



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 AM UTC

PDB ID : 3CD7 / pdb\_00003cd7  
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 : 2.05 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](mailto: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>.

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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

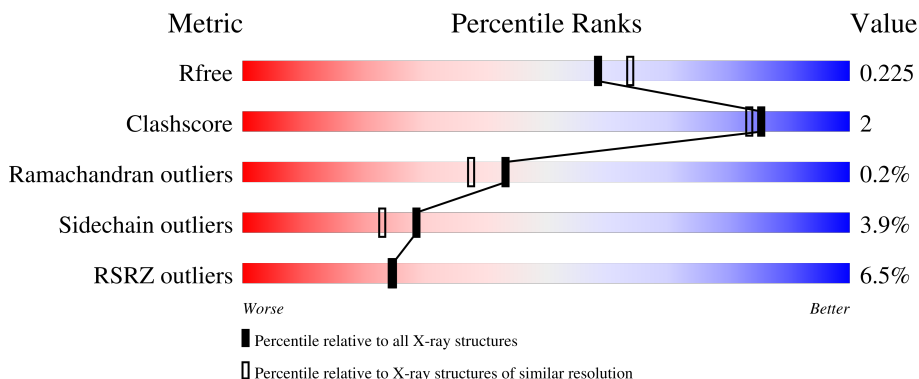
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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  $\geq 3$ , 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 12542 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	392	2903	1806	511	557	29	0	0	0
1	B	401	2979	1859	524	567	29	0	0	0
1	C	416	3087	1923	540	594	30	0	0	0
1	D	394	2920	1818	514	559	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

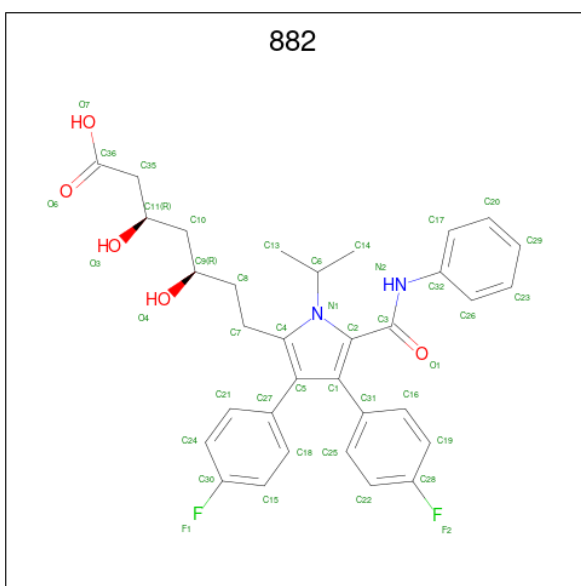
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered 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-[5-(ANILINOCARBONYL)-3,4-BIS(4-FLUOROPHENYL)-1-ISOPROPYL-1H-PYRROL-2-YL]-3,5-DIHYDROXYHEPTANOIC ACID (CCD ID: 882) (formula: C<sub>33</sub>H<sub>34</sub>F<sub>2</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total	C	F	N	O	0	0
			42	33	2	2	5		
2	A	1	Total	C	F	N	O	0	0
			42	33	2	2	5		
2	C	1	Total	C	F	N	O	0	0
			42	33	2	2	5		
2	D	1	Total	C	F	N	O	0	0
			42	33	2	2	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		

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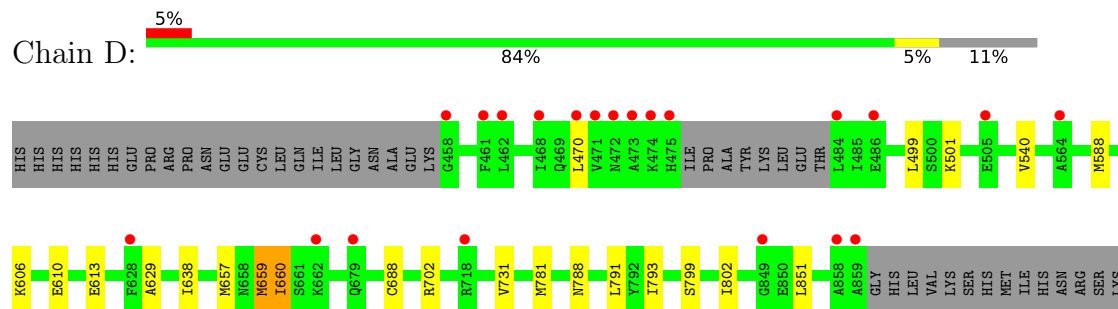
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	113	Total 113	O 113	0	0
3	C	109	Total 109	O 109	0	0
3	D	131	Total 131	O 131	0	0



SER  
LYS  
ILE  
ASN

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



ILE  
ASN

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73Å 176.96Å 76.73Å 90.00° 118.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	79.7 (30.00-2.05) 74.8 (30.00-2.22)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.223 , 0.263 0.226 , 0.225	Depositor DCC
$R_{free}$ test set	3233 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h-l,k,h 0.012 for l,k,-h-l 0.029 for h,-k,-h-l 0.034 for -h-l,-k,l 0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:  
882

