Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:47 AM EDT

PDB ID	:	3CDA
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	:	2.07 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

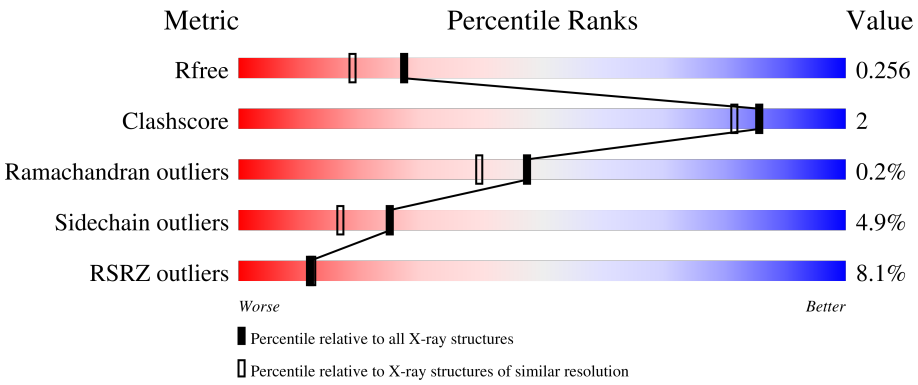
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	10% 81% 12% • •
1	B	441	4% 87% 8% 5%
1	C	441	10% 89% 5% 5%
1	D	441	7% 82% 7% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12971 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	422	3141	1957	552	602	30	0	0	0
1	B	421	3133	1951	551	601	30	0	0	0
1	C	417	3096	1929	542	595	30	0	0	0
1	D	395	2928	1824	515	560	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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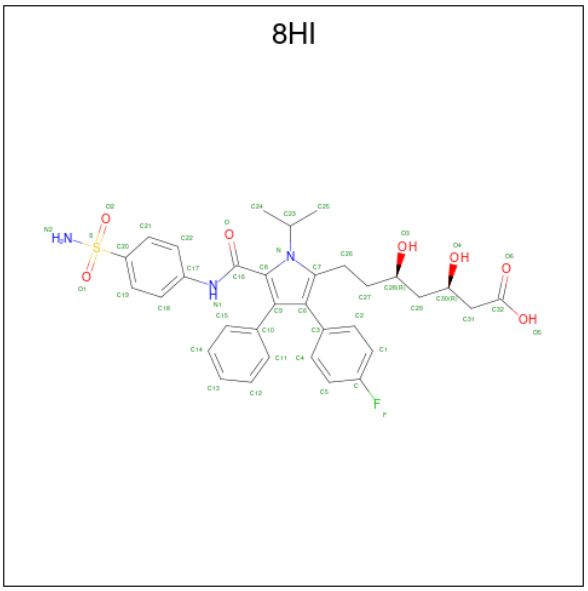
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is (3R,5R)-7-{3-(4-fluorophenyl)-1-(1-methylethyl)-4-phenyl-5-[(4-sulfamoyl phenyl)carbamoyl]-1H-pyrrol-2-yl}-3,5-dihydroxyheptanoic acid (three-letter code: 8HI) (formula: $C_{33}H_{36}FN_3O_7S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	45	33	1	3	7	1	0	0
			Total	C	F	N	O	S		
2	B	1	45	33	1	3	7	1	0	0
			Total	C	F	N	O	S		
2	C	1	45	33	1	3	7	1	0	0
			Total	C	F	N	O	S		
2	D	1	45	33	1	3	7	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	129	129	129	0	0

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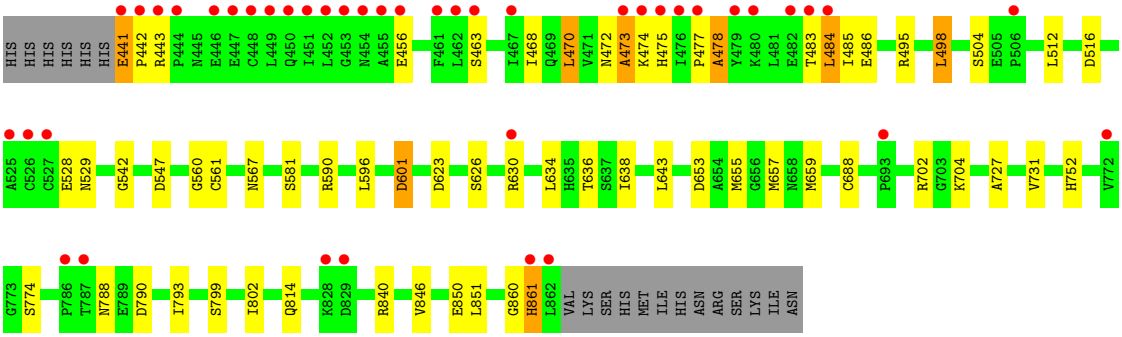
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	134	134	134	0	0
			Total	O		
3	C	98	98	98	0	0
			Total	O		
3	D	132	132	132	0	0

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.

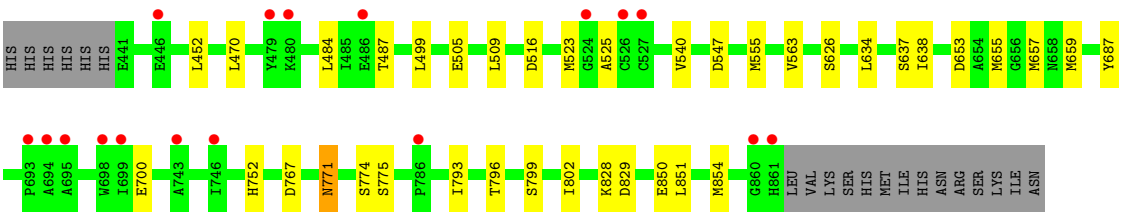
• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain A:



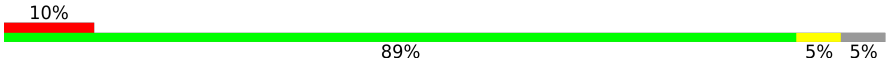
• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

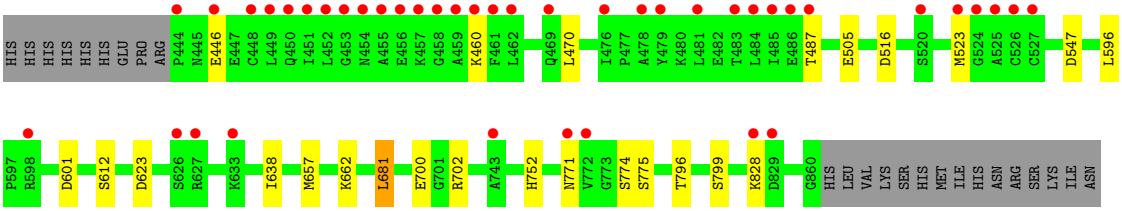
Chain B:



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

Chain C:

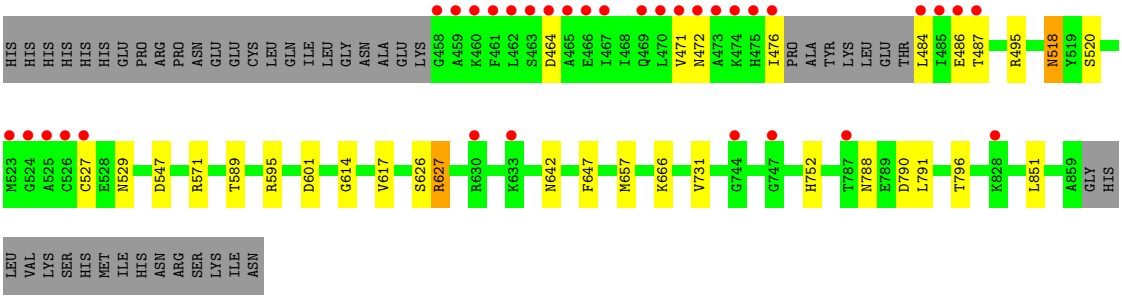




• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain D:

7%
82%
7%
10%


HIS HIS HIS HIS HIS GLU PRO ARG PRO ASN GLU GLU CYS LEU GLN ILE LEU GLY ASN ALA GLU LYS G458 A459 K460 F461 L462 S463 D464 A465 E466 I467 I468 Q469 L470 V471 N472 A473 K474 H475 I476 PRO ALA TYR LYS LEU GLU THR L484 I485 E486 T487 R495 N518 Y519 S520
M523 G524 A525 C526 C527 E528 N529 D547 R571 T589 R595 D601 G614 V617 S626 R627 R630 K633 N642 F647 M657 K666 V731 G744 G747 H752 T787 N788 E789 D790 L791 T796 K828 L851 A859 GLY HIS
LEU VAL LYS SER HIS MET ILE HIS ASN ARG SER LYS ILE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.61Å 172.25Å 75.62Å 90.00° 118.04° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 43.53 – 2.07	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.07) 90.5 (43.53-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 2.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.257 0.215 , 0.256	Depositor DCC
R_{free} test set	2066 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12971	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 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 8HI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/3187	0.64	6/4309 (0.1%)
1	B	0.36	0/3179	0.62	5/4298 (0.1%)
1	C	0.36	0/3140	0.61	4/4244 (0.1%)
1	D	0.37	0/2968	0.63	4/4010 (0.1%)
All	All	0.37	0/12474	0.63	19/16861 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	547	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	623	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	547	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	623	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	790	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	516	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	547	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	516	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	547	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	516	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	829	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	767	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	653	ASP	CB-CG-OD2	5.13	122.91	118.30
1	D	790	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	653	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	601	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	601	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	601	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	464	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3141	0	3178	26	0
1	B	3133	0	3167	16	0
1	C	3096	0	3135	7	0
1	D	2928	0	2968	10	0
2	A	45	0	35	0	0
2	B	45	0	35	0	0
2	C	45	0	35	1	0
2	D	45	0	35	1	0
3	A	129	0	0	1	0
3	B	134	0	0	2	0
3	C	98	0	0	0	0
3	D	132	0	0	1	0
All	All	12971	0	12588	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:655:MET:SD	1:A:657:MET:HG2	2.14	0.87
1:C:771:ASN:OD1	1:C:775:SER:OG	1.96	0.83
1:B:775:SER:OG	3:B:993:HOH:O	2.02	0.76
1:B:771:ASN:HB2	3:B:993:HOH:O	1.92	0.69
1:B:655:MET:SD	1:B:657:MET:HG2	2.34	0.67
1:A:470:LEU:O	1:A:474:LYS:O	2.22	0.58
1:A:590:ARG:NH2	1:A:657:MET:HE3	2.21	0.56
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.87	0.55
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.89	0.55
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.88	0.55
1:B:700:GLU:OE2	1:C:700:GLU:OE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:MET:CE	1:B:563:VAL:HA	2.38	0.54
1:A:477:PRO:O	1:A:478:ALA:HB2	2.08	0.54
1:A:472:ASN:O	1:A:473:ALA:CB	2.57	0.52
1:C:702:ARG:O	1:C:799:SER:HA	2.10	0.51
1:D:627:ARG:HG2	3:D:911:HOH:O	2.09	0.51
2:D:3:8HI:C16	2:D:3:8HI:H24A	2.40	0.51
1:A:477:PRO:O	1:A:478:ALA:CB	2.60	0.49
1:B:638:ILE:O	1:C:796:THR:HG21	2.13	0.48
1:B:796:THR:HG21	1:C:638:ILE:O	2.13	0.48
1:C:774:SER:HA	1:C:799:SER:O	2.13	0.48
1:A:638:ILE:O	1:D:796:THR:HG21	2.12	0.48
1:D:495:ARG:HG2	1:D:529:ASN:OD1	2.13	0.48
1:A:793:ILE:HD13	1:A:851:LEU:HG	1.96	0.48
1:A:474:LYS:O	1:A:475:HIS:HB2	2.13	0.48
1:A:727:ALA:O	1:A:731:VAL:HG23	2.14	0.47
1:A:441:GLU:N	1:A:442:PRO:CD	2.77	0.47
1:D:471:VAL:HA	1:D:476:ILE:HG23	1.96	0.47
2:C:4:8HI:O	2:C:4:8HI:H25A	2.14	0.47
1:A:581:SER:OG	1:A:840:ARG:HD2	2.16	0.46
1:D:589:THR:HA	1:D:647:PHE:O	2.16	0.46
1:A:529:ASN:ND2	1:B:540:VAL:O	2.47	0.46
1:A:636:THR:HG23	1:A:643:LEU:CD1	2.46	0.45
1:A:860:GLY:O	1:A:861:HIS:HB2	2.16	0.45
1:A:774:SER:HA	1:A:799:SER:O	2.16	0.45
1:B:555:MET:HE3	1:B:563:VAL:HA	1.98	0.44
1:A:542:GLY:H	1:A:567:ASN:HD22	1.65	0.44
1:A:702:ARG:O	1:A:799:SER:HA	2.17	0.44
1:A:590:ARG:NH2	1:A:657:MET:CE	2.81	0.43
1:D:518:ASN:ND2	1:D:520:SER:OG	2.47	0.43
1:B:850:GLU:O	1:B:854:MET:HG2	2.19	0.43
1:D:614:GLY:O	1:D:617:VAL:HG22	2.20	0.42
1:A:596:LEU:HB3	1:A:601:ASP:HB2	2.00	0.42
1:B:655:MET:HA	1:B:802:ILE:O	2.19	0.42
1:B:637:SER:HB2	1:B:687:TYR:OH	2.19	0.42
1:B:499:LEU:HD23	1:B:509:LEU:HD11	2.02	0.41
1:A:560:GLY:O	1:A:561:CYS:HB2	2.20	0.41
1:B:774:SER:HA	1:B:799:SER:O	2.21	0.41
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.50	0.41
1:D:642:ASN:N	1:D:642:ASN:HD22	2.17	0.41
1:A:846:VAL:O	1:A:850:GLU:HG2	2.22	0.40
1:A:474:LYS:O	1:A:475:HIS:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:ILE:HD13	1:B:851:LEU:HG	2.02	0.40
1:A:657:MET:HE2	3:A:978:HOH:O	2.21	0.40
1:D:595:ARG:HE	1:D:642:ASN:ND2	2.19	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	420/441 (95%)	398 (95%)	19 (4%)	3 (1%)	22	11
1	B	419/441 (95%)	404 (96%)	14 (3%)	1 (0%)	47	39
1	C	415/441 (94%)	399 (96%)	16 (4%)	0	100	100
1	D	391/441 (89%)	376 (96%)	15 (4%)	0	100	100
All	All	1645/1764 (93%)	1577 (96%)	64 (4%)	4 (0%)	47	39

