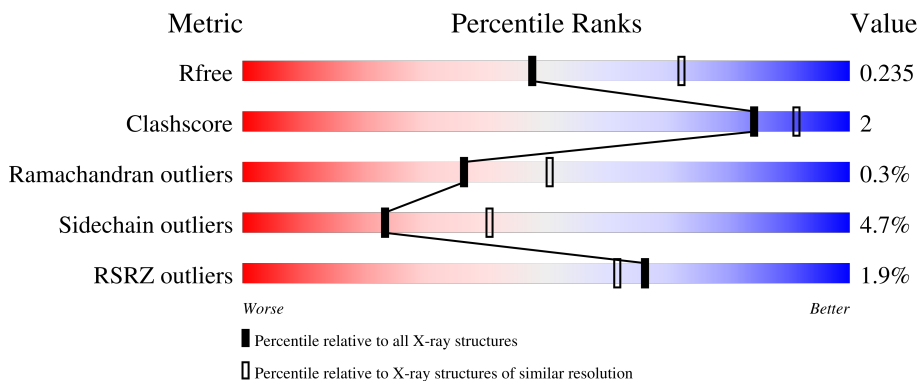
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 13075 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	3136	1952	552	602	30	0	1	0
1	C	414	3079	1918	541	590	30	0	1	0
1	D	396	2934	1826	518	561	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

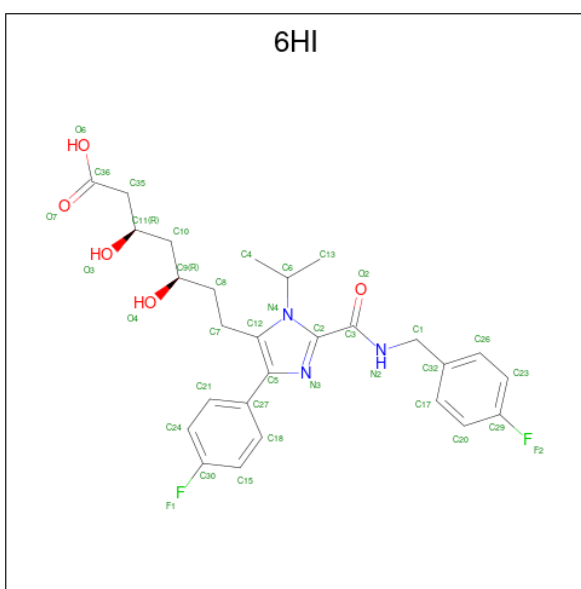
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered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

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

- Molecule 2 is (3R,5R)-7-{2-[(4-fluorobenzyl)carbamoyl]-4-(4-fluorophenyl)-1-(1-methylethyl)-1H-imidazol-5-yl}-3,5-dihydroxyheptanoic acid (CCD ID: 6HI) (formula: C₂₇H₃₁F₂N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	B	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	B	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	C	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	D	1	Total	C	F	N	O	0	0
			37	27	2	3	5		

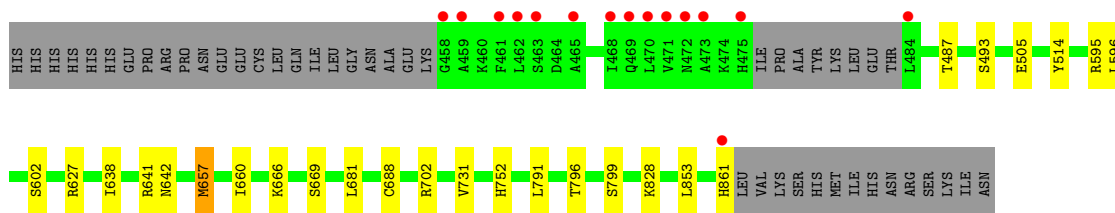
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	167	Total 167	O 167	0	0
3	C	118	Total 118	O 118	0	0
3	D	175	Total 175	O 175	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 173.96Å 76.40Å 90.00° 119.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.40) 97.7 (50.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.238 0.192 , 0.235	Depositor DCC
R_{free} test set	3290 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.7	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 0.021 for h,-k,-h-l 0.020 for l,-k,h 0.020 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13075	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 3.97% 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: 6HI

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	0.55	1/3179 (0.0%)	0.81	0/4298
1	B	0.55	1/3187 (0.0%)	0.80	0/4309
1	C	0.51	0/3127	0.79	0/4225
1	D	0.53	0/2975	0.79	0/4019
All	All	0.53	2/12468 (0.0%)	0.80	0/16851

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-7.80	1.60	1.79
1	A	657	MET	SD-CE	5.19	1.92	1.79