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	0.52	0/2943	0.80	1/3977 (0.0%)
1	B	0.51	1/3022 (0.0%)	0.79	0/4084
1	C	0.52	0/3130	0.79	0/4230
1	D	0.52	0/2960	0.80	0/3999
All	All	0.52	1/12055 (0.0%)	0.80	1/16290 (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	-5.47	1.65	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	ILE	N-CA-C	5.59	115.69	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	2903	0	2933	14	0
1	B	2979	0	3020	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3087	0	3121	21	0
1	D	2920	0	2957	9	0
2	A	84	0	66	1	0
2	C	42	0	33	1	0
2	D	42	0	33	1	0
3	A	132	0	0	0	0
3	B	113	0	0	0	0
3	C	109	0	0	0	0
3	D	131	0	0	0	0
All	All	12542	0	12163	53	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 (53) 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	2.27	0.74
1:A:817:CYS:HA	1:A:820:MET:HE3	1.68	0.74
1:A:771:ASN:OD1	1:A:775:SER:OG	2.10	0.69
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.73	0.69
1:C:655:MET:SD	1:C:657:MET:HG2	2.35	0.67
1:C:445:ASN:HD22	1:C:469:GLN:HE21	1.44	0.65
1:C:523:MET:HE1	1:C:530:VAL:CG2	2.29	0.63
1:C:771:ASN:OD1	1:C:775:SER:OG	2.17	0.62
1:C:456:GLU:C	1:C:458:GLY:N	2.60	0.59
1:B:655:MET:SD	1:B:657:MET:HG2	2.43	0.57
1:C:655:MET:HE1	1:C:657:MET:HG3	1.90	0.54
1:D:629:ALA:HB2	1:D:659:MET:HE3	1.88	0.54
1:C:523:MET:HE1	1:C:530:VAL:HG23	1.89	0.53
1:C:774:SER:HA	1:C:799:SER:O	2.08	0.53
1:D:781:MET:HE2	1:D:793:ILE:HD12	1.92	0.51
1:C:487:THR:HG23	1:C:490:ARG:HB2	1.92	0.51
1:B:555:MET:CE	1:B:563:VAL:HA	2.41	0.51
1:A:590:ARG:NH2	1:A:657:MET:HE3	2.27	0.49
1:B:655:MET:HE1	1:B:657:MET:HG3	1.95	0.49
1:D:606:LYS:NZ	1:D:610:GLU:OE2	2.43	0.49
2:C:4:882:H133	2:C:4:882:O1	2.12	0.49
1:C:731:VAL:HG12	1:C:854:MET:HE1	1.95	0.48
1:B:606:LYS:NZ	1:B:610:GLU:OE2	2.47	0.47
1:A:796:THR:HG21	1:D:638:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:TYR:CD1	1:B:535:PRO:HB3	2.49	0.47
1:B:700:GLU:OE2	1:C:700:GLU:OE2	2.33	0.46
1:A:596:LEU:HB3	1:A:601:ASP:HB2	1.98	0.46
1:B:592:PRO:HD2	1:B:645:ILE:O	2.15	0.46
1:B:555:MET:HE1	1:B:563:VAL:HA	1.97	0.46
1:C:470:LEU:O	1:C:473:ALA:O	2.34	0.45
1:A:541:ALA:HA	1:A:567:ASN:HD22	1.82	0.45
1:A:542:GLY:H	1:A:567:ASN:ND2	2.13	0.45
1:C:719:GLU:O	1:C:722:LYS:NZ	2.48	0.45
1:C:651:SER:HA	1:C:659:MET:HE3	1.98	0.44
1:C:820:MET:HE3	1:D:499:LEU:HD21	1.98	0.44
1:B:774:SER:HA	1:B:799:SER:O	2.18	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.17	0.43
1:D:588:MET:HB3	1:D:660:ILE:HD13	2.00	0.43
1:B:817:CYS:HA	1:B:820:MET:HE3	2.01	0.43
1:C:754:ALA:HB1	1:C:771:ASN:HD21	1.84	0.42
1:A:590:ARG:NH2	1:A:657:MET:CE	2.82	0.42
1:A:808:GLY:O	1:A:814:GLN:HG3	2.18	0.42
1:C:531:ILE:HD13	1:D:540:VAL:CG2	2.50	0.42
2:D:3:882:H133	2:D:3:882:O1	2.20	0.41
1:A:637:SER:HB2	1:A:687:TYR:OH	2.20	0.41
1:C:560:GLY:O	1:C:561:CYS:HB2	2.21	0.41
1:D:702:ARG:O	1:D:799:SER:HA	2.20	0.41
1:A:702:ARG:O	1:A:799:SER:HA	2.21	0.41
1:C:593:VAL:HG13	1:C:681:LEU:HB3	2.03	0.41
1:A:655:MET:HE1	1:A:657:MET:HG3	2.03	0.41
2:A:2:882:H133	2:A:2:882:O1	2.22	0.40
1:B:838:LEU:O	1:B:842:VAL:HG23	2.22	0.40
1:C:756:ILE:HD12	1:C:756:ILE:N	2.36	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	388/441 (88%)	374 (96%)	13 (3%)	1 (0%)	36	30
1	B	397/441 (90%)	381 (96%)	15 (4%)	1 (0%)	36	30
1	C	412/441 (93%)	391 (95%)	20 (5%)	1 (0%)	43	37
1	D	390/441 (88%)	375 (96%)	15 (4%)	0	100	100
All	All	1587/1764 (90%)	1521 (96%)	63 (4%)	3 (0%)	43	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	ASN
1	B	525	ALA
1	A	860	GLY