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/355 (95%)	311 (93%)	25 (7%)	13 6
1	B	335/355 (94%)	323 (96%)	12 (4%)	35 28
1	C	331/355 (93%)	318 (96%)	13 (4%)	32 25
1	D	313/355 (88%)	298 (95%)	15 (5%)	25 18
All	All	1315/1420 (93%)	1250 (95%)	65 (5%)	25 17

All (65) 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	463	SER
1	A	470	LEU
1	A	483	THR
1	A	484	LEU
1	A	485	ILE
1	A	486	GLU
1	A	495	ARG
1	A	498	LEU
1	A	504	SER
1	A	512	LEU
1	A	528	GLU
1	A	626	SER
1	A	630	ARG
1	A	634	LEU
1	A	659	MET
1	A	688	CYS
1	A	704	LYS
1	A	752	HIS
1	A	788	ASN
1	A	802	ILE
1	A	814	GLN
1	A	861	HIS
1	B	452	LEU
1	B	470	LEU
1	B	484	LEU
1	B	487	THR
1	B	505	GLU
1	B	523	MET

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Mol	Chain	Res	Type
1	B	626	SER
1	B	634	LEU
1	B	659	MET
1	B	752	HIS
1	B	771	ASN
1	B	828	LYS
1	C	446	GLU
1	C	460	LYS
1	C	470	LEU
1	C	487	THR
1	C	505	GLU
1	C	523	MET
1	C	596	LEU
1	C	612	SER
1	C	657	MET
1	C	662	LYS
1	C	681	LEU
1	C	752	HIS
1	C	828	LYS
1	D	472	ASN
1	D	484	LEU
1	D	486	GLU
1	D	487	THR
1	D	518	ASN
1	D	527	CYS
1	D	571	ARG
1	D	626	SER
1	D	627	ARG
1	D	657	MET
1	D	666	LYS
1	D	752	HIS
1	D	788	ASN
1	D	791	LEU
1	D	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN

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Mol	Chain	Res	Type
1	A	635	HIS
1	A	788	ASN
1	B	472	ASN
1	B	510	GLN
1	B	819	GLN
1	B	830	ASN
1	C	472	ASN
1	C	679	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	672	HIS
1	D	810	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	8HI	D	3	-	42,48,48	1.74	3 (7%)	60,69,69	1.42	6 (10%)
2	8HI	C	4	-	42,48,48	1.77	3 (7%)	60,69,69	1.49	7 (11%)
2	8HI	B	1	-	42,48,48	1.74	3 (7%)	60,69,69	1.69	9 (15%)
2	8HI	A	2	-	42,48,48	1.83	3 (7%)	60,69,69	1.54	10 (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	8HI	D	3	-	-	2/33/39/39	0/4/4/4
2	8HI	C	4	-	-	4/33/39/39	0/4/4/4
2	8HI	B	1	-	-	4/33/39/39	0/4/4/4
2	8HI	A	2	-	-	2/33/39/39	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	8HI	C20-S	-10.46	1.60	1.77
2	C	4	8HI	C20-S	-10.27	1.61	1.77
2	D	3	8HI	C20-S	-9.89	1.61	1.77
2	B	1	8HI	C20-S	-9.83	1.61	1.77
2	A	2	8HI	C9-C6	-2.93	1.37	1.43
2	C	4	8HI	C9-C6	-2.71	1.37	1.43
2	D	3	8HI	C9-C6	-2.67	1.37	1.43
2	B	1	8HI	C9-C6	-2.62	1.37	1.43
2	D	3	8HI	C17-N1	-2.50	1.36	1.41
2	C	4	8HI	C17-N1	-2.38	1.36	1.41
2	A	2	8HI	C17-N1	-2.36	1.36	1.41
2	B	1	8HI	C17-N1	-2.29	1.37	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	8HI	O2-S-O1	-7.06	107.16	118.76
2	C	4	8HI	O2-S-O1	-6.06	108.81	118.76
2	A	2	8HI	O2-S-O1	-5.58	109.59	118.76
2	D	3	8HI	O2-S-O1	-5.24	110.15	118.76
2	A	2	8HI	O1-S-C20	4.42	112.28	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	8HI	O2-S-C20	3.98	111.79	107.35
2	D	3	8HI	O1-S-C20	3.70	111.48	107.35
2	B	1	8HI	C9-C8-C16	-3.36	124.38	131.00
2	C	4	8HI	C9-C8-C16	-3.18	124.73	131.00
2	D	3	8HI	C9-C8-C16	-3.06	124.98	131.00
2	A	2	8HI	C9-C8-C16	-3.02	125.04	131.00
2	C	4	8HI	C2-C3-C6	-2.72	116.28	120.79
2	B	1	8HI	C7-N-C23	-2.69	121.47	126.89
2	C	4	8HI	C26-C7-C6	-2.68	125.77	130.34
2	A	2	8HI	C26-C27-C28	-2.67	109.91	115.05
2	C	4	8HI	O1-S-C20	2.64	110.30	107.35
2	B	1	8HI	C2-C3-C6	-2.60	116.47	120.79
2	B	1	8HI	O1-S-C20	2.51	110.15	107.35
2	D	3	8HI	C26-C7-C6	-2.51	126.06	130.34
2	A	2	8HI	C26-C7-C6	-2.46	126.14	130.34
2	B	1	8HI	C24-C23-N	-2.42	108.68	111.52
2	A	2	8HI	O1-S-N2	2.42	110.95	107.36
2	D	3	8HI	C26-C27-C28	-2.40	110.44	115.05
2	D	3	8HI	C2-C3-C6	-2.37	116.86	120.79
2	A	2	8HI	C2-C3-C6	-2.34	116.92	120.79
2	C	4	8HI	C26-C27-C28	-2.21	110.80	115.05
2	A	2	8HI	C7-N-C23	-2.17	122.51	126.89
2	C	4	8HI	C1-C-C5	-2.16	119.96	122.83
2	B	1	8HI	C26-C7-C6	-2.13	126.70	130.34
2	B	1	8HI	C1-C-C5	-2.04	120.11	122.83
2	A	2	8HI	C1-C-C5	-2.02	120.14	122.83
2	A	2	8HI	C30-C29-C28	-2.02	111.10	114.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	8HI	C26-C27-C28-O3
2	B	1	8HI	C26-C27-C28-O3
2	C	4	8HI	C26-C27-C28-O3
2	A	2	8HI	C26-C27-C28-C29
2	B	1	8HI	C26-C27-C28-C29
2	D	3	8HI	C26-C27-C28-O3
2	C	4	8HI	C26-C27-C28-C29
2	D	3	8HI	C26-C27-C28-C29
2	B	1	8HI	C24-C23-N-C7
2	B	1	8HI	C25-C23-N-C7

