



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:54 PM UTC

PDB ID : 3CCW / pdb_00003ccw
Title : Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors
Authors : Pavlovsky, A.; Sarver, R.W.; Harris, M.S.; Finzel, B.C.
Deposited on : 2008-02-26
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

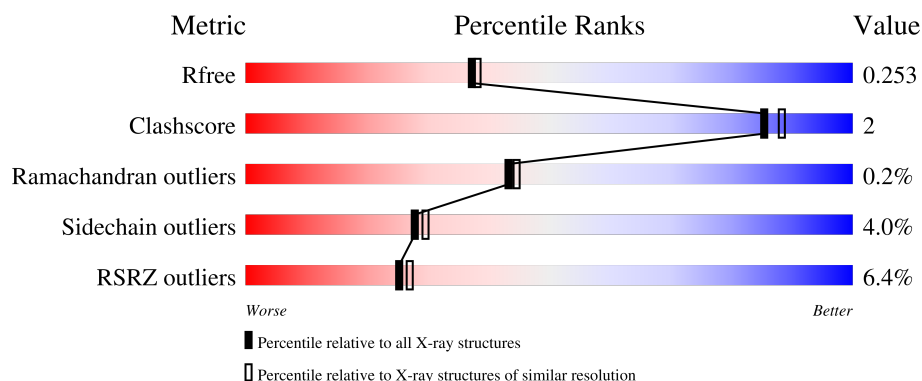
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	441	6% 87% 7% 5%
1	B	441	4% 87% 7% 5%
1	C	441	9% 88% 5% 6%
1	D	441	5% 83% 5% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12823 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	414	Total	C	N	O	S	0	0	0
			3073	1915	538	590	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:

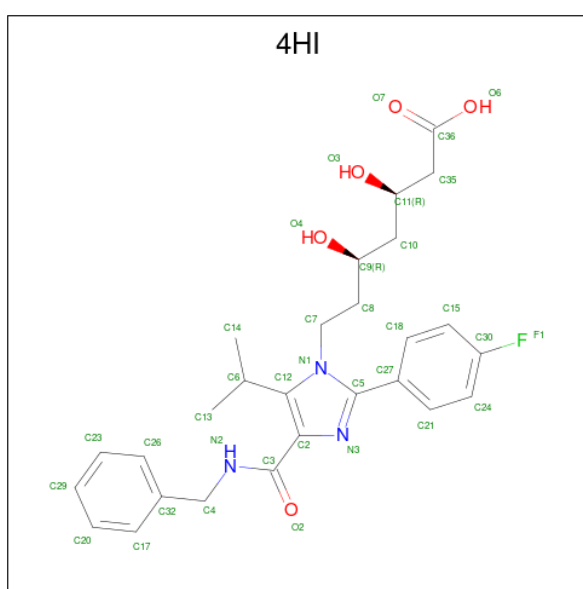
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered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



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

- Molecule 3 is water.

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

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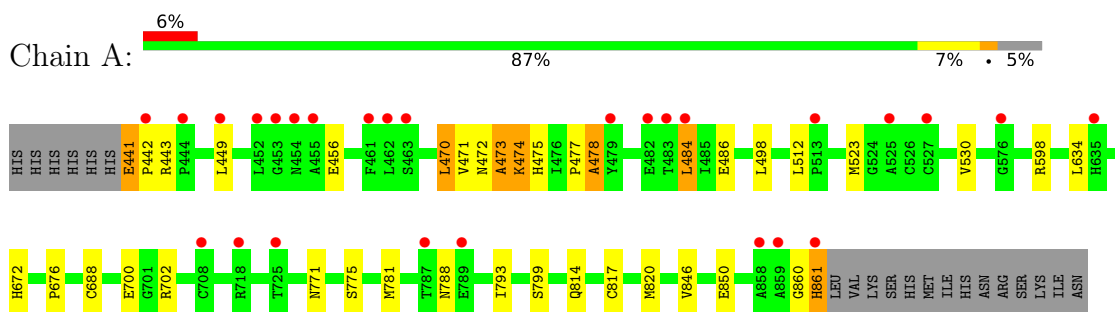
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	89	Total 89	O 89	0	0
3	D	109	Total 109	O 109	0	0

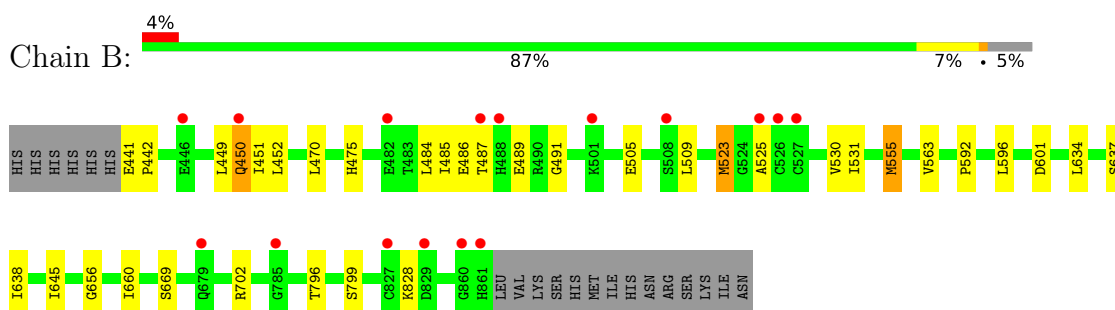
3 Residue-property plots [i](#)

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.