### 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	310/355 (87%)	297 (96%)	13 (4%)	26	20
1	B	318/355 (90%)	305 (96%)	13 (4%)	27	21
1	C	330/355 (93%)	317 (96%)	13 (4%)	28	23
1	D	312/355 (88%)	301 (96%)	11 (4%)	32	27
All	All	1270/1420 (89%)	1220 (96%)	50 (4%)	28	23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	A	485	ILE
1	A	486	GLU
1	A	498	LEU
1	A	512	LEU
1	A	540	VAL
1	A	630	ARG
1	A	634	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	704	LYS
1	A	788	ASN
1	A	802	ILE
1	A	814	GLN
1	A	851	LEU
1	B	470	LEU
1	B	482	GLU
1	B	505	GLU
1	B	523	MET
1	B	540	VAL
1	B	613	GLU
1	B	634	LEU
1	B	662	LYS
1	B	669	SER
1	B	746	ILE
1	B	756	ILE
1	B	771	ASN
1	B	828	LYS
1	C	445	ASN
1	C	452	LEU
1	C	460	LYS
1	C	470	LEU
1	C	476	ILE
1	C	487	THR
1	C	505	GLU
1	C	523	MET
1	C	657	MET
1	C	660	ILE
1	C	662	LYS
1	C	681	LEU
1	C	725	THR
1	D	470	LEU
1	D	501	LYS
1	D	613	GLU
1	D	657	MET
1	D	659	MET
1	D	660	ILE
1	D	688	CYS
1	D	788	ASN
1	D	791	LEU
1	D	802	ILE
1	D	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	567	ASN
1	A	635	HIS
1	A	732	ASN
1	A	736	ASN
1	A	788	ASN
1	A	861	HIS
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	632	GLN
1	C	469	GLN
1	C	472	ASN
1	C	488	HIS
1	C	497	GLN
1	C	679	GLN
1	C	819	GLN
1	D	472	ASN
1	D	488	HIS
1	D	518	ASN
1	D	632	GLN
1	D	770	GLN
1	D	788	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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	882	A	2	-	45,45,45	0.85	2 (4%)	53,63,63	1.63	8 (15%)
2	882	D	3	-	45,45,45	0.88	2 (4%)	53,63,63	1.85	8 (15%)
2	882	A	1	-	45,45,45	0.82	2 (4%)	53,63,63	1.84	9 (16%)
2	882	C	4	-	45,45,45	0.82	2 (4%)	53,63,63	1.73	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	882	A	2	-	-	5/33/33/33	0/4/4/4
2	882	D	3	-	-	3/33/33/33	0/4/4/4
2	882	A	1	-	-	6/33/33/33	0/4/4/4
2	882	C	4	-	-	5/33/33/33	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	882	C1-C5	-2.33	1.36	1.46
2	D	3	882	C1-C5	-2.26	1.36	1.46
2	A	2	882	C1-C5	-2.19	1.36	1.46
2	C	4	882	C1-C5	-2.14	1.36	1.46
2	D	3	882	C2-N1	-2.08	1.36	1.41
2	A	1	882	C2-N1	-2.08	1.36	1.41
2	A	2	882	C2-N1	-2.03	1.36	1.41
2	C	4	882	C2-N1	-2.01	1.36	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	882	C3-C2-N1	6.87	129.91	122.33
2	D	3	882	C3-C2-N1	6.60	129.62	122.33
2	A	2	882	C3-C2-N1	6.10	129.06	122.33
2	C	4	882	C3-C2-N1	5.90	128.84	122.33
2	D	3	882	C2-C3-N2	5.05	122.14	115.32
2	A	1	882	C2-C3-N2	4.92	121.96	115.32
2	C	4	882	C2-C3-N2	4.61	121.54	115.32
2	A	2	882	C2-C3-N2	4.23	121.03	115.32
2	D	3	882	C21-C27-C5	-4.17	114.23	120.79
2	A	1	882	O1-C3-C2	-3.77	114.62	121.96
2	C	4	882	C32-N2-C3	-3.74	120.81	127.45
2	D	3	882	O1-C3-C2	-3.53	115.09	121.96
2	C	4	882	O1-C3-C2	-3.31	115.52	121.96
2	C	4	882	C21-C27-C5	-3.26	115.66	120.79
2	A	2	882	C21-C27-C5	-3.25	115.68	120.79
2	A	1	882	C32-N2-C3	-3.24	121.70	127.45
2	D	3	882	C18-C27-C5	3.17	125.78	120.79
2	A	1	882	C21-C27-C5	-3.15	115.83	120.79
2	A	2	882	O1-C3-C2	-3.03	116.05	121.96
2	D	3	882	C9-C10-C11	-2.87	109.74	114.28
2	A	1	882	C7-C8-C9	-2.83	108.23	113.58
2	D	3	882	C7-C8-C9	-2.59	108.69	113.58
2	A	2	882	C32-N2-C3	-2.59	122.86	127.45
2	A	1	882	C14-C6-N1	-2.46	108.25	111.69
2	D	3	882	C32-N2-C3	-2.45	123.11	127.45
2	A	1	882	C9-C10-C11	-2.40	110.48	114.28
2	C	4	882	C18-C27-C5	2.38	124.53	120.79
2	C	4	882	C7-C8-C9	-2.37	109.10	113.58
2	A	2	882	C19-C28-C22	-2.34	119.73	122.80
2	C	4	882	C19-C28-C22	-2.17	119.95	122.80
2	A	2	882	C25-C22-C28	2.14	120.58	118.38
2	A	1	882	C18-C15-C30	2.08	120.51	118.38
2	A	2	882	C18-C27-C5	2.06	124.02	120.79

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	882	C7-C8-C9-O4
2	C	4	882	C7-C8-C9-O4
2	A	2	882	C7-C8-C9-C10
2	C	4	882	C7-C8-C9-C10
2	D	3	882	C7-C8-C9-O4