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Mol	Chain	Res	Type	Atoms
2	C	4	8HI	C24-C23-N-C7
2	C	4	8HI	C25-C23-N-C7

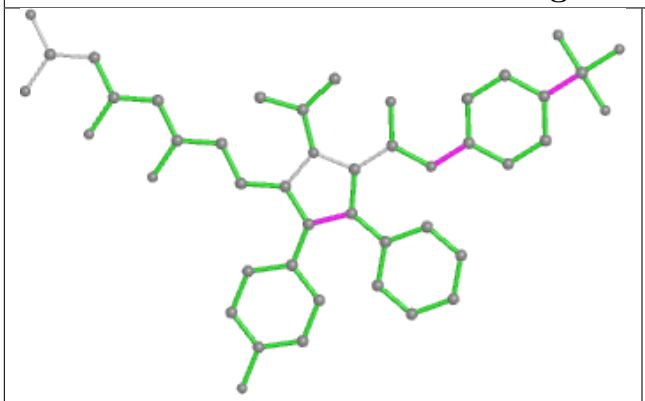
There are no ring outliers.

2 monomers are involved in 2 short contacts:

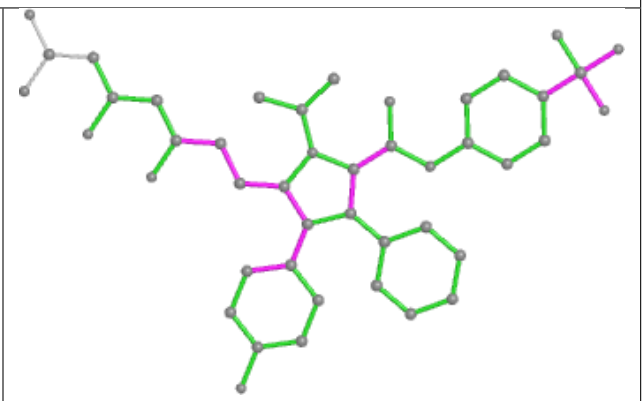
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	8HI	1	0
2	C	4	8HI	1	0

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 then 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.