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	0	3167	19	0
1	B	3136	0	3169	18	0
1	C	3079	0	3119	13	0
1	D	2934	0	2967	10	0
2	B	74	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	37	0	30	1	0
2	D	37	0	30	2	0
3	A	185	0	0	0	0
3	B	167	0	0	1	0
3	C	118	0	0	2	0
3	D	175	0	0	1	0
All	All	13075	0	12542	58	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 (58) 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:657:MET:HE1	1:A:690:ASP:OD2	1.94	0.68
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.27	0.64
1:C:771:ASN:OD1	1:C:775:SER:OG	2.18	0.61
1:B:752:HIS:HE1	1:B:849:GLY:C	2.09	0.60
2:B:2:6HI:H4A	2:B:2:6HI:H7A	1.83	0.59
1:C:523:MET:HE1	1:C:530:VAL:HG21	1.83	0.58
2:C:4:6HI:H4A	2:C:4:6HI:H7A	1.84	0.57
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.87	0.56
1:A:655:MET:SD	1:A:657:MET:HG3	2.47	0.55
2:B:1:6HI:H7A	2:B:1:6HI:H4A	1.88	0.55
1:D:657:MET:HG3	3:D:929:HOH:O	2.05	0.55
2:D:3:6HI:H4A	2:D:3:6HI:H7A	1.89	0.54
1:A:470:LEU:O	1:A:474:LYS:O	2.25	0.53
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.89	0.53
1:B:796:THR:HG21	1:C:638:ILE:O	2.09	0.53
1:A:820:MET:HE1	1:B:531:ILE:HD11	1.92	0.51
1:B:655:MET:SD	1:B:657:MET:HG2	2.51	0.51
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.91	0.51
1:A:820:MET:HE2	1:B:509:LEU:CD2	2.43	0.49
1:B:731:VAL:HG12	1:B:854:MET:HE1	1.93	0.49
1:C:523:MET:HE2	3:C:919:HOH:O	2.13	0.48
1:A:474:LYS:O	1:A:475:HIS:HB2	2.13	0.48
1:A:472:ASN:O	1:A:473:ALA:CB	2.61	0.47
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.49	0.47
1:B:638:ILE:O	1:C:796:THR:HG21	2.14	0.47
1:A:477:PRO:O	1:A:478:ALA:HB2	2.14	0.47
1:A:472:ASN:O	1:A:473:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:HIS:CE1	3:B:884:HOH:O	2.67	0.47
1:B:752:HIS:O	1:B:752:HIS:CG	2.68	0.46
2:D:3:6HI:H8A	2:D:3:6HI:H13B	1.96	0.46
1:A:817:CYS:HA	1:A:820:MET:HE3	1.96	0.46
1:D:702:ARG:O	1:D:799:SER:HA	2.15	0.46
1:C:793:ILE:HD13	1:C:851:LEU:HG	1.98	0.46
1:A:474:LYS:O	1:A:475:HIS:CB	2.64	0.45
1:A:638:ILE:O	1:D:796:THR:HG21	2.17	0.45
1:A:774:SER:HA	1:A:799:SER:O	2.17	0.45
1:A:819:GLN:HB3	1:B:508:SER:HB3	1.98	0.45
1:B:752:HIS:HE1	1:B:849:GLY:O	2.01	0.44
1:B:541:ALA:HB2	1:B:555:MET:HE2	2.00	0.43
1:D:595:ARG:HE	1:D:642:ASN:ND2	2.16	0.43
1:D:595:ARG:HE	1:D:642:ASN:HD21	1.66	0.43
1:D:596:LEU:HD13	1:D:602:SER:HA	2.01	0.43
1:B:555:MET:HE1	1:B:563:VAL:HA	2.01	0.42
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.55	0.42
1:C:702:ARG:O	1:C:799:SER:HA	2.18	0.42
1:C:470:LEU:O	1:C:473:ALA:O	2.38	0.42
1:B:672:HIS:CE1	1:B:676:PRO:HA	2.55	0.42
1:C:781:MET:HE2	1:C:793:ILE:HD12	2.02	0.42
1:B:752:HIS:CE1	1:B:849:GLY:C	2.94	0.41
1:D:596:LEU:O	1:D:641:ARG:HB2	2.19	0.41
1:A:592:PRO:HD2	1:A:645:ILE:O	2.20	0.41
1:A:771:ASN:OD1	1:A:775:SER:OG	2.39	0.41
1:D:752:HIS:CD2	1:D:853:LEU:HD23	2.56	0.41
1:B:702:ARG:O	1:B:799:SER:HA	2.20	0.41
1:B:555:MET:HE3	1:B:563:VAL:HG22	2.02	0.41
1:C:661:SER:HB3	3:C:988:HOH:O	2.19	0.41
1:A:482:GLU:OE2	1:A:495:ARG:NH2	2.55	0.40
1:B:765:GLY:CA	1:B:814:GLN:HG2	2.52	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%)	17 (4%)	4 (1%)	12	20
1	B	420/441 (95%)	405 (96%)	15 (4%)	0	100	100
1	C	411/441 (93%)	398 (97%)	13 (3%)	0	100	100
1	D	392/441 (89%)	375 (96%)	16 (4%)	1 (0%)	36	50
All	All	1642/1764 (93%)	1576 (96%)	61 (4%)	5 (0%)	36	50