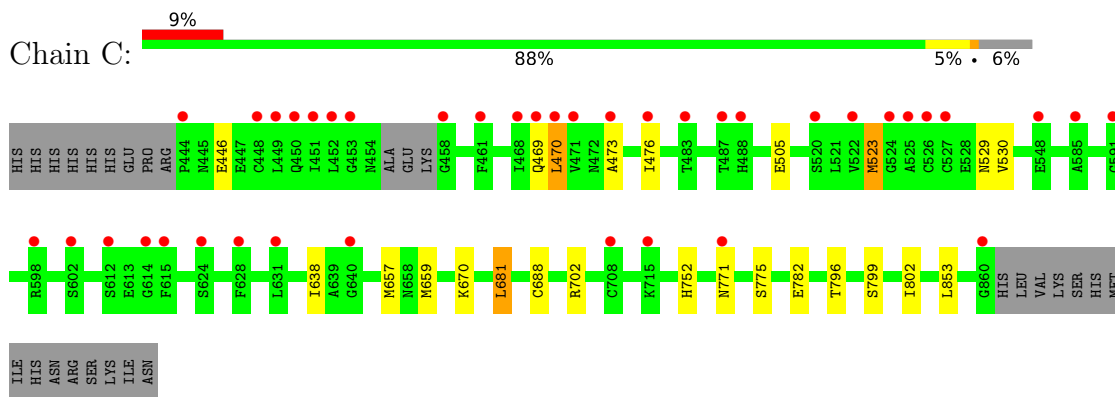
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



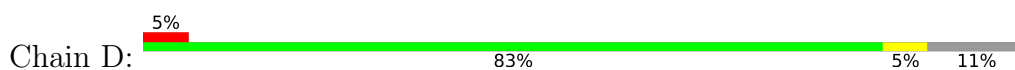
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

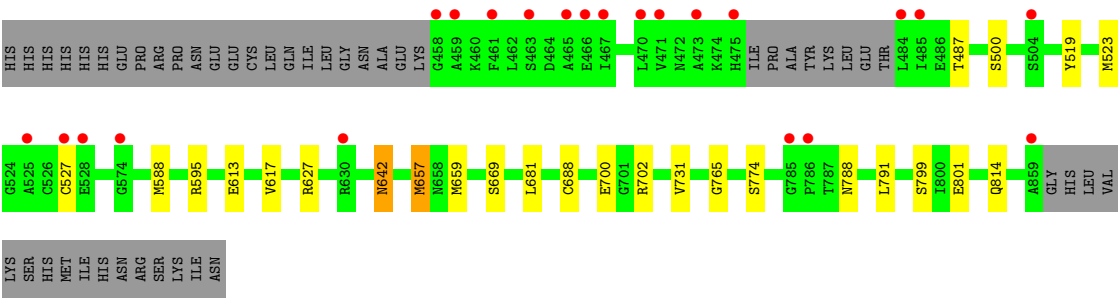


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- 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	73.93Å 174.38Å 76.08Å 90.00° 118.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (50.00-2.10) 88.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.252 0.220 , 0.253	Depositor DCC
R_{free} test set	2647 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.027 for h,-k,-h-l 0.027 for -h-l,-k,l 0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4HI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/3179	0.81	0/4298
1	B	0.55	1/3179 (0.0%)	0.80	0/4298
1	C	0.51	0/3116	0.78	1/4211 (0.0%)
1	D	0.52	0/2960	0.79	0/3999
All	All	0.53	1/12434 (0.0%)	0.79	1/16806 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	MET	SD-CE	-9.14	1.56	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	802	ILE	N-CA-C	5.11	115.01	107.75