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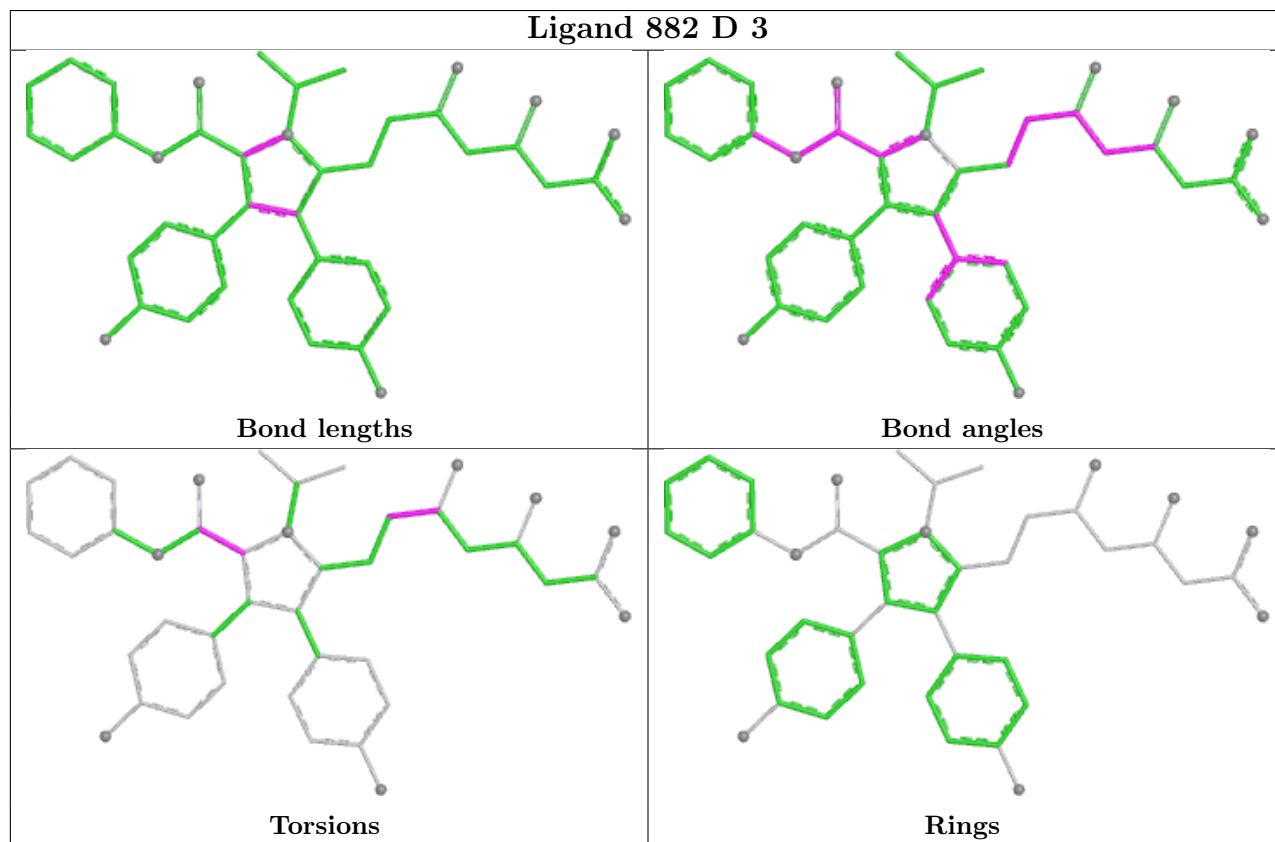
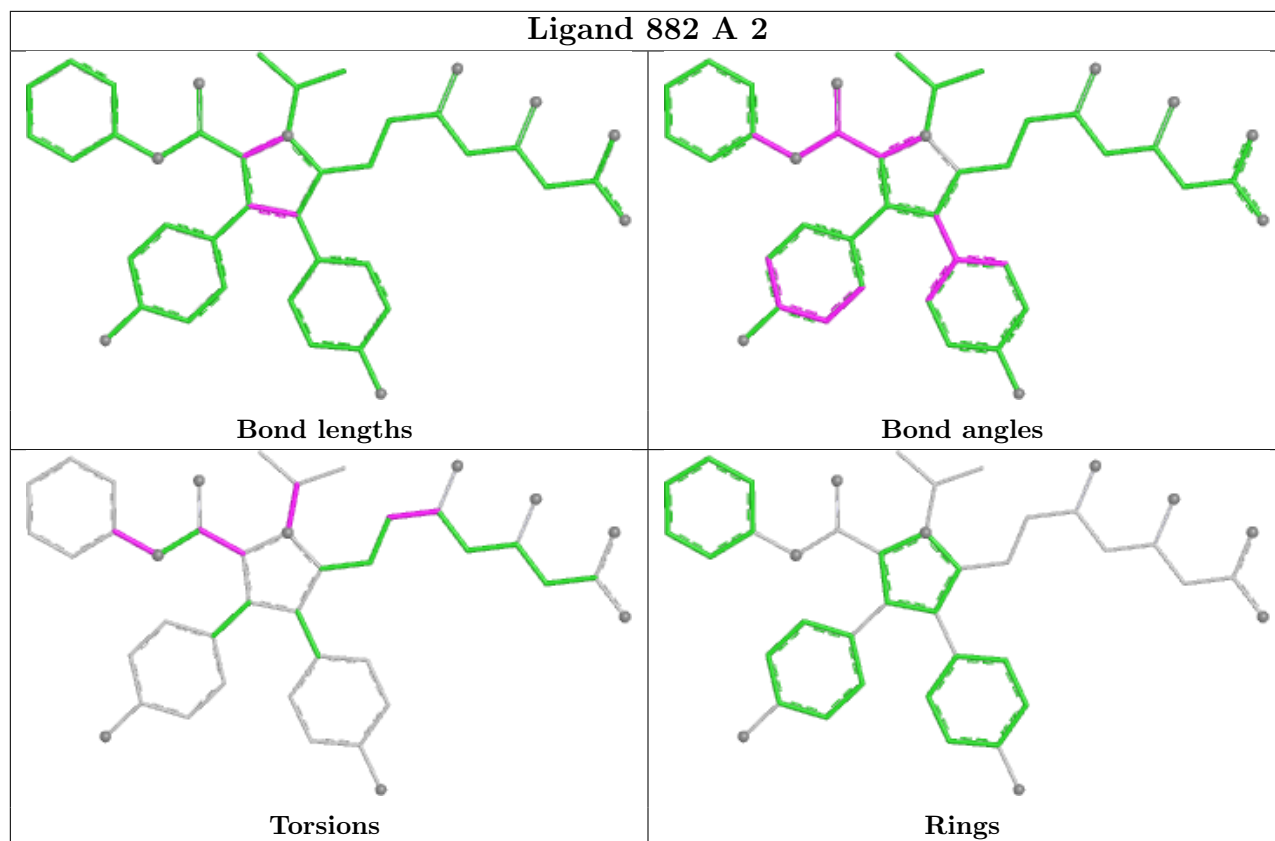
Mol	Chain	Res	Type	Atoms
2	A	1	882	C7-C8-C9-O4
2	A	1	882	N1-C2-C3-O1
2	A	1	882	N1-C2-C3-N2
2	A	2	882	N1-C2-C3-N2
2	C	4	882	N1-C2-C3-N2
2	D	3	882	N1-C2-C3-N2
2	A	1	882	C7-C8-C9-C10
2	D	3	882	C7-C8-C9-C10
2	C	4	882	C26-C32-N2-C3
2	C	4	882	C17-C32-N2-C3
2	A	1	882	C1-C2-C3-N2
2	A	2	882	C14-C6-N1-C4
2	A	2	882	C26-C32-N2-C3
2	A	1	882	C4-C7-C8-C9