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/355 (94%)	318 (95%)	17 (5%)	21	37
1	B	336/355 (95%)	319 (95%)	17 (5%)	21	37
1	C	330/355 (93%)	314 (95%)	16 (5%)	23	40
1	D	313/355 (88%)	300 (96%)	13 (4%)	26	45
All	All	1314/1420 (92%)	1251 (95%)	63 (5%)	23	40

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	470	LEU

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Mol	Chain	Res	Type
1	A	482	GLU
1	A	486	GLU
1	A	498	LEU
1	A	509	LEU
1	A	512	LEU
1	A	627	ARG
1	A	630	ARG
1	A	634	LEU
1	A	638	ILE
1	A	657	MET
1	A	661	SER
1	A	688	CYS
1	A	704	LYS
1	A	814	GLN
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	482	GLU
1	B	484	LEU
1	B	486	GLU
1	B	505	GLU
1	B	523	MET
1	B	613	GLU
1	B	634	LEU
1	B	661	SER
1	B	669	SER
1	B	728	MET
1	B	771[A]	ASN
1	B	771[B]	ASN
1	B	802	ILE
1	B	828	LYS
1	C	446	GLU
1	C	450	GLN
1	C	470	LEU
1	C	523	MET
1	C	580	SER
1	C	598	ARG
1	C	638	ILE
1	C	649	SER
1	C	657	MET
1	C	659	MET
1	C	660	ILE

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Mol	Chain	Res	Type
1	C	662	LYS
1	C	666	LYS
1	C	681	LEU
1	C	688	CYS
1	C	715	LYS
1	D	487	THR
1	D	493	SER
1	D	505	GLU
1	D	627	ARG
1	D	638	ILE
1	D	657	MET
1	D	660	ILE
1	D	666	LYS
1	D	669	SER
1	D	688	CYS
1	D	791	LEU
1	D	828	LYS
1	D	861	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	A	679	GLN
1	A	819	GLN
1	B	450	GLN
1	B	472	ASN
1	B	529	ASN
1	B	648	GLN
1	B	752	HIS
1	B	770	GLN
1	B	788	ASN
1	B	819	GLN
1	C	445	ASN
1	C	469	GLN
1	C	472	ASN
1	C	497	GLN
1	C	632	GLN
1	C	658	ASN

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Mol	Chain	Res	Type
1	C	736	ASN
1	C	819	GLN
1	D	472	ASN
1	D	518	ASN
1	D	642	ASN
1	D	672	HIS
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	6HI	D	3	-	39,39,39	1.61	2 (5%)	46,54,54	1.71	5 (10%)
2	6HI	C	4	-	39,39,39	1.66	3 (7%)	46,54,54	1.73	6 (13%)
2	6HI	B	1	-	39,39,39	1.73	3 (7%)	46,54,54	1.73	9 (19%)
2	6HI	B	2	-	39,39,39	1.76	2 (5%)	46,54,54	1.59	6 (13%)

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	6HI	D	3	-	-	9/30/30/30	0/3/3/3
2	6HI	C	4	-	-	7/30/30/30	0/3/3/3
2	6HI	B	1	-	-	8/30/30/30	0/3/3/3
2	6HI	B	2	-	-	4/30/30/30	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	6HI	C5-C12	9.44	1.49	1.38
2	B	1	6HI	C5-C12	9.01	1.49	1.38
2	C	4	6HI	C5-C12	8.64	1.48	1.38
2	D	3	6HI	C5-C12	8.24	1.48	1.38
2	D	3	6HI	C5-N3	-3.61	1.32	1.38
2	B	2	6HI	C5-N3	-3.39	1.33	1.38
2	B	1	6HI	C5-N3	-3.37	1.33	1.38
2	C	4	6HI	C5-N3	-3.12	1.33	1.38
2	B	1	6HI	C7-C12	2.19	1.53	1.50
2	C	4	6HI	C7-C12	2.10	1.52	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	6HI	C27-C5-N3	6.78	129.55	119.53
2	C	4	6HI	C27-C5-N3	6.60	129.29	119.53
2	B	1	6HI	C27-C5-N3	5.75	128.03	119.53
2	B	2	6HI	C27-C5-N3	5.34	127.42	119.53
2	D	3	6HI	C27-C5-C12	-4.32	121.06	129.56
2	C	4	6HI	C27-C5-C12	-4.05	121.59	129.56
2	B	1	6HI	C27-C5-C12	-3.42	122.82	129.56
2	D	3	6HI	O2-C3-C2	-3.31	116.58	121.74
2	B	2	6HI	C27-C5-C12	-3.21	123.23	129.56
2	C	4	6HI	O2-C3-C2	-2.78	117.41	121.74
2	C	4	6HI	C8-C7-C12	-2.74	107.76	113.36
2	B	2	6HI	C8-C7-C12	-2.66	107.92	113.36
2	B	1	6HI	C7-C8-C9	2.62	118.53	113.58
2	D	3	6HI	C8-C7-C12	-2.54	108.17	113.36
2	B	1	6HI	C8-C7-C12	-2.38	108.50	113.36
2	B	2	6HI	O2-C3-C2	-2.35	118.08	121.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	6HI	C23-C29-C20	-2.34	119.73	122.80
2	B	1	6HI	C24-C30-C15	-2.33	119.74	122.80
2	B	1	6HI	O6-C36-C35	2.28	121.09	114.00
2	B	1	6HI	C3-C2-N3	-2.28	120.98	124.20
2	B	2	6HI	C5-C12-N4	-2.21	103.03	105.17
2	B	1	6HI	C5-C12-N4	-2.15	103.09	105.17
2	C	4	6HI	O6-C36-C35	2.13	120.61	114.00
2	D	3	6HI	C10-C11-C35	-2.05	108.77	112.96
2	C	4	6HI	C10-C11-C35	-2.02	108.83	112.96
2	B	2	6HI	O6-C36-C35	2.01	120.24	114.00