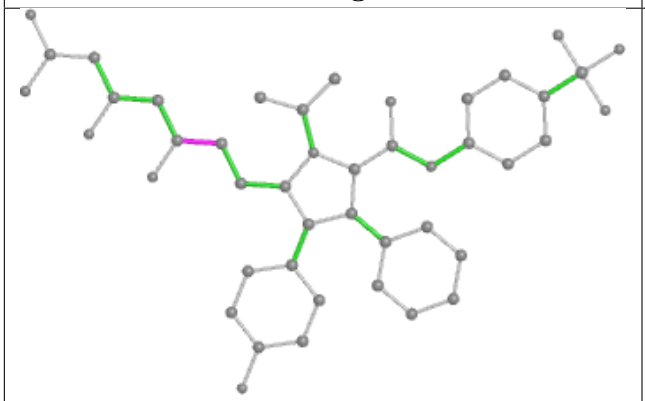
Ligand 8HI D 3



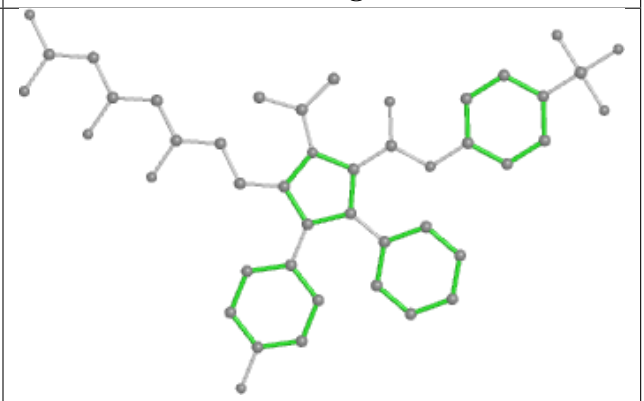
Bond lengths



Bond angles

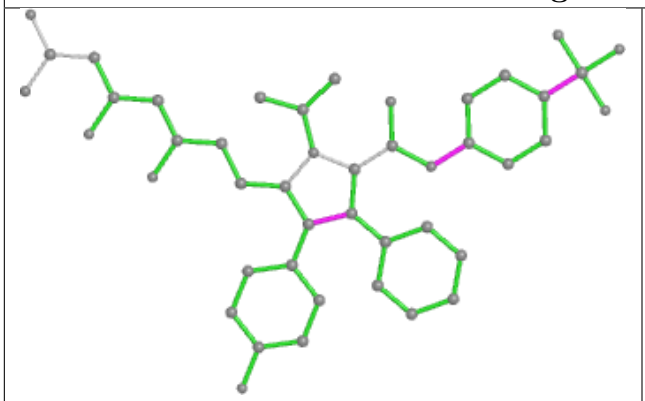


Torsions

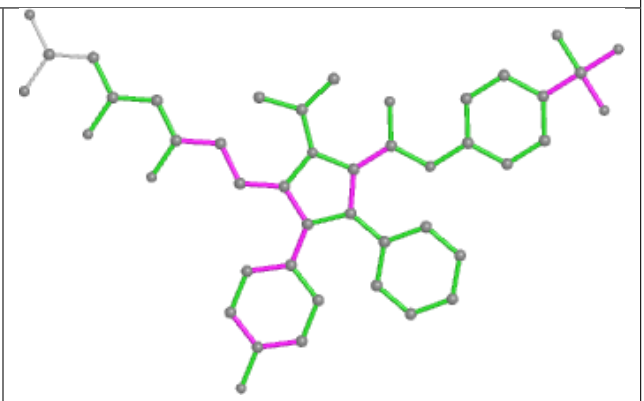


Rings

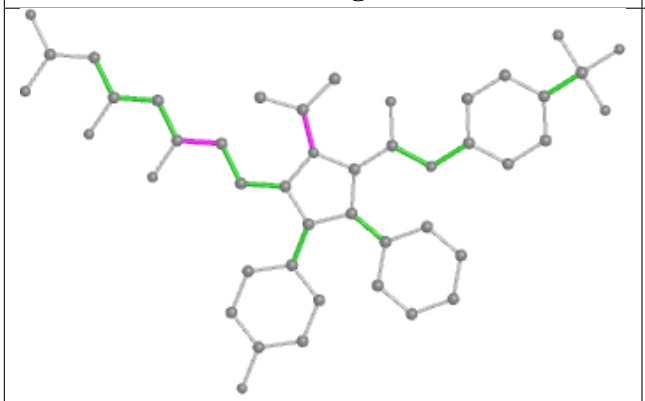
Ligand 8HI C 4



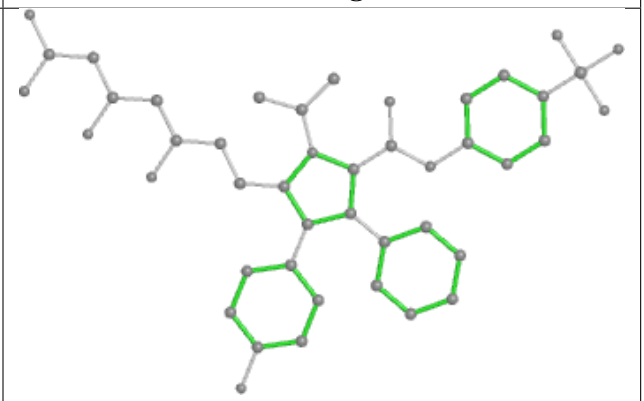
Bond lengths



Bond angles

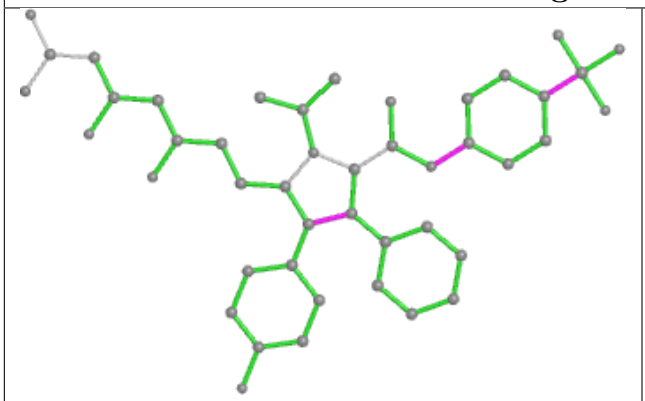


Torsions

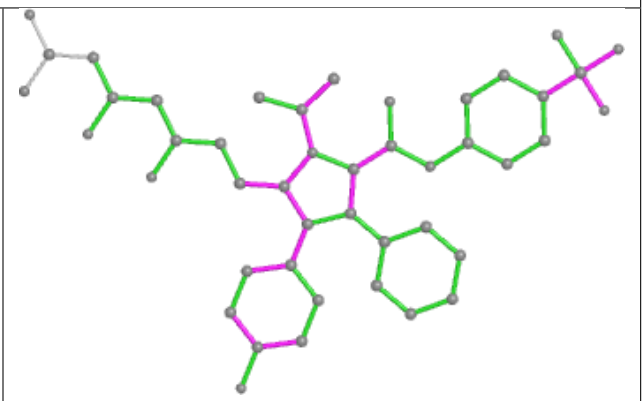


Rings

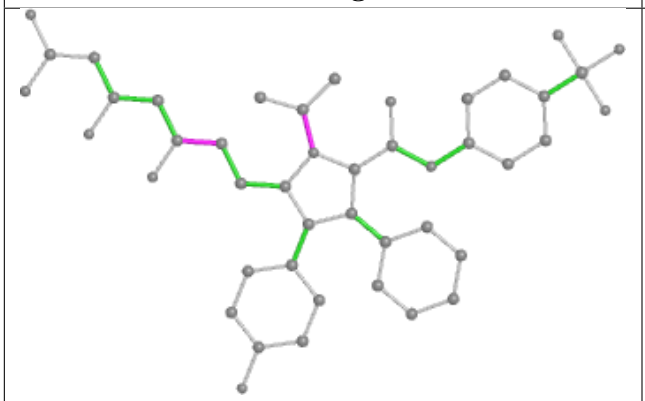
Ligand 8HI B 1



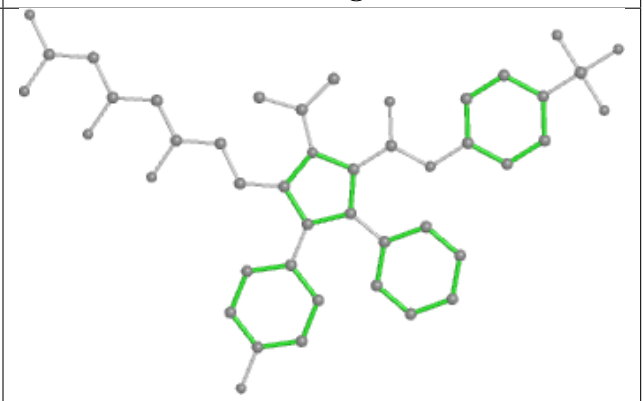
Bond lengths



Bond angles

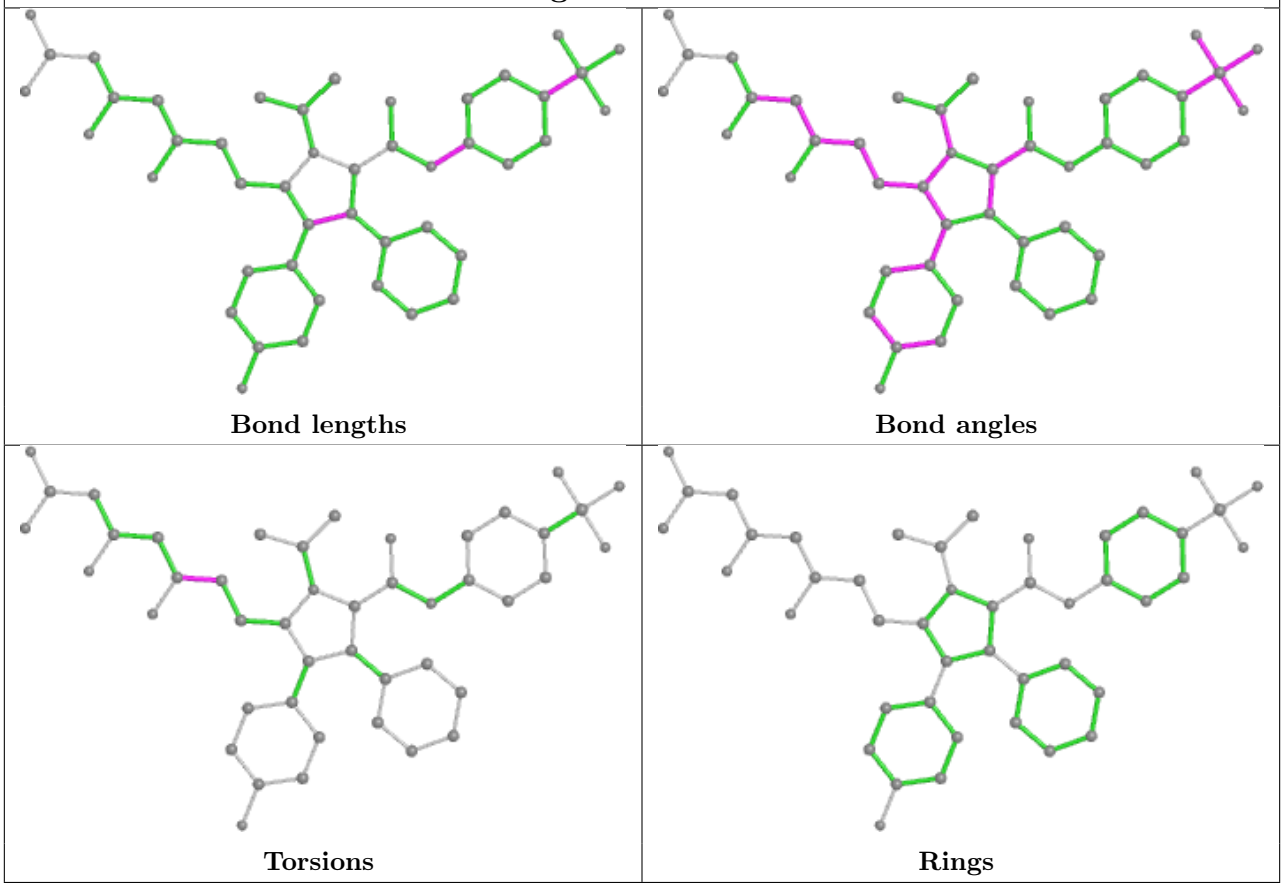


Torsions



Rings

Ligand 8HI A 2



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	422/441 (95%)	0.40	42 (9%)	7	7	24, 35, 56, 63	0
1	B	421/441 (95%)	0.23	17 (4%)	38	40	25, 35, 48, 57	0
1	C	417/441 (94%)	0.54	42 (10%)	7	7	23, 36, 59, 65	0
1	D	395/441 (89%)	0.48	33 (8%)	11	11	24, 35, 59, 64	0
All	All	1655/1764 (93%)	0.41	134 (8%)	12	12	23, 35, 56, 65	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	CYS	13.0
1	D	461	PHE	10.0
1	C	455	ALA	9.0
1	B	861	HIS	8.5
1	D	475	HIS	8.2
1	C	461	PHE	8.1
1	A	861	HIS	7.9
1	D	458	GLY	7.8
1	D	525	ALA	7.5
1	C	525	ALA	7.5
1	D	486	GLU	7.1
1	A	527	CYS	6.7
1	D	470	LEU	6.6
1	C	483	THR	6.5
1	D	485	ILE	6.4
1	D	465	ALA	6.3
1	D	459	ALA	6.2
1	D	484	LEU	6.2
1	A	862	LEU	5.9
1	C	458	GLY	5.8
1	C	527	CYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	451	ILE	5.2
1	C	456	GLU	5.2
1	D	523	MET	5.2
1	D	463	SER	5.1
1	C	457	LYS	5.0
1	C	524	GLY	5.0
1	C	452	LEU	5.0
1	A	444	PRO	5.0
1	C	481	LEU	4.9
1	D	469	GLN	4.8
1	D	460	LYS	4.6
1	A	452	LEU	4.5
1	C	484	LEU	4.5
1	A	461	PHE	4.4
1	A	456	GLU	4.3
1	D	462	LEU	4.3