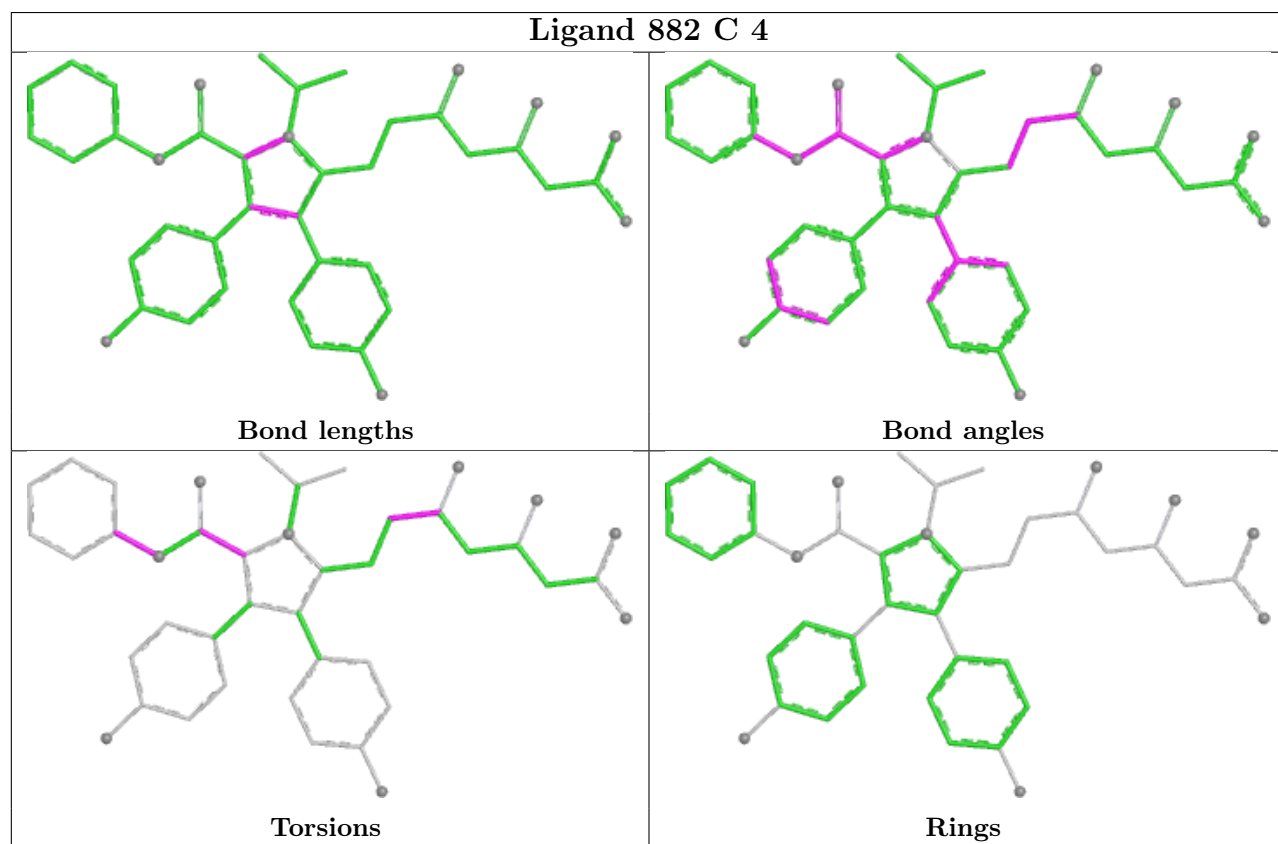
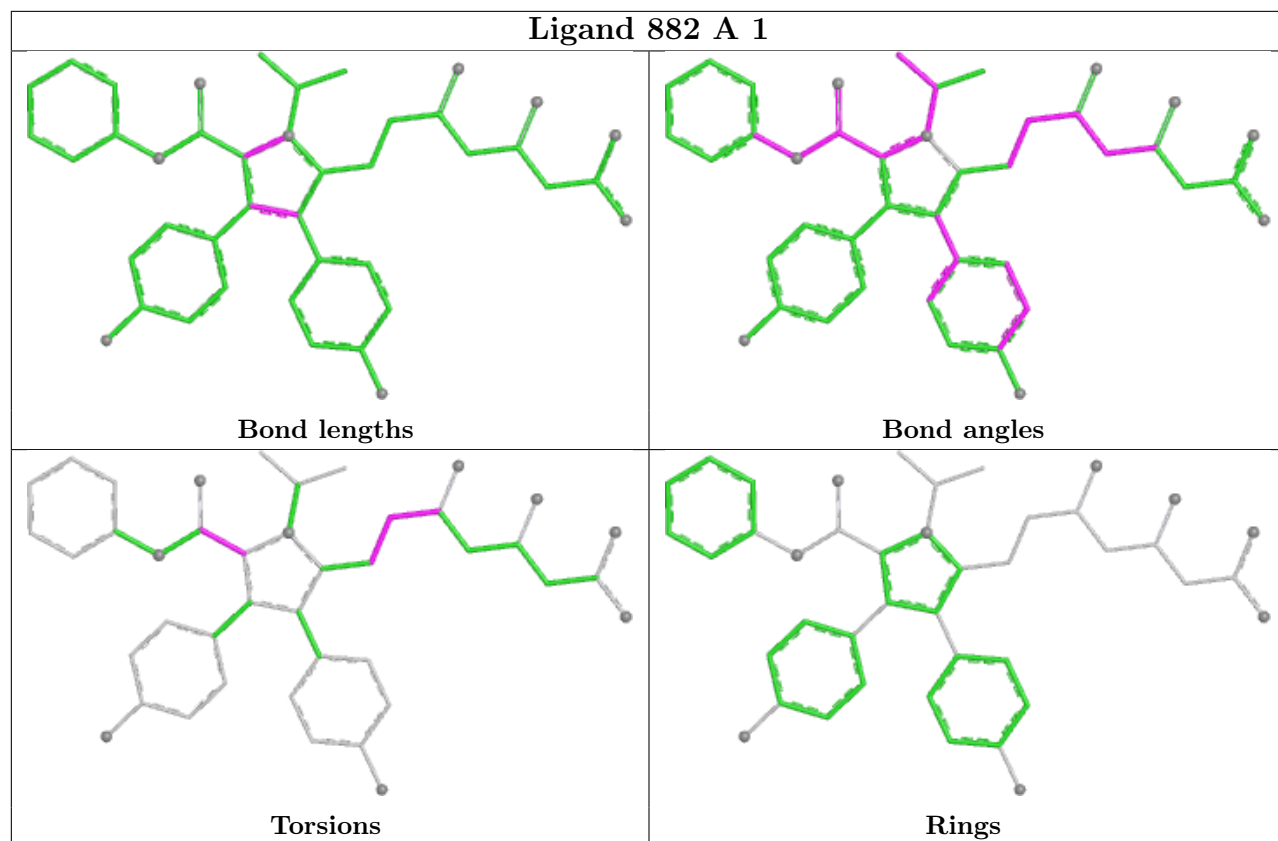
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	882	1	0
2	D	3	882	1	0
2	C	4	882	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	392/441 (88%)	0.38	17 (4%) 40 40	22, 32, 55, 70	0
1	B	401/441 (90%)	0.62	40 (9%) 12 12	22, 37, 71, 89	0
1	C	416/441 (94%)	0.31	26 (6%) 26 26	19, 31, 60, 85	0
1	D	394/441 (89%)	0.29	21 (5%) 32 32	19, 31, 53, 90	0
All	All	1603/1764 (90%)	0.40	104 (6%) 25 24	19, 33, 58, 90	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	GLY	5.7
1	B	479	TYR	5.5
1	B	478	ALA	5.0
1	B	861	HIS	5.0
1	B	473	ALA	4.9
1	C	444	PRO	4.8
1	A	860	GLY	4.7
1	D	475	HIS	4.4
1	D	470	LEU	4.4
1	B	485	ILE	4.4
1	D	461	PHE	4.3
1	B	476	ILE	4.1
1	C	458	GLY	4.0
1	A	861	HIS	3.9
1	A	486	GLU	3.9
1	A	461	PHE	3.8
1	B	461	PHE	3.8
1	B	481	LEU	3.6
1	A	470	LEU	3.6
1	D	849	GLY	3.5
1	B	525	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	477	PRO	3.4
1	C	598	ARG	3.3
1	A	473	ALA	3.3
1	B	475	HIS	3.3
1	A	469	GLN	3.2
1	B	465	ALA	3.2
1	C	451	ILE	3.2
1	B	483	THR	3.2
1	D	859	ALA	3.1
1	A	859	ALA	3.1
1	D	468	ILE	3.1
1	C	829	ASP	3.0
1	B	488	HIS	3.0
1	C	449	LEU	3.0
1	B	522	VAL	2.9
1	C	679	GLN	2.9
1	C	860	GLY	2.9
1	B	829	ASP	2.8
1	D	718	ARG	2.8
1	C	485	ILE	2.8
1	C	455	ALA	2.7
1	B	469	GLN	2.6
1	A	525	ALA	2.6
1	A	462	LEU	2.6
1	C	473	ALA	2.6
1	C	524	GLY	2.6
1	C	617	VAL	2.6
1	C	447	GLU	2.6
1	B	503	LEU	2.5
1	B	514	TYR	2.5
1	B	786	PRO	2.5
1	B	484	LEU	2.5
1	C	456	GLU	2.4
1	C	859	ALA	2.4
1	C	448	CYS	2.4
1	A	717	VAL	2.4
1	D	474	LYS	2.4
1	D	505	GLU	2.3
1	D	462	LEU	2.3
1	B	470	LEU	2.3
1	D	484	LEU	2.3
1	A	463	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	628	PHE	2.3
1	D	679	GLN	2.3
1	B	803	GLY	2.3
1	A	504	SER	2.2
1	A	786	PRO	2.2
1	C	822	GLY	2.2
1	B	463	SER	2.2
1	B	460	LYS	2.2
1	C	479	TYR	2.2
1	C	445	ASN	2.2
1	A	485	ILE	2.2
1	B	467	ILE	2.2
1	C	450	GLN	2.2
1	D	564	ALA	2.2
1	B	517	TYR	2.2
1	D	472	ASN	2.2
1	C	487	THR	2.2
1	B	466	GLU	2.1
1	B	468	ILE	2.1
1	C	461	PHE	2.1
1	C	677	GLU	2.1
1	D	471	VAL	2.1
1	D	458	GLY	2.1
1	C	475	HIS	2.1
1	D	473	ALA	2.1
1	A	598	ARG	2.1
1	D	486	GLU	2.1
1	B	721	LEU	2.1
1	B	548	GLU	2.1
1	B	577	GLY	2.1
1	B	480	LYS	2.1
1	D	628	PHE	2.1
1	A	465	ALA	2.1
1	D	858	ALA	2.1
1	B	512	LEU	2.0
1	B	526	CYS	2.0
1	B	515	ARG	2.0
1	C	718	ARG	2.0
1	B	624	SER	2.0
1	B	462	LEU	2.0
1	D	662	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

