



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:21 am BST

PDB ID : 3LU6  
Title : Human serum albumin in complex with compound 1  
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Deposited on : 2010-02-17  
Resolution : 2.70 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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

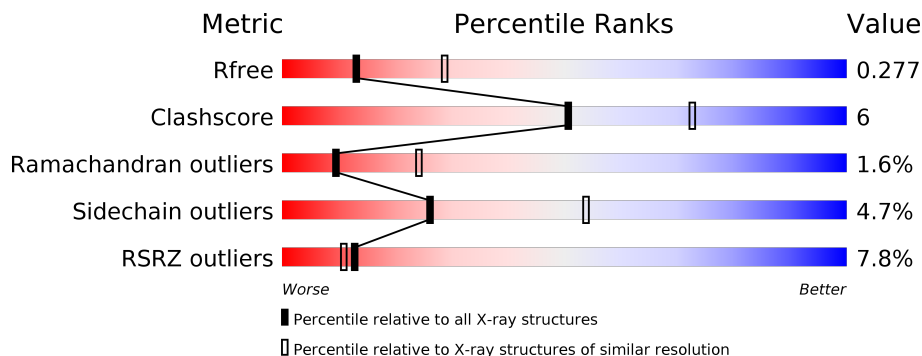
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	585	
1	B	585	

## 2 Entry composition [i](#)

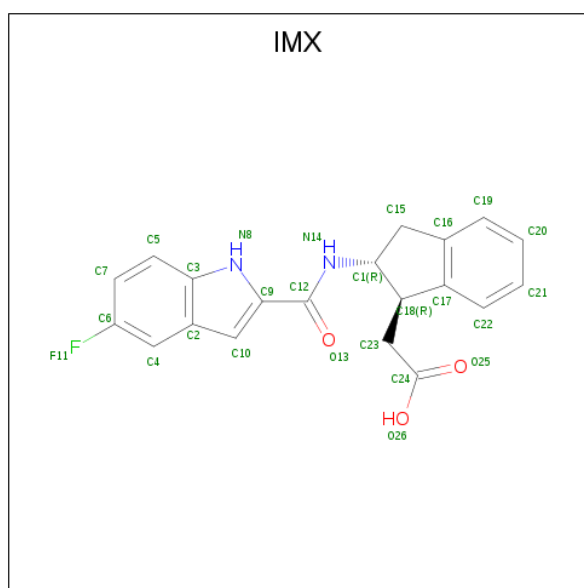
There are 3 unique types of molecules in this entry. The entry contains 9322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			
1	B	578	Total	C	N	O	S	0	1	0
			4605	2907	777	880	41			

- Molecule 2 is [(1R,2R)-2-[(5-fluoro-1H-indol-2-yl)carbonyl]amino]-2,3-dihydro-1H-inden-1-yl]acetic acid (three-letter code: IMX) (formula: C<sub>20</sub>H<sub>17</sub>FN<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total	C	F	N	O	0	0
			26	20	1	2	3		
2	A	1	Total	C	F	N	O	0	0
			26	20	1	2	3		
2	B	1	Total	C	F	N	O	0	0
			26	20	1	2	3		
2	B	1	Total	C	F	N	O	0	0
			26	20	1	2	3		