1	C	479	TYR	4.3
1	C	450	GLN	4.2
1	D	473	ALA	4.2
1	C	462	LEU	4.0
1	D	466	GLU	4.0
1	D	472	ASN	4.0
1	A	475	HIS	3.9
1	D	476	ILE	3.8
1	C	453	GLY	3.8
1	A	455	ALA	3.8
1	C	444	PRO	3.8
1	A	446	GLU	3.8
1	C	485	ILE	3.7
1	A	450	GLN	3.7
1	A	476	ILE	3.7
1	A	525	ALA	3.6
1	C	478	ALA	3.6
1	D	464	ASP	3.5
1	A	447	GLU	3.4
1	A	462	LEU	3.4
1	D	474	LYS	3.4
1	D	828	LYS	3.4
1	D	487	THR	3.4
1	D	471	VAL	3.3
1	C	526	CYS	3.3
1	C	460	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	483	THR	3.2
1	A	480	LYS	3.2
1	B	479	TYR	3.1
1	A	453	GLY	3.0
1	C	469	GLN	3.0
1	C	487	THR	3.0
1	D	524	GLY	3.0
1	C	829	ASP	3.0
1	C	523	MET	2.9
1	A	828	LYS	2.9
1	A	506	PRO	2.9
1	A	443	ARG	2.9
1	B	486	GLU	2.8
1	C	454	ASN	2.7
1	B	698	TRP	2.7
1	C	448	CYS	2.7
1	A	829	ASP	2.7
1	B	524	GLY	2.7
1	A	448	CYS	2.7
1	A	449	LEU	2.7
1	C	486	GLU	2.7
1	A	463	SER	2.7
1	B	446	GLU	2.7
1	C	828	LYS	2.6
1	A	526	CYS	2.6
1	C	743	ALA	2.5
1	C	449	LEU	2.5
1	A	772	VAL	2.5
1	C	627	ARG	2.5
1	C	476	ILE	2.5
1	D	467	ILE	2.4
1	D	526	CYS	2.4
1	A	693	PRO	2.4
1	B	743	ALA	2.4
1	B	699	ILE	2.4
1	B	527	CYS	2.4
1	A	630	ARG	2.4
1	B	746	ILE	2.4
1	B	526	CYS	2.3
1	B	695	ALA	2.3
1	A	441	GLU	2.3
1	A	454	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	2.3
1	A	786	PRO	2.3
1	D	630	ARG	2.3
1	A	479	TYR	2.3
1	D	744	GLY	2.3
1	A	473	ALA	2.2
1	A	442	PRO	2.2
1	C	633	LYS	2.2
1	C	520	SER	2.2
1	A	467	ILE	2.2
1	B	694	ALA	2.2
1	A	482	GLU	2.2
1	B	693	PRO	2.2
1	A	474	LYS	2.2
1	C	771	ASN	2.2
1	C	626	SER	2.2
1	C	459	ALA	2.1
1	B	480	LYS	2.1
1	B	860	GLY	2.1
1	D	633	LYS	2.1
1	B	786	PRO	2.1
1	A	787	THR	2.1
1	C	598	ARG	2.0
1	A	451	ILE	2.0
1	D	787	THR	2.0
1	C	446	GLU	2.0
1	C	772	VAL	2.0
1	A	477	PRO	2.0
1	D	747	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