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	21	0
1	B	3133	0	3167	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3073	0	3110	9	0
1	D	2920	0	2957	11	0
2	B	72	0	62	3	0
2	C	36	0	31	0	0
2	D	36	0	31	0	0
3	A	109	0	0	0	0
3	B	113	0	0	0	0
3	C	89	0	0	1	0
3	D	109	0	0	2	0
All	All	12823	0	12525	55	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 (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:O	1:A:474:LYS:O	2.07	0.72
1:C:771:ASN:OD1	1:C:775:SER:OG	2.11	0.67
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.83	0.60
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.86	0.57
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.86	0.57
1:B:555:MET:HE1	1:B:563:VAL:HA	1.87	0.57
1:A:860:GLY:O	1:A:861:HIS:HB2	2.05	0.57
1:D:642:ASN:HD22	1:D:642:ASN:N	2.01	0.57
1:B:523:MET:HE1	1:B:530:VAL:HB	1.88	0.56
2:B:2:4HI:H7	2:B:2:4HI:H13B	1.87	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.08	0.54
1:B:555:MET:CE	1:B:563:VAL:HA	2.38	0.54
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.90	0.53
1:A:820:MET:HE2	1:B:509:LEU:CD2	2.38	0.53
1:D:657:MET:HG3	3:D:197:HOH:O	2.08	0.53
1:A:771:ASN:OD1	1:A:775:SER:OG	2.27	0.53
1:A:472:ASN:O	1:A:473:ALA:CB	2.57	0.52
2:B:2:4HI:H8A	2:B:2:4HI:H14B	1.92	0.52
1:A:441:GLU:N	1:A:442:PRO:CD	2.72	0.52
1:A:474:LYS:O	1:A:475:HIS:HB2	2.09	0.52
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.41	0.50
1:B:449:LEU:HD11	1:B:475:HIS:ND1	2.26	0.50
1:A:477:PRO:O	1:A:478:ALA:CB	2.59	0.49
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.95	0.48
1:B:450:GLN:HG3	1:B:451:ILE:N	2.29	0.48
1:A:702:ARG:O	1:A:799:SER:HA	2.14	0.48
1:C:529:ASN:ND2	3:C:252:HOH:O	2.48	0.46
1:C:470:LEU:O	1:C:473:ALA:O	2.34	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.16	0.46
1:B:555:MET:CE	1:B:563:VAL:HG22	2.46	0.46
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.98	0.46
1:B:638:ILE:O	1:C:796:THR:HG21	2.16	0.45
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.45
2:B:1:4HI:H7	2:B:1:4HI:H13B	1.98	0.45
1:A:781:MET:HE2	1:A:793:ILE:HD12	1.98	0.45
1:A:820:MET:HE1	1:B:531:ILE:HD11	1.97	0.45
1:B:592:PRO:HD2	1:B:645:ILE:O	2.17	0.45
1:D:519:TYR:O	1:D:523:MET:HG2	2.17	0.45
1:A:846:VAL:O	1:A:850:GLU:HG2	2.17	0.45
1:A:471:VAL:HG11	1:A:498:LEU:CD2	2.45	0.44
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.52	0.44
1:D:700:GLU:OE1	3:D:369:HOH:O	2.21	0.44
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:A:820:MET:HE2	1:B:509:LEU:HD21	2.00	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.43
1:A:449:LEU:HD11	1:A:475:HIS:ND1	2.34	0.43
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.53	0.43
1:B:656:GLY:O	1:B:660:ILE:HG12	2.19	0.42
1:A:817:CYS:HA	1:A:820:MET:HE3	2.00	0.42
1:D:588:MET:HE1	1:D:801:GLU:HG2	2.02	0.42
1:D:702:ARG:O	1:D:799:SER:HA	2.20	0.42
1:B:596:LEU:HB3	1:B:601:ASP:HB2	2.02	0.41
1:D:765:GLY:HA2	1:D:814:GLN:HG2	2.03	0.41
1:B:441:GLU:N	1:B:442:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/441 (95%)	398 (95%)	18 (4%)	3 (1%)	18	15
1	B	419/441 (95%)	406 (97%)	12 (3%)	1 (0%)	43	44
1	C	410/441 (93%)	397 (97%)	13 (3%)	0	100	100
1	D	390/441 (88%)	377 (97%)	13 (3%)	0	100	100
All	All	1638/1764 (93%)	1578 (96%)	56 (3%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	28
1	B	335/355 (94%)	322 (96%)	13 (4%)	28	31
1	C	329/355 (93%)	317 (96%)	12 (4%)	31	34
1	D	312/355 (88%)	299 (96%)	13 (4%)	26	28
All	All	1311/1420 (92%)	1259 (96%)	52 (4%)	28	29

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	456	GLU
1	A	470	LEU

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Mol	Chain	Res	Type
1	A	474	LYS
1	A	484	LEU
1	A	486	GLU
1	A	512	LEU
1	A	598	ARG
1	A	634	LEU
1	A	688	CYS
1	A	788	ASN
1	A	814	GLN
1	A	861	HIS
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	489	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	637	SER
1	B	669	SER
1	B	828	LYS
1	C	446	GLU
1	C	469	GLN
1	C	470	LEU
1	C	476	ILE
1	C	505	GLU
1	C	523	MET
1	C	657	MET
1	C	659	MET
1	C	670	LYS
1	C	681	LEU
1	C	688	CYS
1	C	782	GLU
1	D	487	THR
1	D	500	SER
1	D	527	CYS
1	D	613	GLU
1	D	617	VAL
1	D	627	ARG
1	D	642	ASN