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	6HI	N3-C2-C3-O2
2	B	2	6HI	N3-C2-C3-O2
2	C	4	6HI	N3-C2-C3-O2
2	D	3	6HI	N3-C2-C3-O2
2	C	4	6HI	C18-C27-C5-N3
2	C	4	6HI	C21-C27-C5-N3
2	D	3	6HI	C21-C27-C5-N3
2	D	3	6HI	C18-C27-C5-N3
2	C	4	6HI	C21-C27-C5-C12
2	C	4	6HI	C18-C27-C5-C12
2	D	3	6HI	C21-C27-C5-C12
2	D	3	6HI	C18-C27-C5-C12
2	D	3	6HI	C2-C3-N2-C1
2	D	3	6HI	N4-C2-C3-O2
2	B	1	6HI	C12-C7-C8-C9
2	B	1	6HI	C7-C8-C9-O4
2	C	4	6HI	C11-C35-C36-O7
2	D	3	6HI	C11-C35-C36-O7
2	C	4	6HI	C11-C35-C36-O6
2	B	1	6HI	C18-C27-C5-C12
2	B	1	6HI	C11-C35-C36-O6
2	D	3	6HI	C11-C35-C36-O6
2	B	2	6HI	C18-C27-C5-C12
2	B	2	6HI	N4-C2-C3-O2
2	B	2	6HI	C18-C27-C5-N3
2	B	1	6HI	C21-C27-C5-C12
2	B	1	6HI	C11-C35-C36-O7