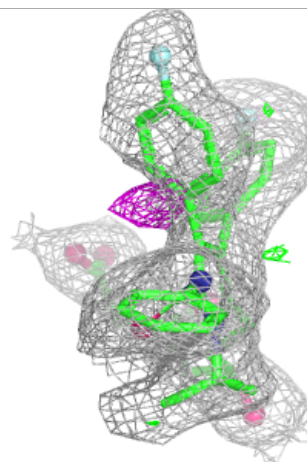
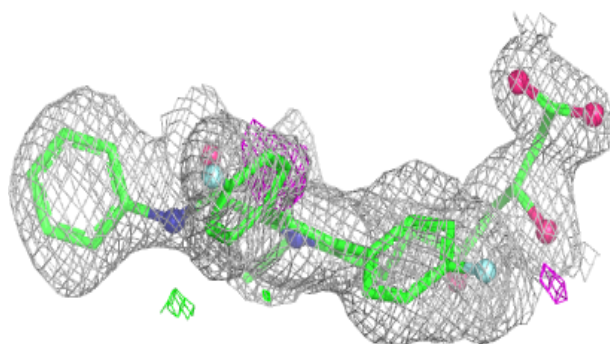
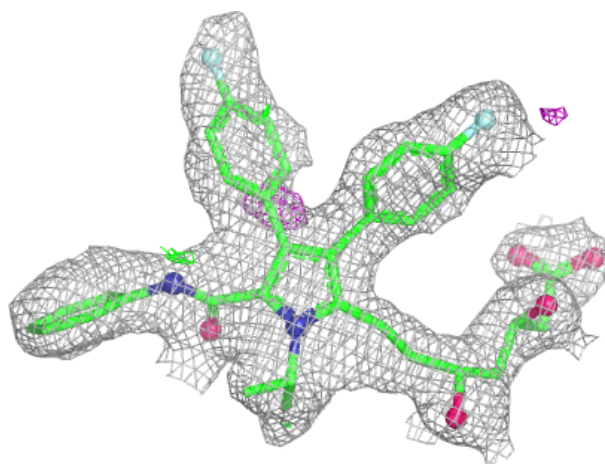
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	882	C	4	42/42	0.90	0.09	27,35,37,38	0
2	882	A	2	42/42	0.91	0.08	25,31,35,39	0
2	882	A	1	42/42	0.91	0.09	24,35,41,44	0
2	882	D	3	42/42	0.94	0.08	21,27,32,32	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.