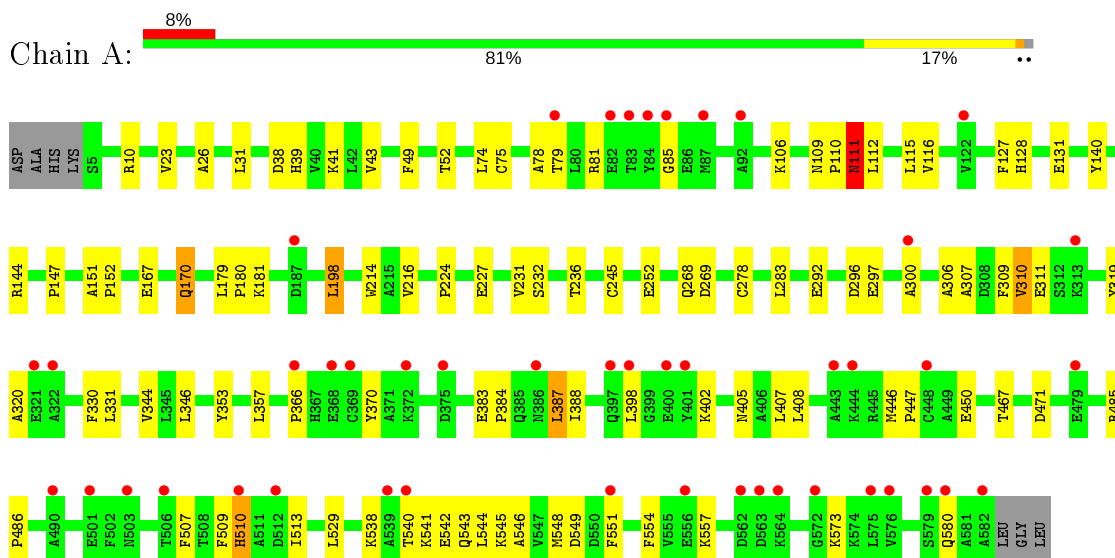
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	A	6	Total O 6 6	0	0
3	B	8	Total O 8 8	0	0

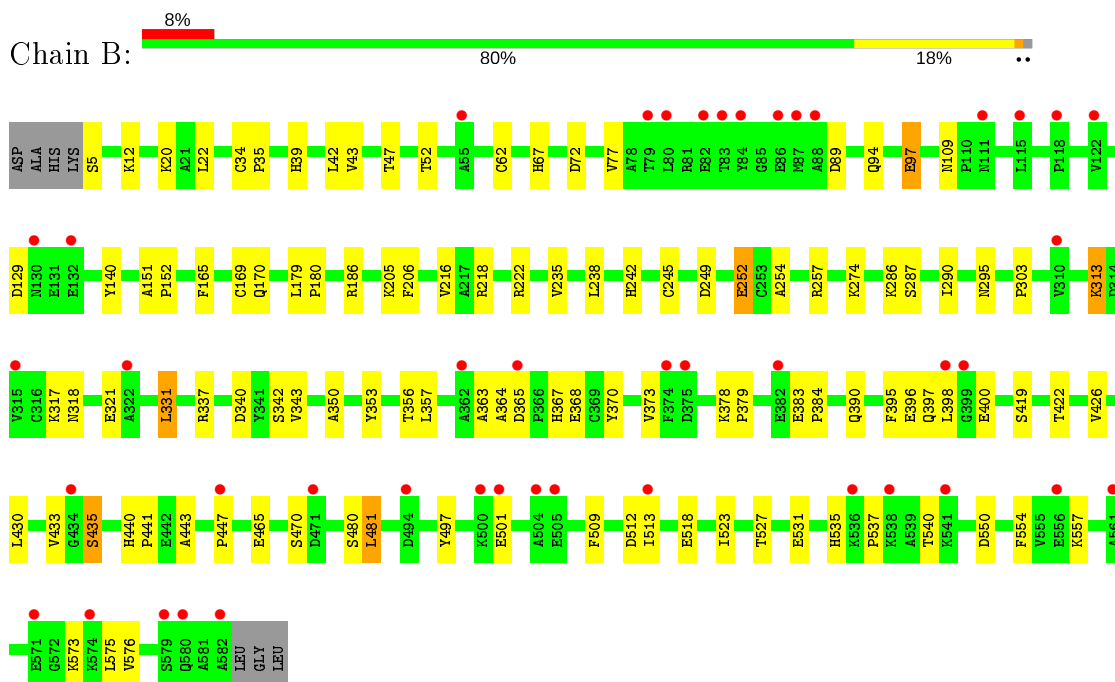
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serum albumin



- Molecule 1: Serum albumin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.56Å 59.87Å 95.57Å 74.51° 86.57° 74.47°	Depositor
Resolution (Å)	55.64 – 2.70 55.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.64-2.70) 81.4 (55.68-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.236 , 0.275 0.235 , 0.277	Depositor DCC
$R_{free}$ test set	1479 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.075 for -h,-k,-k+1	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: IMX

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	0.49	0/4688	0.58	0/6324
1	B	0.47	0/4697	0.59	0/6336
All	All	0.48	0/9385	0.58	0/12660

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	363	ALA	Peptide

### 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	4599	0	4518	49	0
1	B	4605	0	4526	56	0
2	A	52	0	32	2	0
2	B	52	0	32	3	0
3	A	6	0	0	0	0
3	B	8	0	0	1	0
All	All	9322	0	9108	104	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 6.