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Mol	Chain	Res	Type
1	D	657	MET
1	D	659	MET
1	D	669	SER
1	D	688	CYS
1	D	788	ASN
1	D	791	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	567	ASN
1	A	635	HIS
1	A	672	HIS
1	A	788	ASN
1	B	472	ASN
1	B	529	ASN
1	B	632	GLN
1	B	819	GLN
1	C	469	GLN
1	C	472	ASN
1	C	770	GLN
1	D	472	ASN
1	D	518	ASN
1	D	552	GLN
1	D	632	GLN
1	D	642	ASN
1	D	736	ASN
1	D	788	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	4HI	B	1	-	37,38,38	0.80	1 (2%)	50,52,52	1.58	10 (20%)
2	4HI	B	2	-	37,38,38	0.77	1 (2%)	50,52,52	1.72	8 (16%)
2	4HI	C	4	-	37,38,38	0.78	1 (2%)	50,52,52	1.66	9 (18%)
2	4HI	D	3	-	37,38,38	0.78	1 (2%)	50,52,52	1.64	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4HI	B	1	-	-	6/30/30/30	0/3/3/3
2	4HI	B	2	-	-	2/30/30/30	0/3/3/3
2	4HI	C	4	-	-	7/30/30/30	0/3/3/3
2	4HI	D	3	-	-	7/30/30/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	4HI	C2-N3	-2.45	1.33	1.38
2	B	1	4HI	C2-N3	-2.36	1.33	1.38
2	D	3	4HI	C2-N3	-2.09	1.34	1.38
2	B	2	4HI	C2-N3	-2.06	1.34	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	4HI	C3-C2-C12	-5.38	122.62	128.20
2	C	4	4HI	C3-C2-C12	-4.50	123.53	128.20
2	D	3	4HI	C3-C2-C12	-4.27	123.77	128.20
2	D	3	4HI	C4-N2-C3	4.11	127.94	122.07
2	D	3	4HI	C8-C7-N1	-3.93	105.29	112.16
2	B	1	4HI	C3-C2-C12	-3.92	124.14	128.20
2	B	2	4HI	C3-C2-N3	3.91	128.16	121.06
2	B	2	4HI	C4-N2-C3	3.80	127.49	122.07
2	C	4	4HI	C4-N2-C3	3.47	127.02	122.07
2	C	4	4HI	C3-C2-N3	3.46	127.34	121.06
2	B	1	4HI	C4-N2-C3	3.35	126.86	122.07
2	B	2	4HI	C27-C5-N1	3.34	130.12	125.46
2	B	1	4HI	C8-C7-N1	-3.31	106.37	112.16
2	D	3	4HI	C27-C5-N1	3.11	129.81	125.46
2	D	3	4HI	C3-C2-N3	3.10	126.68	121.06
2	B	1	4HI	C3-C2-N3	3.00	126.51	121.06
2	D	3	4HI	C6-C12-N1	2.99	130.31	123.67
2	C	4	4HI	C6-C12-N1	2.78	129.84	123.67
2	C	4	4HI	C27-C5-N1	2.75	129.30	125.46
2	B	2	4HI	C6-C12-N1	2.69	129.65	123.67
2	B	2	4HI	C8-C7-N1	-2.60	107.62	112.16
2	B	2	4HI	N1-C5-N3	-2.59	109.58	111.42
2	C	4	4HI	C8-C7-N1	-2.57	107.67	112.16
2	C	4	4HI	C12-C2-N3	-2.46	109.11	111.12
2	B	1	4HI	C27-C5-N1	2.42	128.84	125.46
2	B	1	4HI	C6-C12-N1	2.36	128.91	123.67
2	B	2	4HI	C12-C2-N3	-2.34	109.22	111.12
2	B	1	4HI	C13-C6-C12	-2.32	108.38	112.92
2	D	3	4HI	N1-C5-N3	-2.29	109.80	111.42
2	D	3	4HI	C7-N1-C5	-2.27	124.44	127.65
2	B	1	4HI	C12-C2-N3	-2.18	109.34	111.12
2	C	4	4HI	C13-C6-C12	-2.17	108.67	112.92
2	C	4	4HI	C7-N1-C5	-2.17	124.58	127.65
2	B	1	4HI	C24-C30-C15	-2.16	119.97	122.80
2	B	1	4HI	N1-C5-N3	-2.12	109.91	111.42

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	4HI	N3-C2-C3-O2
2	B	1	4HI	C12-C2-C3-O2
2	B	2	4HI	N3-C2-C3-O2