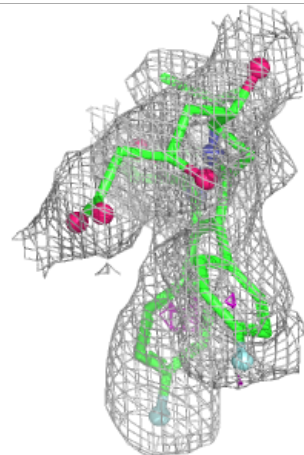
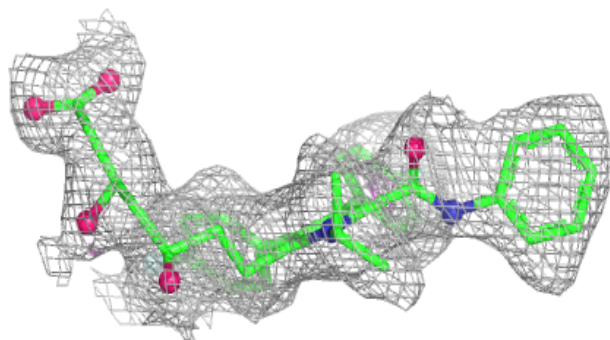
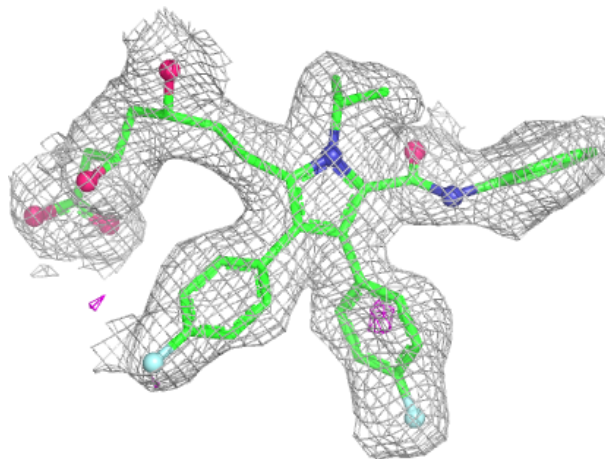
**Electron density around 882 C 4:**