All (104) 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:320:ALA:O	1:B:364:ALA:HB2	1.84	0.78
1:A:320:ALA:O	1:B:364:ALA:CB	2.43	0.65
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.77	0.65
1:B:430:LEU:O	1:B:433:VAL:HG12	2.00	0.62
1:B:317:LYS:NZ	1:B:321:GLU:OE2	2.32	0.60
1:B:370:TYR:O	1:B:373:VAL:HG23	2.03	0.58
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.86	0.57
1:A:75:CYS:O	1:A:79:THR:OG1	2.20	0.57
1:B:342:SER:CB	1:B:447:PRO:HA	2.35	0.56
1:B:573:LYS:O	1:B:576:VAL:HG22	2.07	0.55
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.89	0.54
1:B:12:LYS:NZ	3:B:594:HOH:O	2.39	0.54
1:B:353:TYR:CE2	1:B:357:LEU:HD11	2.43	0.53
1:B:422:THR:O	1:B:426:VAL:HG23	2.08	0.53
1:B:206:PHE:CE2	1:B:481:LEU:HB2	2.44	0.53
1:A:402:LYS:HA	1:A:405:ASN:HD22	1.73	0.53
1:B:317:LYS:HG2	1:B:321:GLU:OE2	2.09	0.53
1:A:127:PHE:O	1:A:131:GLU:HB3	2.08	0.52
1:A:81:ARG:HB2	1:A:85:GLY:HA2	1.92	0.52
1:B:5:SER:HA	1:B:62:CYS:O	2.09	0.52
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.93	0.51
1:A:510:HIS:O	1:A:513:ILE:HG22	2.11	0.51
1:B:353:TYR:CZ	1:B:357:LEU:HD11	2.46	0.51
1:A:306:ALA:O	1:A:310:VAL:N	2.44	0.50
1:A:546:ALA:O	1:A:549:ASP:HB2	2.12	0.50
1:A:140:TYR:CZ	1:A:144:ARG:HD2	2.47	0.50
1:A:319:TYR:CD1	1:A:357:LEU:HD12	2.48	0.49
1:B:440:HIS:HB3	1:B:441:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.95	0.49
1:B:242:HIS:HE2	2:B:586:IMX:C24	2.26	0.48
1:B:67:HIS:CE1	1:B:249:ASP:OD1	2.66	0.48
1:B:216:VAL:HG21	2:B:587:IMX:C4	2.43	0.48
1:A:111:ASN:N	1:A:111:ASN:OD1	2.44	0.48
1:B:34:CYS:SG	1:B:77:VAL:HG11	2.53	0.48
1:B:342:SER:HB2	1:B:447:PRO:HA	1.96	0.48
1:A:296:ASP:OD1	1:A:297:GLU:N	2.47	0.48
1:B:550:ASP:O	1:B:554:PHE:HB3	2.14	0.47
1:B:531:GLU:O	1:B:535:HIS:ND1	2.48	0.47
1:A:198:LEU:HD22	2:A:586:IMX:F11	2.05	0.47
1:B:317:LYS:CG	1:B:321:GLU:OE2	2.63	0.47
1:B:303:PRO:O	1:B:337:ARG:NH1	2.48	0.47
1:B:523:ILE:O	1:B:527:THR:OG1	2.31	0.46
1:A:542:GLU:O	1:A:544:LEU:N	2.48	0.46
1:A:179:LEU:N	1:A:180:PRO:HD2	2.30	0.46
1:A:214:TRP:CH2	1:A:344:VAL:HG12	2.50	0.46
1:B:42:LEU:HD11	1:B:77:VAL:HG21	1.98	0.45
1:B:35:PRO:HA	1:B:140:TYR:OH	2.16	0.45
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.98	0.45
1:A:106:LYS:NZ	1:A:147:PRO:O	2.43	0.45
1:B:365:ASP:HB3	1:B:368:GLU:HB3	1.97	0.45
1:A:529:LEU:HB2	1:A:548:MET:SD	2.56	0.45
1:A:110:PRO:O	1:A:112:LEU:N	2.50	0.45
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.99	0.45
1:B:512:ASP:OD1	1:B:513:ILE:N	2.50	0.45
1:A:344:VAL:CG2	1:A:450:GLU:HG3	2.47	0.44
1:B:400:GLU:OE1	1:B:435:SER:OG	2.34	0.44
1:A:140:TYR:CE2	1:A:144:ARG:HD2	2.52	0.44
1:A:353:TYR:CE2	1:A:357:LEU:HD11	2.52	0.44