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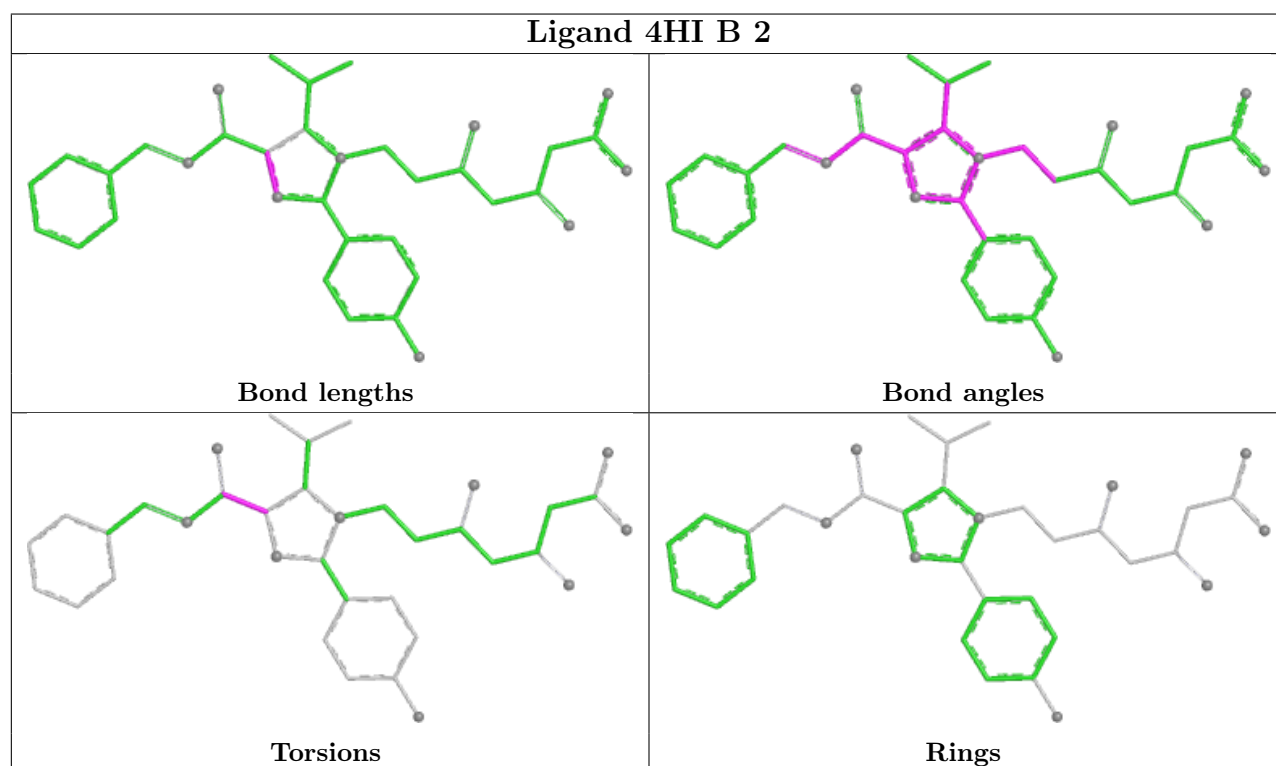
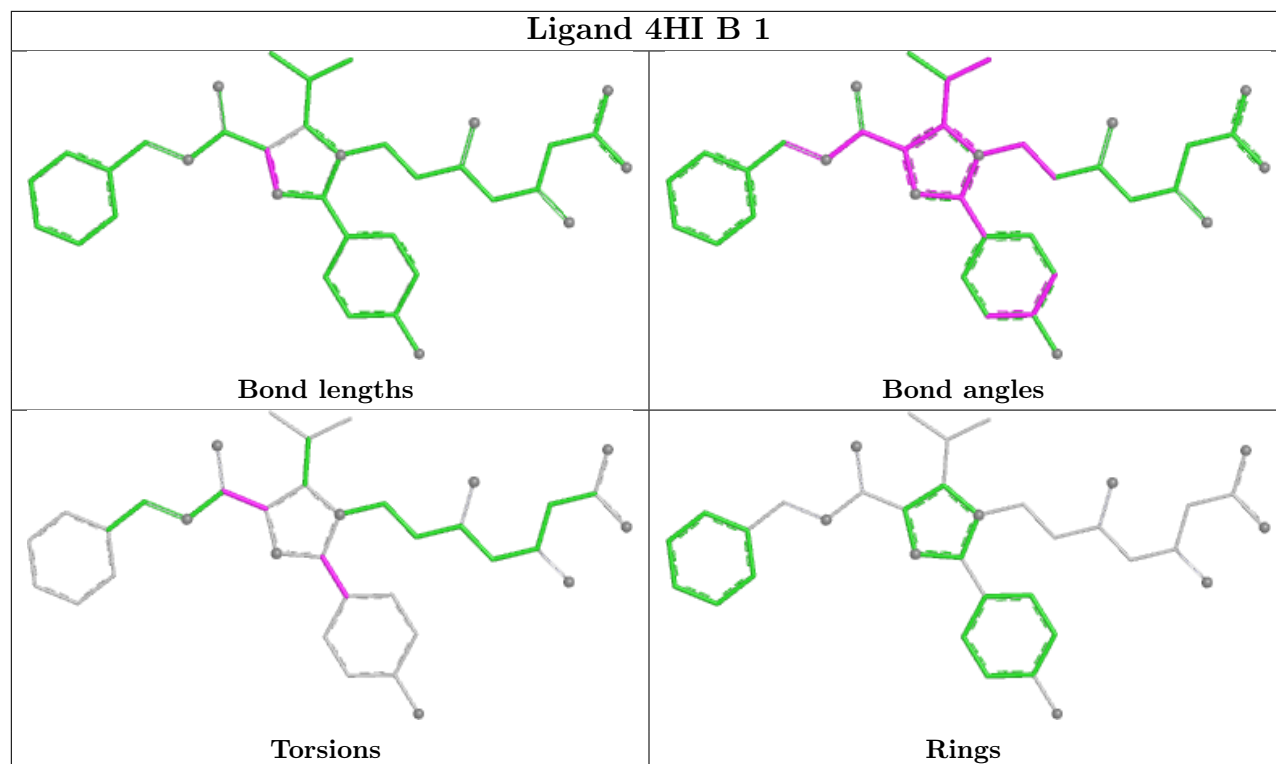
Mol	Chain	Res	Type	Atoms
2	B	2	4HI	C12-C2-C3-O2
2	C	4	4HI	N3-C2-C3-O2
2	C	4	4HI	C12-C2-C3-O2
2	D	3	4HI	N3-C2-C3-O2
2	D	3	4HI	C12-C2-C3-O2
2	B	1	4HI	N3-C2-C3-N2
2	D	3	4HI	C18-C27-C5-N3
2	D	3	4HI	C21-C27-C5-N3
2	D	3	4HI	C18-C27-C5-N1
2	D	3	4HI	C21-C27-C5-N1
2	C	4	4HI	C18-C27-C5-N3
2	C	4	4HI	C21-C27-C5-N3
2	C	4	4HI	C21-C27-C5-N1
2	C	4	4HI	N3-C2-C3-N2
2	D	3	4HI	N3-C2-C3-N2
2	B	1	4HI	C21-C27-C5-N3
2	B	1	4HI	C18-C27-C5-N3
2	C	4	4HI	C18-C27-C5-N1
2	B	1	4HI	C12-C2-C3-N2