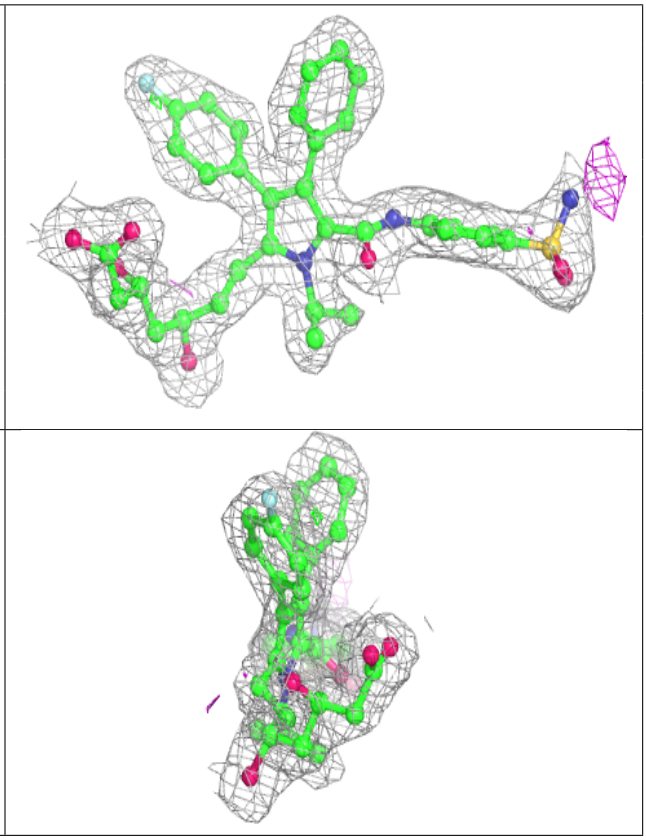
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

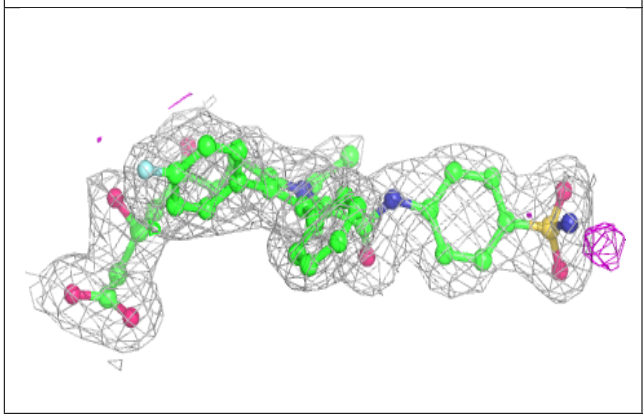
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	8HI	A	2	45/45	0.93	0.12	26,30,35,36	0
2	8HI	C	4	45/45	0.93	0.11	28,31,36,37	0
2	8HI	D	3	45/45	0.93	0.12	25,32,34,36	0
2	8HI	B	1	45/45	0.94	0.12	27,34,37,38	0

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 8HI A 2:

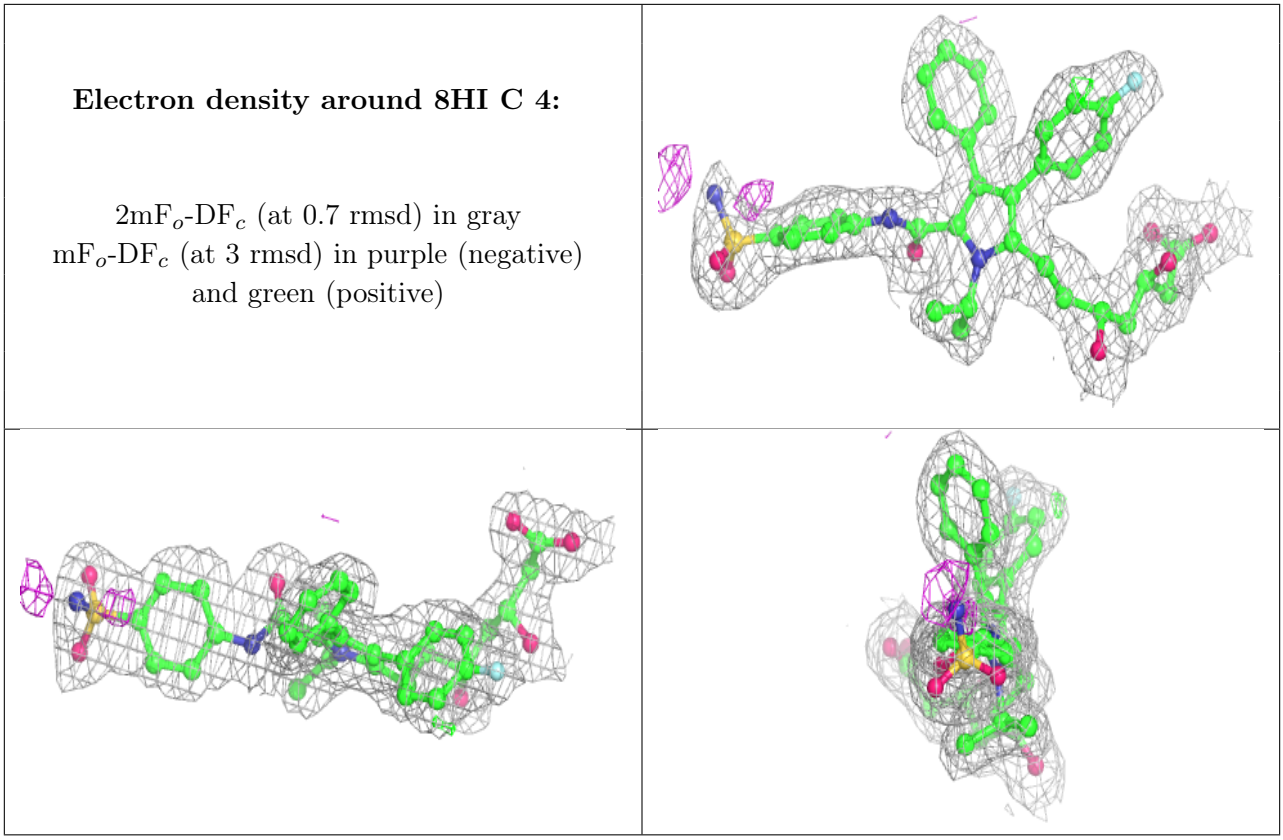
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