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.83	0.44
1:A:388:ILE:HG13	1:A:446:MET:HA	2.00	0.44
1:B:331:LEU:HD13	1:B:350:ALA:HB2	2.00	0.44
1:B:554:PHE:CD1	1:B:575:LEU:HD11	2.53	0.44
1:B:252:GLU:OE1	1:B:252:GLU:N	2.51	0.44
1:A:31:LEU:HD12	1:A:74:LEU:HD22	2.01	0.43
2:A:587:IMX:O13	2:A:587:IMX:H15A	2.18	0.43
1:A:38:ASP:O	1:A:41:LYS:HB3	2.18	0.43
1:A:446:MET:SD	1:A:446:MET:C	2.97	0.43
1:B:365:ASP:OD2	1:B:368:GLU:HB2	2.18	0.43
1:B:22:LEU:HD11	1:B:254:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:HA	1:A:408:LEU:HD12	2.00	0.42
1:B:238:LEU:HD11	2:B:586:IMX:C24	2.49	0.42
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.01	0.42
1:B:39:HIS:O	1:B:43:VAL:HG23	2.20	0.42
1:B:557:LYS:HB2	1:B:557:LYS:NZ	2.35	0.42
1:A:167:GLU:OE1	1:A:181:LYS:NZ	2.53	0.42
1:A:49:PHE:O	1:A:52:THR:OG1	2.30	0.42
1:A:507:PHE:HB3	1:A:551:PHE:CZ	2.54	0.42
1:A:10:ARG:NH2	1:A:252:GLU:HB3	2.35	0.42
1:A:23:VAL:O	1:A:26:ALA:HB3	2.20	0.42
1:B:151:ALA:HB3	1:B:152:PRO:HD3	2.01	0.42
1:B:313:LYS:HA	1:B:367:HIS:NE2	2.35	0.42
1:A:10:ARG:CZ	1:A:252:GLU:HB3	2.50	0.41
1:B:378:LYS:N	1:B:379:PRO:HD2	2.35	0.41
1:B:94:GLN:O	1:B:97:GLU:HB2	2.20	0.41
1:A:309:PHE:CZ	1:A:330:PHE:HA	2.55	0.41
1:B:218:ARG:HD3	1:B:343:VAL:HG21	2.02	0.41
1:A:39:HIS:O	1:A:43:VAL:HG23	2.21	0.41
1:A:307:ALA:HA	1:A:311:GLU:HB2	2.02	0.41
1:B:395:PHE:C	1:B:397:GLN:H	2.23	0.41
1:B:205:LYS:NZ	1:B:465:GLU:OE2	2.45	0.41
1:A:485:ARG:N	1:A:486:PRO:CD	2.82	0.41
1:B:340:ASP:O	1:B:447:PRO:CG	2.69	0.41
1:B:20:LYS:CE	1:B:47:THR:HG21	2.51	0.41
1:A:227:GLU:O	1:A:231:VAL:HG23	2.20	0.41
1:A:509:PHE:N	1:A:509:PHE:CD1	2.88	0.41
1:B:165:PHE:O	1:B:169:CYS:SG	2.79	0.41
1:B:222:ARG:HG3	1:B:295:ASN:HA	2.02	0.41
1:B:257:ARG:CZ	1:B:287:SER:HB3	2.51	0.41
1:A:545:LYS:O	1:A:549:ASP:N	2.43	0.41
1:B:342:SER:HB3	1:B:447:PRO:HA	2.03	0.41
1:A:387:LEU:HD23	1:A:388:ILE:HD13	2.03	0.40
1:A:446:MET:N	1:A:447:PRO:HD2	2.37	0.40
1:B:286:LYS:HG3	1:B:290:ILE:HD12	2.02	0.40
1:B:378:LYS:N	1:B:379:PRO:CD	2.84	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	576/585 (98%)	514 (89%)	53 (9%)	9 (2%)	9	24
1	B	577/585 (99%)	512 (89%)	56 (10%)	9 (2%)	9	24
All	All	1153/1170 (98%)	1026 (89%)	109 (10%)	18 (2%)	9	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ALA
1	A	538	LYS
1	A	543	GLN
1	B	501	GLU
1	A	111	ASN
1	A	283	LEU
1	B	537	PRO
1	A	310	VAL
1	A	541	LYS
1	B	398	LEU
1	B	481	LEU
1	A	116	VAL
1	B	129	ASP
1	B	396	GLU
1	B	443	ALA
1	B	497	TYR
1	B	480	SER
1	A	366	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	506/511 (99%)	479 (95%)	27 (5%)	22	48
1	B	507/511 (99%)	486 (96%)	21 (4%)	30	59
All	All	1013/1022 (99%)	965 (95%)	48 (5%)	26	54