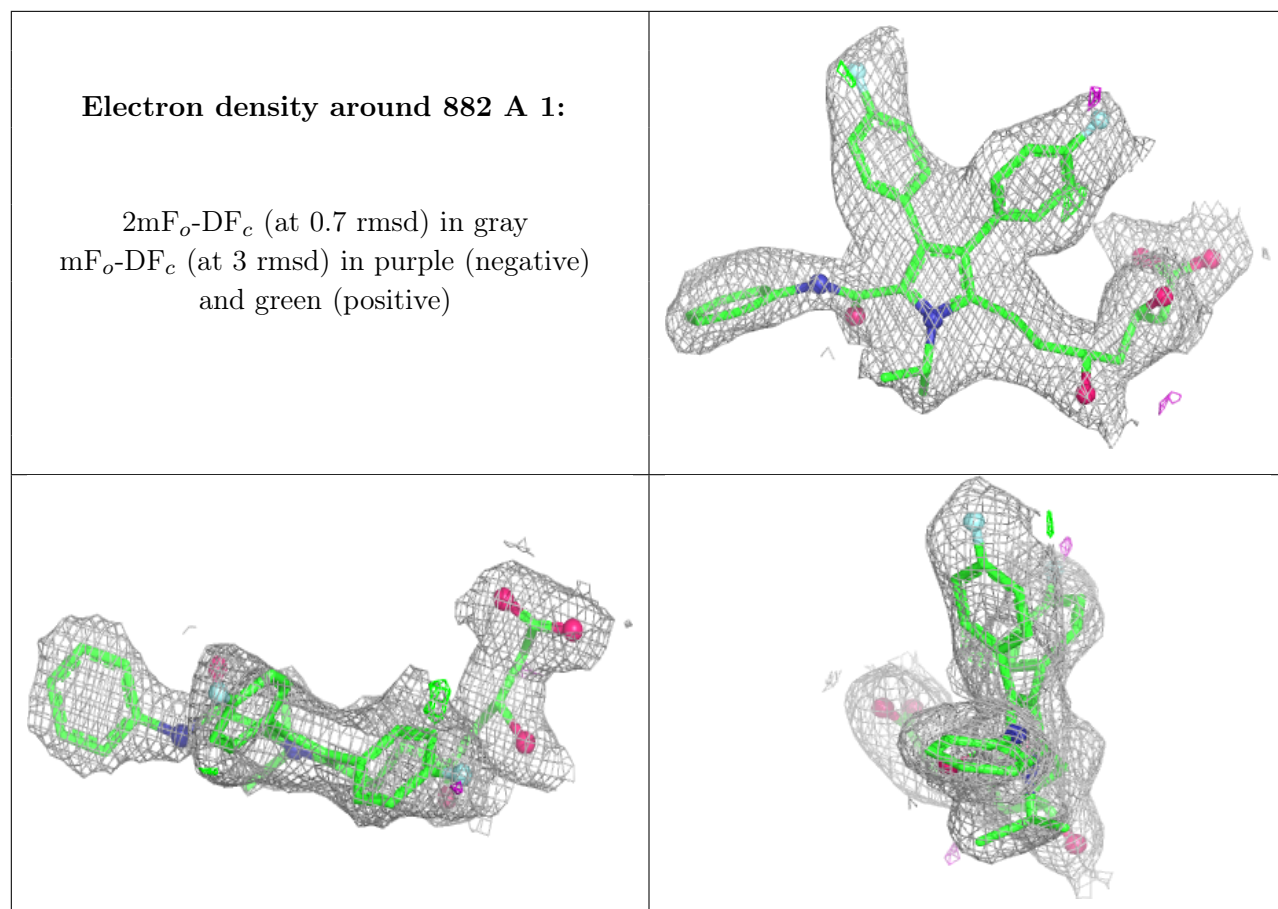
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

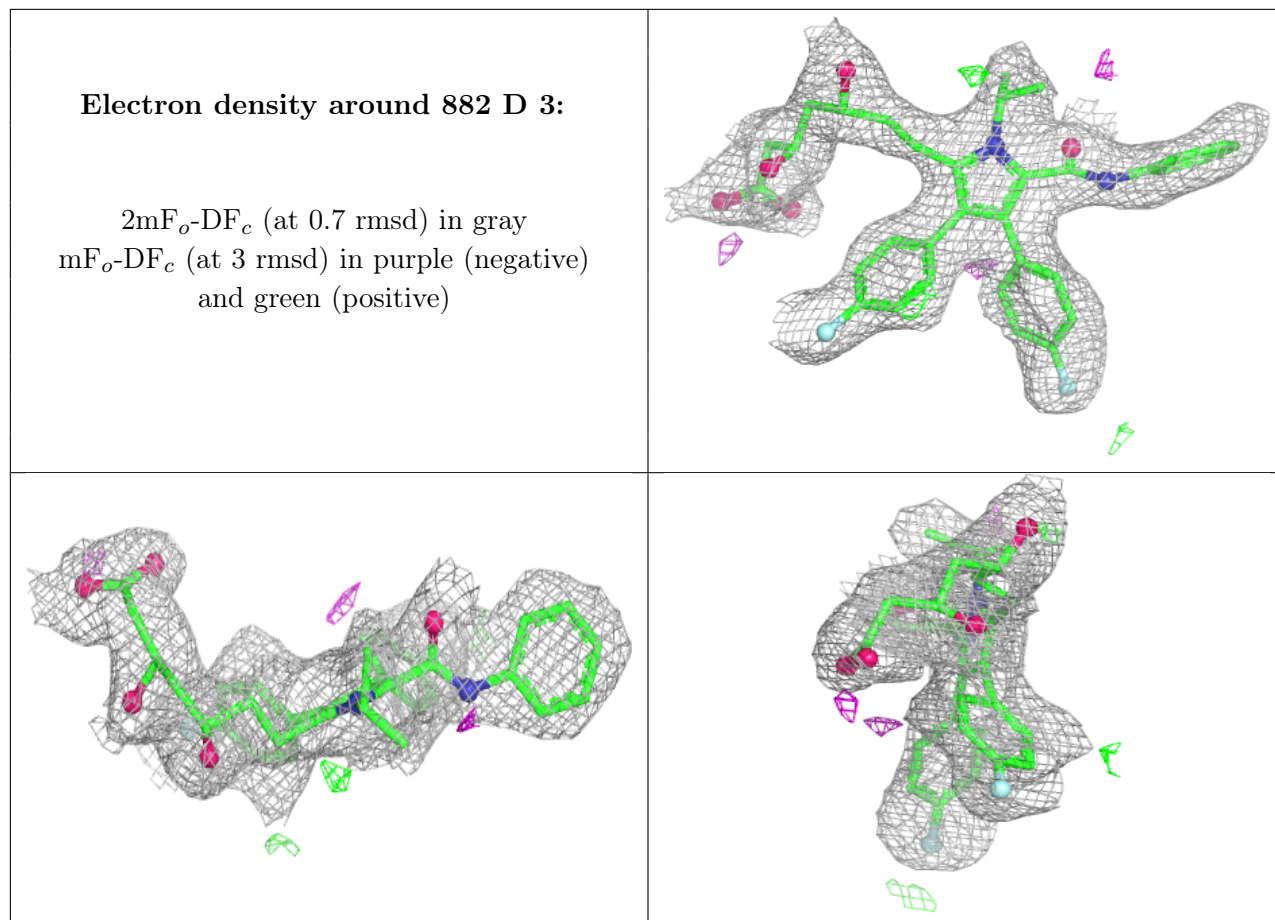


**Electron density around 882 A 2:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.