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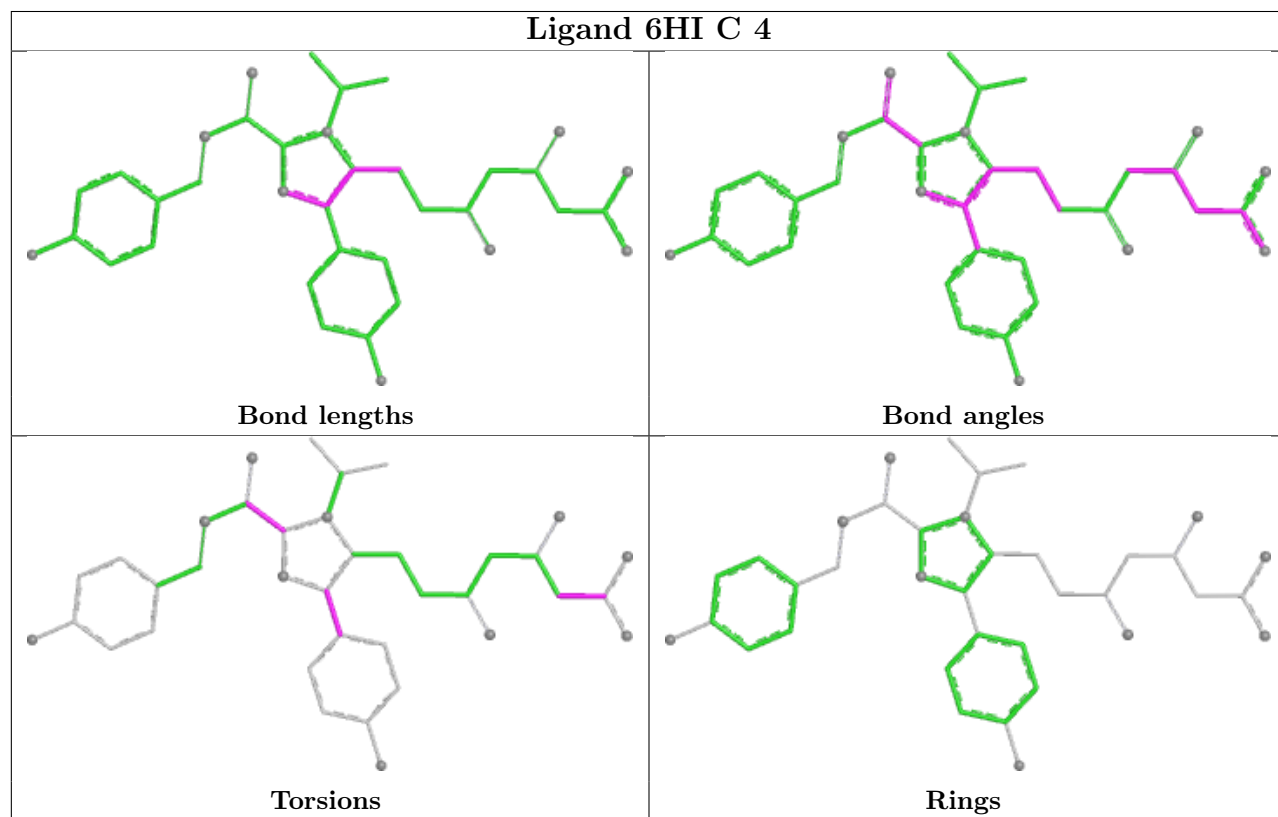
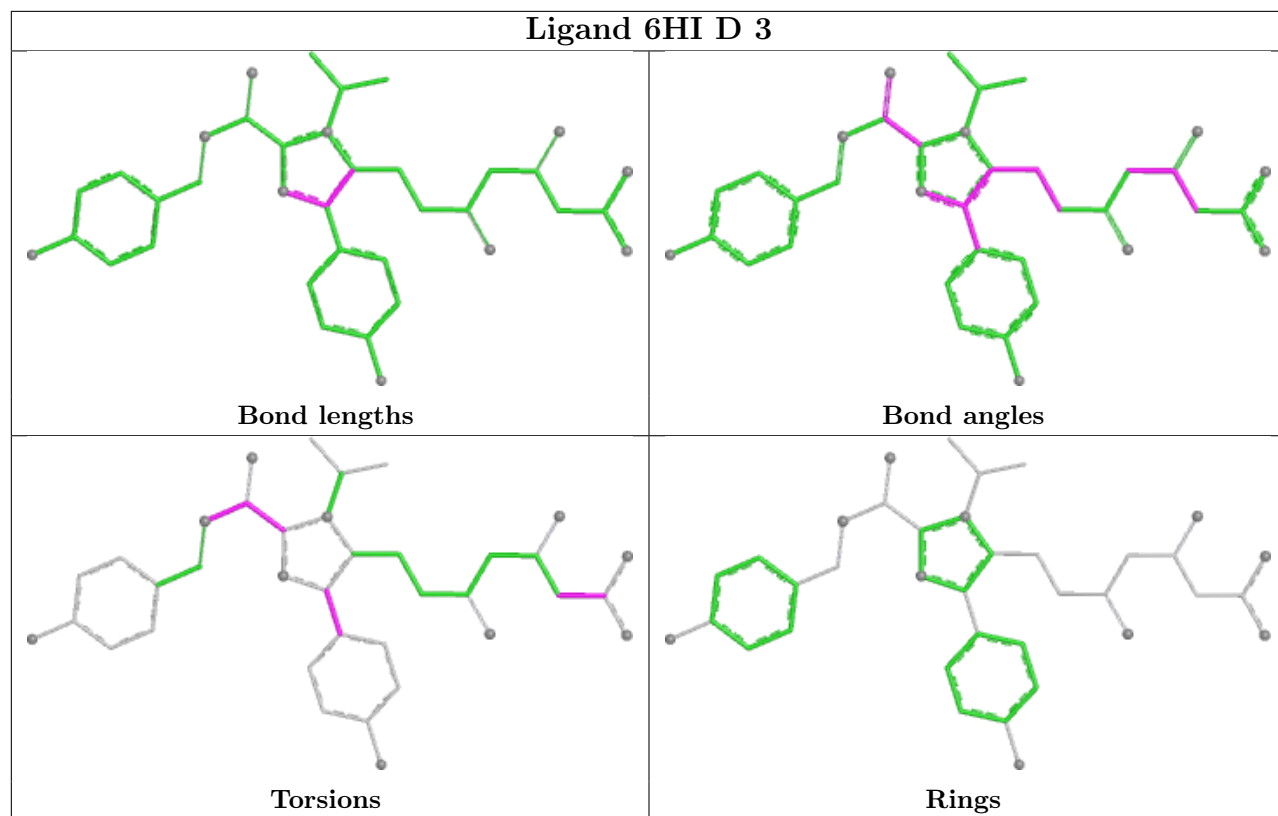
Mol	Chain	Res	Type	Atoms
2	B	1	6HI	C18-C27-C5-N3