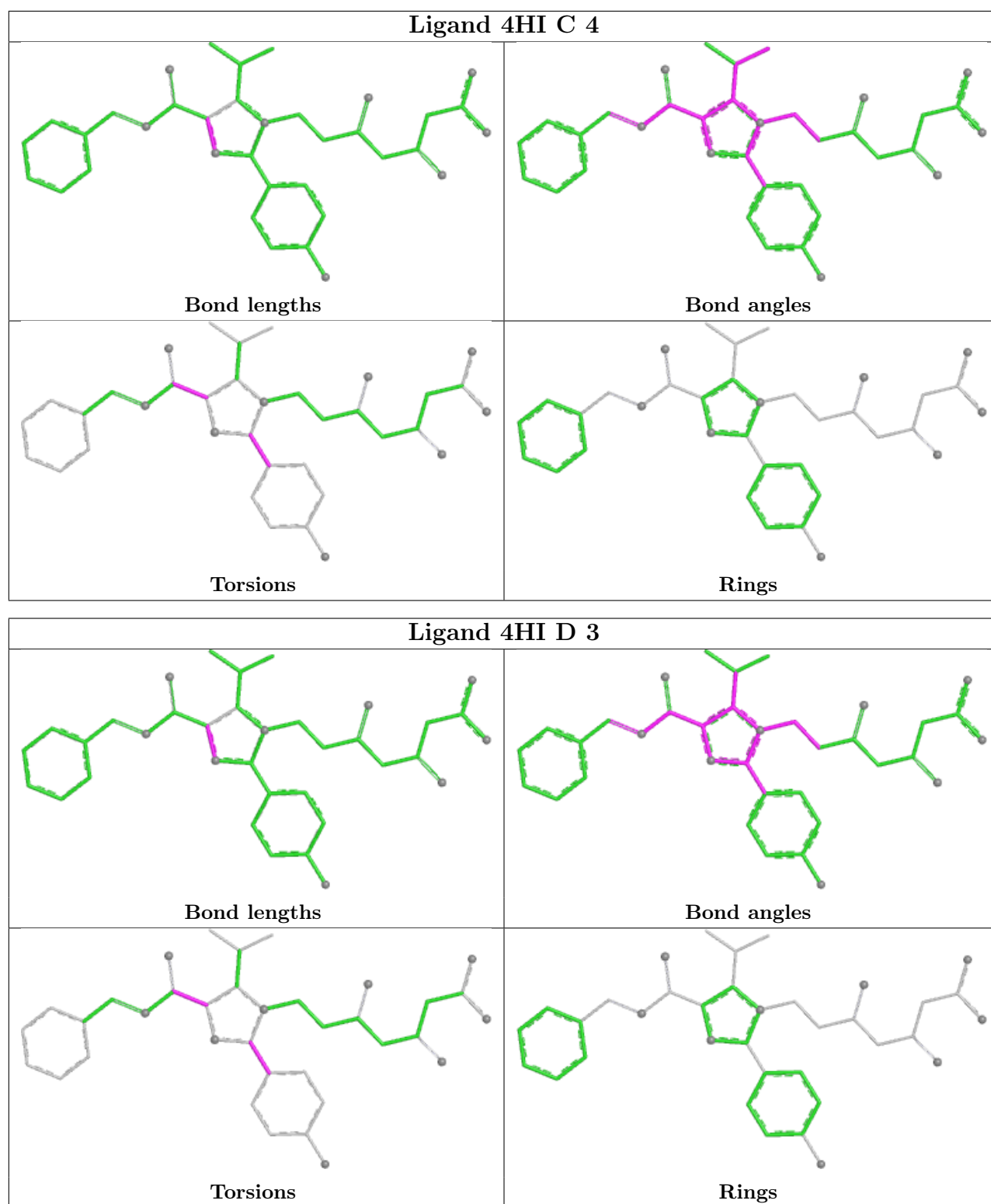
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	4HI	1	0
2	B	2	4HI	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 ⓘ