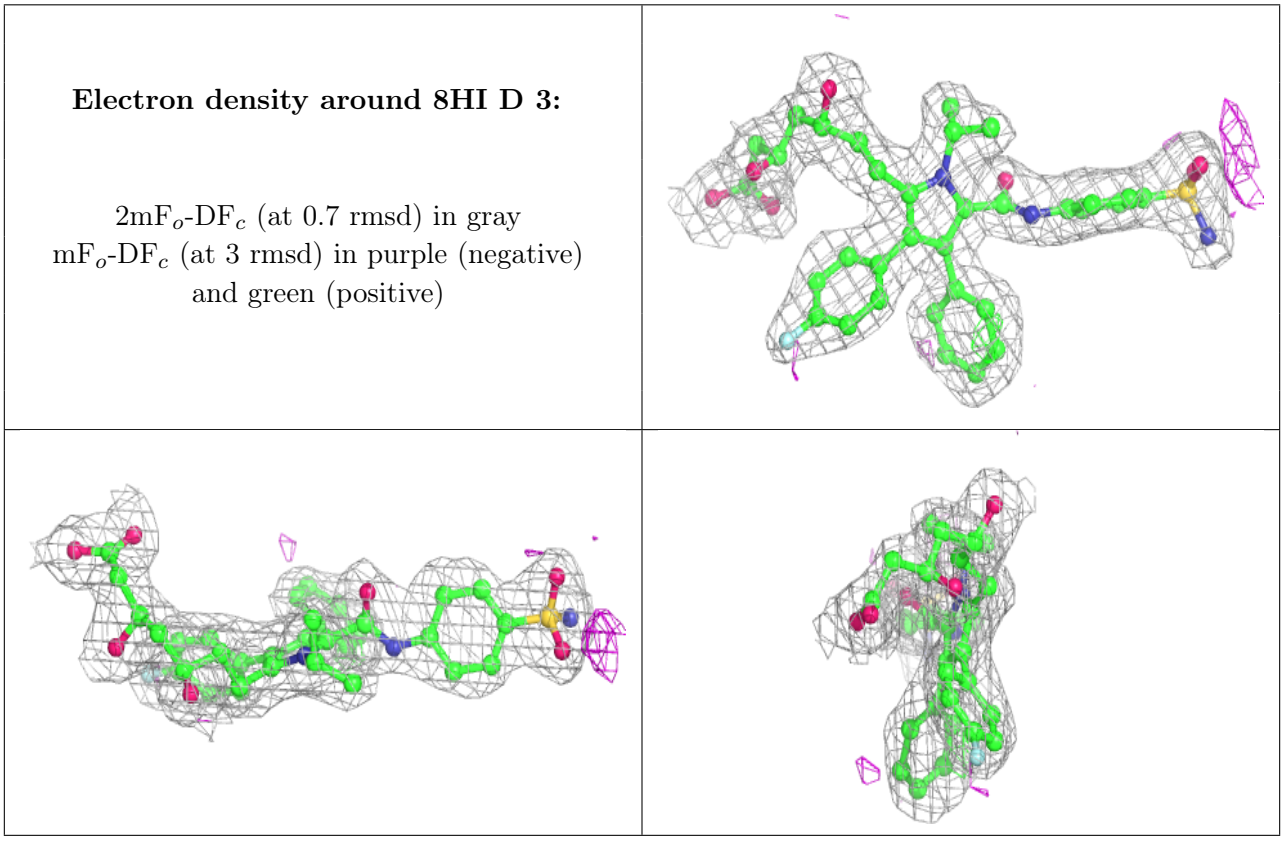
Electron density around 8HI C 4:

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



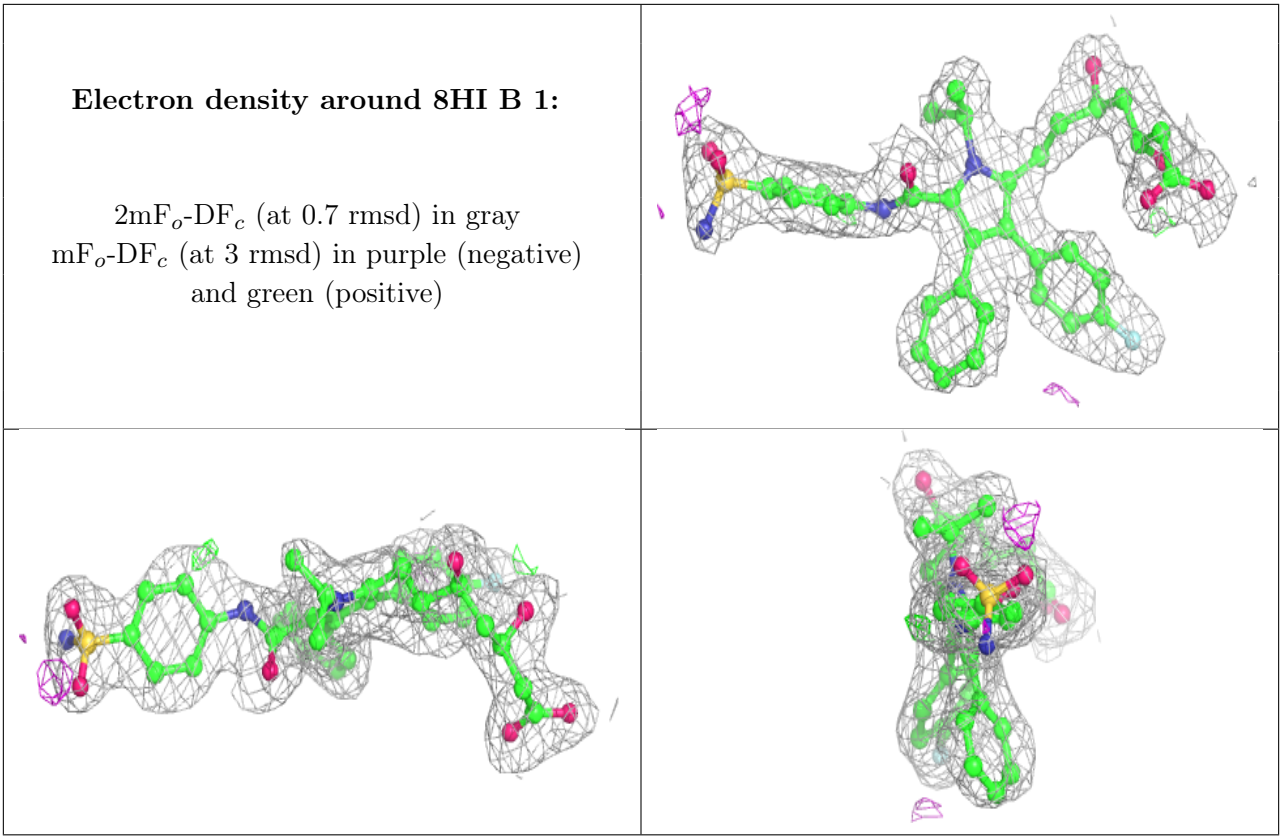
Electron density around 8HI D 3:

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



Electron density around 8HI B 1:

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



6.5 Other polymers (i)

There are no such residues in this entry.