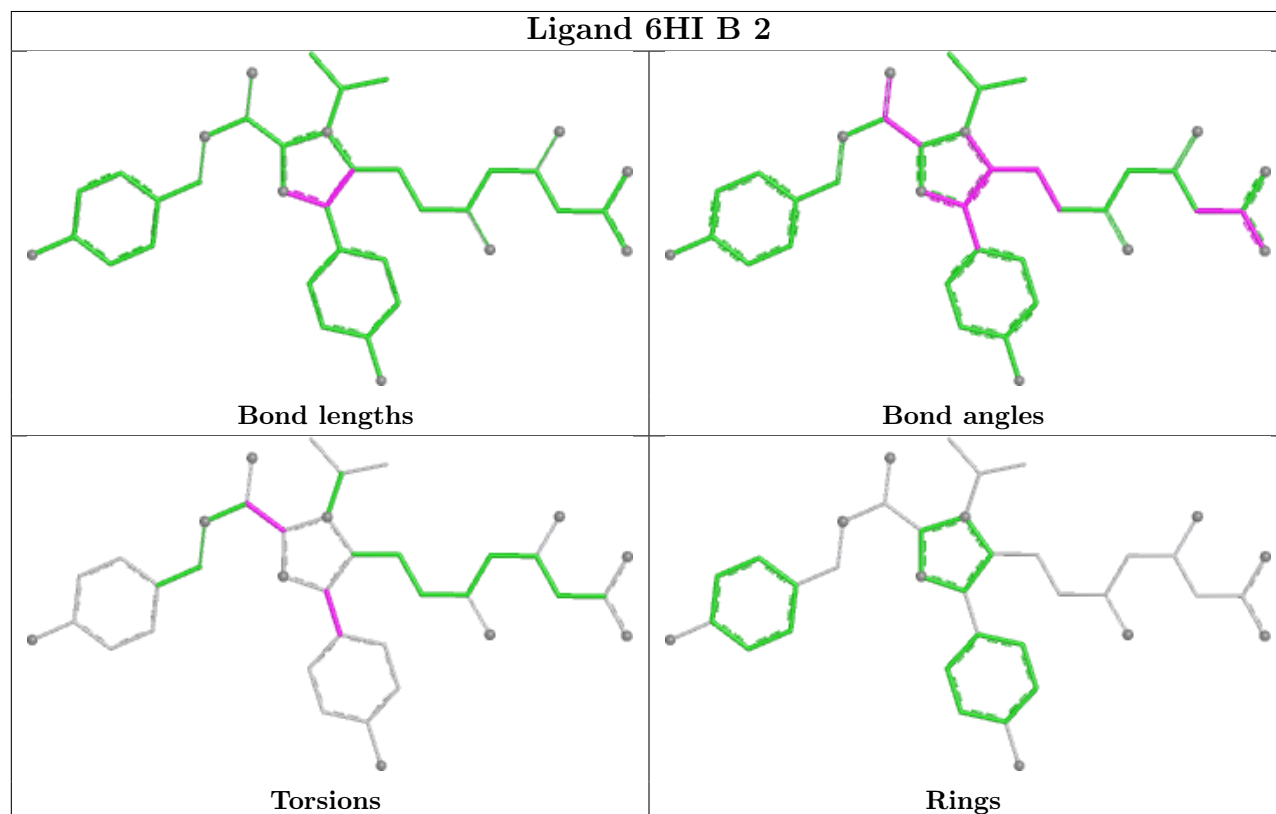
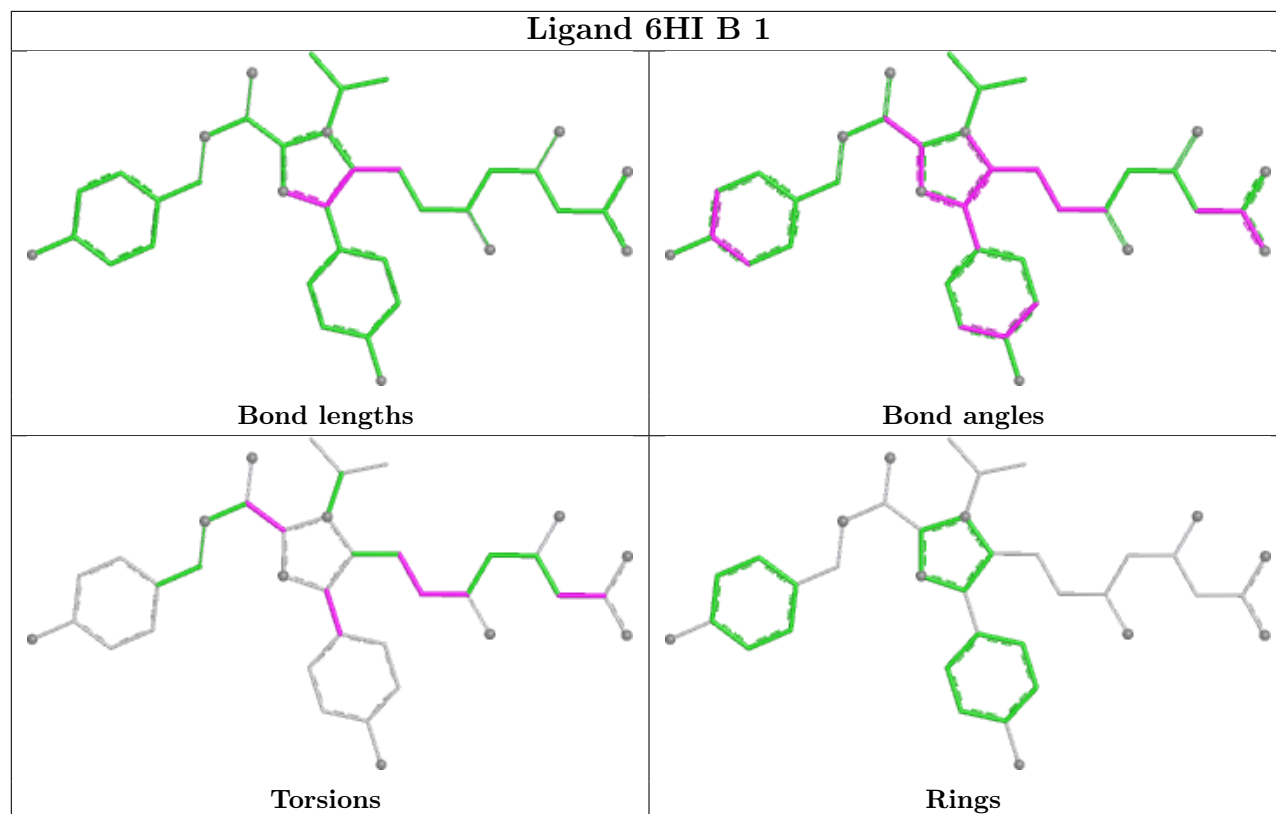
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	6HI	2	0
2	C	4	6HI	1	0
2	B	1	6HI	1	0
2	B	2	6HI	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%)	-0.17	4 (0%) 79 76	22, 33, 63, 71	0
1	B	421/441 (95%)	-0.20	2 (0%) 87 85	21, 34, 46, 59	1 (0%)
1	C	414/441 (93%)	0.03	11 (2%) 56 52	21, 38, 71, 94	2 (0%)
1	D	396/441 (89%)	-0.08	15 (3%) 44 40	21, 34, 70, 99	0
All	All	1652/1764 (93%)	-0.10	32 (1%) 66 62	21, 34, 62, 99	3 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	444	PRO	4.6
1	D	861	HIS	4.3
1	D	458	GLY	4.0
1	D	465	ALA	3.5
1	D	470	LEU	3.4
1	D	461	PHE	3.3
1	C	461	PHE	3.3
1	D	484	LEU	3.3
1	A	861	HIS	3.1
1	B	861	HIS	3.1
1	C	451	ILE	3.0
1	A	483	THR	3.0
1	D	475	HIS	3.0
1	D	462	LEU	2.9
1	B	450	GLN	2.8
1	C	454	ASN	2.7
1	C	448	CYS	2.6
1	C	452	LEU	2.5
1	A	479	TYR	2.4
1	C	449	LEU	2.4
1	C	458	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	459	ALA	2.3
1	D	463	SER	2.3
1	D	469	GLN	2.3
1	D	471	VAL	2.3
1	D	473	ALA	2.3
1	C	453	GLY	2.2
1	A	482	GLU	2.2
1	D	468	ILE	2.2
1	D	472	ASN	2.2
1	C	771	ASN	2.1
1	C	483	THR	2.1