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%)	0.41	27 (6%)	25	27	29, 42, 62, 69	0
1	B	421/441 (95%)	0.38	16 (3%)	44	46	29, 43, 56, 72	0
1	C	414/441 (93%)	0.62	40 (9%)	13	14	30, 46, 83, 103	0
1	D	394/441 (89%)	0.42	22 (5%)	30	32	29, 43, 82, 108	0
All	All	1650/1764 (93%)	0.46	105 (6%)	25	27	29, 43, 66, 108	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	525	ALA	7.2
1	D	527	CYS	5.9
1	D	525	ALA	5.3
1	D	859	ALA	4.6
1	C	524	GLY	4.5
1	C	527	CYS	4.4
1	B	861	HIS	4.4
1	B	525	ALA	4.3
1	C	444	PRO	4.1
1	D	458	GLY	4.0
1	B	488	HIS	4.0
1	A	861	HIS	4.0
1	A	787	THR	3.9
1	A	455	ALA	3.6
1	D	470	LEU	3.6
1	C	449	LEU	3.4
1	A	635	HIS	3.3
1	C	526	CYS	3.3
1	D	459	ALA	3.3
1	B	527	CYS	3.3
1	C	476	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	451	ILE	3.2
1	D	471	VAL	3.1
1	A	479	TYR	3.1
1	D	475	HIS	3.1
1	D	504	SER	3.1
1	B	446	GLU	3.0
1	C	612	SER	3.0
1	C	448	CYS	3.0
1	D	485	ILE	3.0
1	A	576	GLY	2.9
1	C	473	ALA	2.9
1	A	453	GLY	2.9
1	A	708	CYS	2.8
1	B	526	CYS	2.8
1	C	487	THR	2.8
1	C	602	SER	2.8
1	B	679	GLN	2.8
1	A	525	ALA	2.8
1	C	452	LEU	2.7
1	C	461	PHE	2.7
1	A	452	LEU	2.6
1	A	463	SER	2.6
1	A	454	ASN	2.6
1	B	829	ASP	2.6
1	C	453	GLY	2.6
1	D	467	ILE	2.5
1	D	473	ALA	2.5
1	A	462	LEU	2.5
1	C	469	GLN	2.5
1	C	488	HIS	2.5
1	B	487	THR	2.5
1	C	591	GLY	2.5
1	D	465	ALA	2.5
1	C	631	LEU	2.5
1	C	708	CYS	2.4
1	A	859	ALA	2.4
1	A	461	PHE	2.4
1	A	513	PRO	2.4
1	D	484	LEU	2.4
1	A	789	GLU	2.4
1	D	528	GLU	2.4
1	B	450	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	574	GLY	2.4
1	C	860	GLY	2.3
1	A	482	GLU	2.3
1	A	858	ALA	2.3
1	C	458	GLY	2.3
1	C	470	LEU	2.3
1	C	640	GLY	2.3
1	C	450	GLN	2.3
1	C	628	PHE	2.3
1	D	466	GLU	2.3
1	A	483	THR	2.3
1	C	483	THR	2.3
1	A	484	LEU	2.3
1	C	615	PHE	2.2
1	C	522	VAL	2.2
1	D	786	PRO	2.2
1	C	585	ALA	2.2
1	D	463	SER	2.2
1	A	442	PRO	2.2
1	A	718	ARG	2.2
1	D	461	PHE	2.2
1	A	449	LEU	2.2
1	B	508	SER	2.2
1	D	630	ARG	2.2
1	C	471	VAL	2.1
1	C	715	LYS	2.1
1	C	771	ASN	2.1
1	C	614	GLY	2.1
1	B	501	LYS	2.1
1	A	527	CYS	2.1
1	B	827	CYS	2.1
1	C	520	SER	2.1
1	A	725	THR	2.1
1	B	785	GLY	2.1
1	D	785	GLY	2.1
1	C	598	ARG	2.1
1	C	468	ILE	2.0
1	B	482	GLU	2.0
1	C	548	GLU	2.0
1	C	624	SER	2.0
1	A	444	PRO	2.0
1	B	860	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

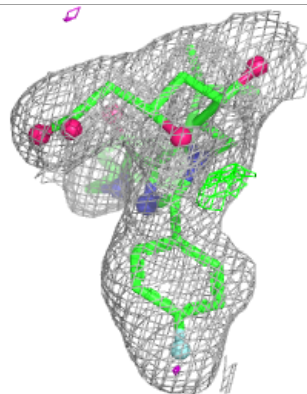
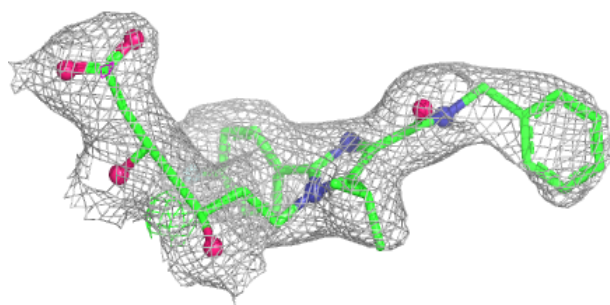
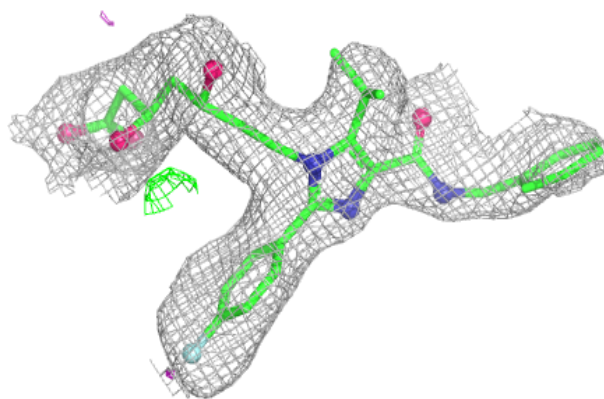
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	4HI	D	3	36/36	0.92	0.09	31,41,44,47	0
2	4HI	C	4	36/36	0.93	0.09	33,45,47,51	0
2	4HI	B	1	36/36	0.94	0.07	32,41,42,44	0
2	4HI	B	2	36/36	0.94	0.08	29,37,43,46	0

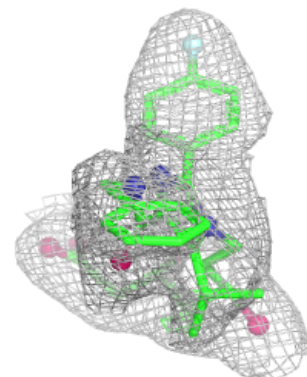
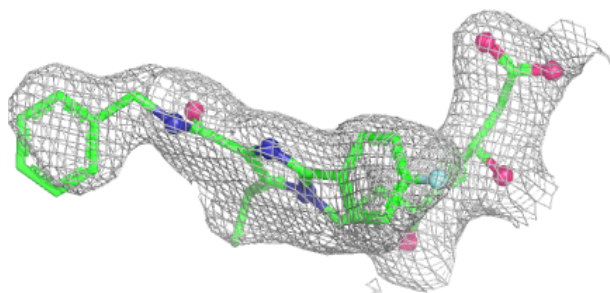
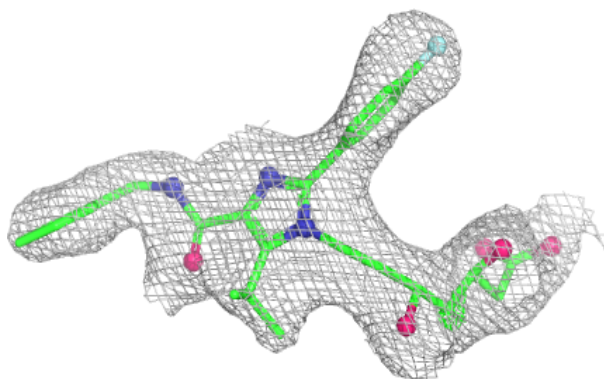
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4HI D 3:

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

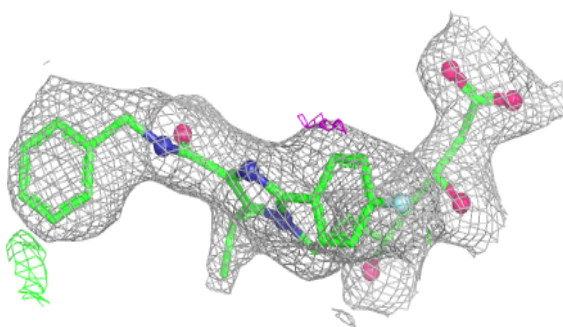
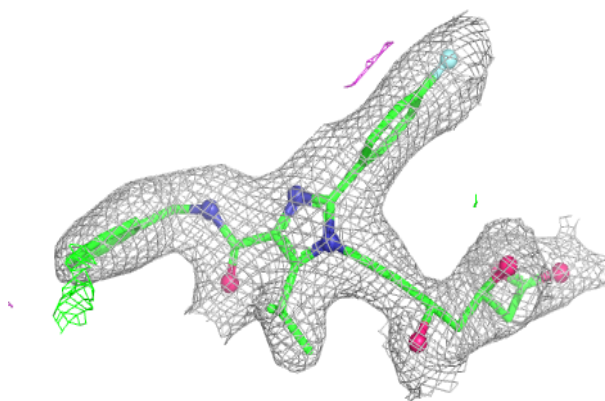
**Electron density around 4HI C 4:**

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

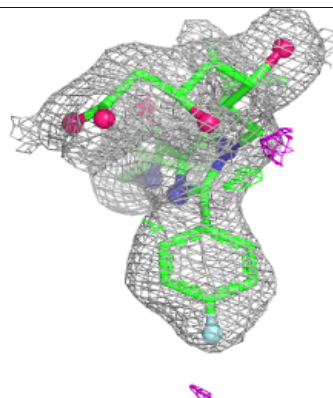
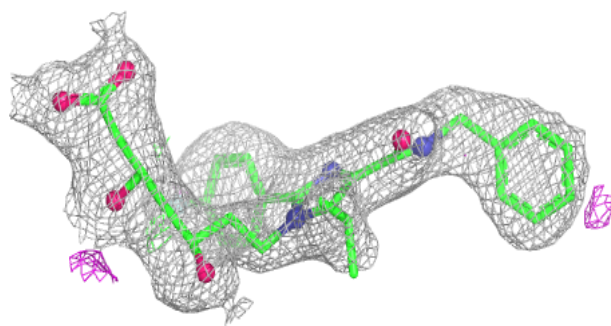
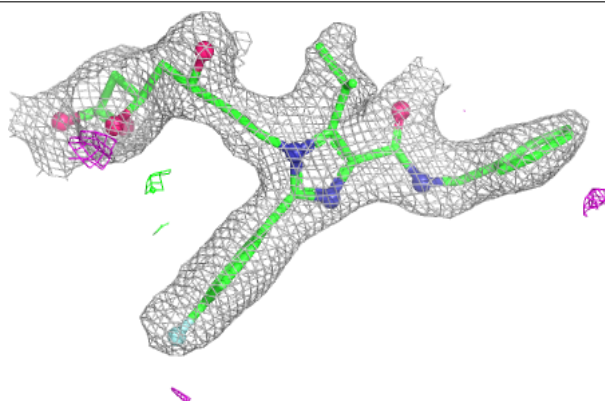


Electron density around 4HI B 1:

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

**Electron density around 4HI 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.