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](#)

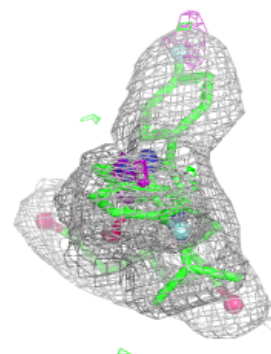
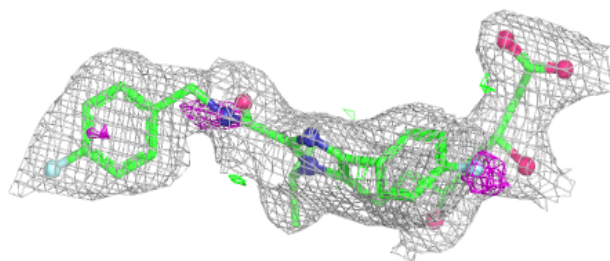
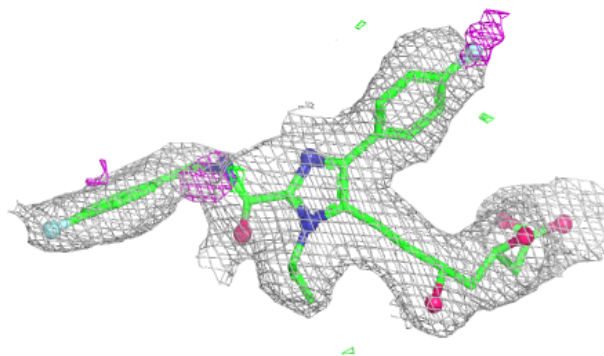
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	6HI	C	4	37/37	0.88	0.10	24,38,42,45	0
2	6HI	B	1	37/37	0.92	0.08	26,33,39,41	0
2	6HI	D	3	37/37	0.92	0.09	23,35,38,39	0
2	6HI	B	2	37/37	0.94	0.07	23,30,36,39	0

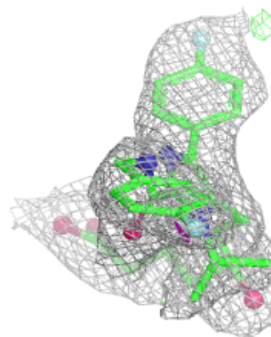
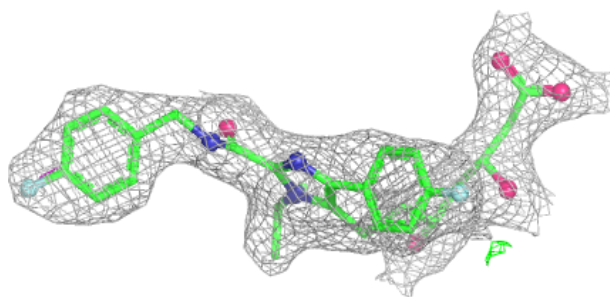
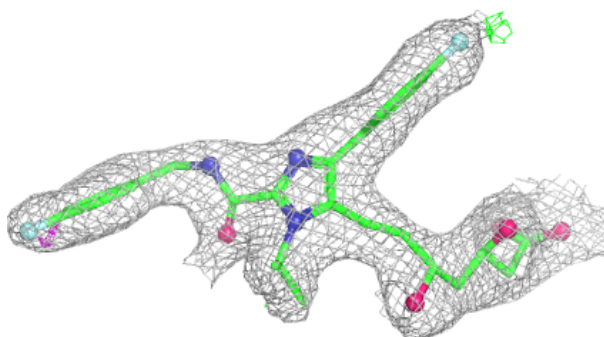
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6HI 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)

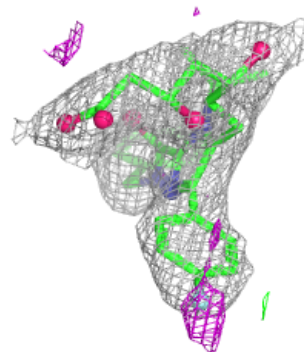
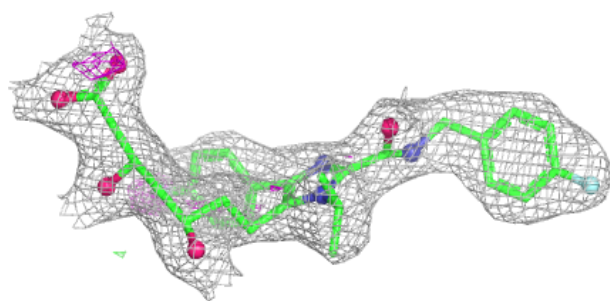
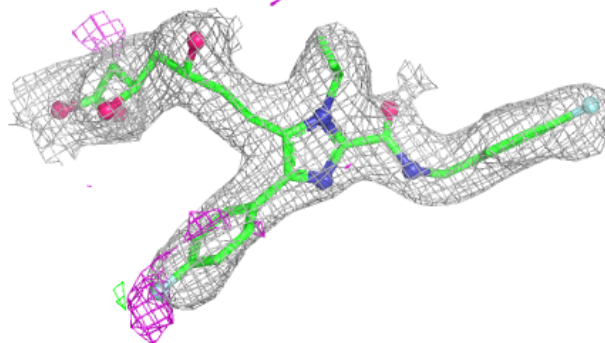
**Electron density around 6HI B 1:**

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

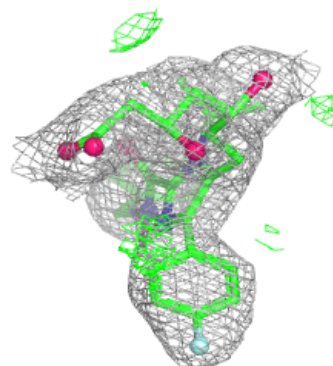
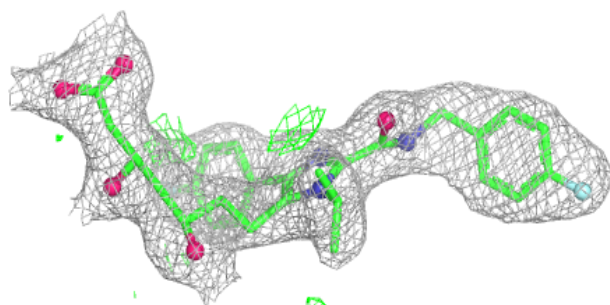
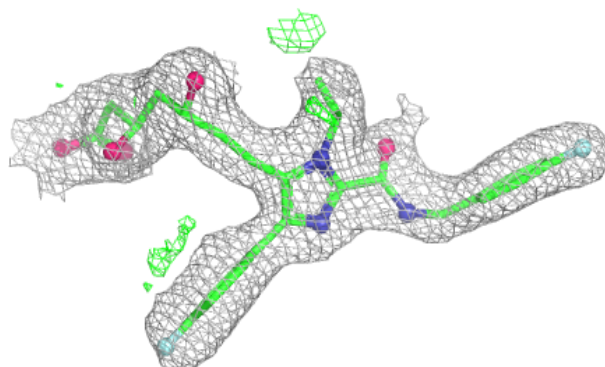


Electron density around 6HI D 3:

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

**Electron density around 6HI 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.