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	111	ASN
1	A	115	LEU
1	A	128	HIS
1	A	170	GLN
1	A	198	LEU
1	A	216	VAL
1	A	232	SER
1	A	236	THR
1	A	245	CYS
1	A	268	GLN
1	A	269	ASP
1	A	278	CYS
1	A	292	GLU
1	A	331	LEU
1	A	346	LEU
1	A	370	TYR
1	A	387	LEU
1	A	407	LEU
1	A	467	THR
1	A	471	ASP
1	A	510	HIS
1	A	540	THR
1	A	554	PHE
1	A	557	LYS
1	A	573	LYS
1	A	580	GLN
1	B	52	THR
1	B	72	ASP
1	B	89	ASP
1	B	97	GLU
1	B	109	ASN
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	186	ARG
1	B	245	CYS
1	B	252	GLU
1	B	274	LYS
1	B	313	LYS
1	B	318	ASN
1	B	331	LEU
1	B	356	THR
1	B	390	GLN
1	B	419	SER
1	B	435	SER
1	B	470	SER
1	B	509	PHE
1	B	518	GLU
1	B	540	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	44	ASN
1	A	109	ASN
1	A	170	GLN
1	A	196	GLN
1	A	386	ASN
1	A	391	ASN
1	A	405	ASN
1	A	483	ASN
1	A	580	GLN
1	B	67	HIS
1	B	94	GLN
1	B	99	ASN
1	B	104	GLN
1	B	109	ASN
1	B	196	GLN
1	B	386	ASN
1	B	391	ASN
1	B	464	HIS
1	B	483	ASN
1	B	522	GLN
1	B	543	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 carbohydrates 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	IMX	A	587	-	23,29,29	1.32	2 (8%)	28,42,42	1.81	8 (28%)
2	IMX	B	586	-	23,29,29	1.23	1 (4%)	28,42,42	1.16	1 (3%)
2	IMX	A	586	-	23,29,29	1.31	3 (13%)	28,42,42	1.21	3 (10%)
2	IMX	B	587	-	23,29,29	1.23	2 (8%)	28,42,42	1.59	5 (17%)

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	IMX	A	587	-	-	4/7/24/24	0/4/4/4
2	IMX	B	586	-	-	2/7/24/24	0/4/4/4
2	IMX	A	586	-	-	3/7/24/24	0/4/4/4
2	IMX	B	587	-	-	4/7/24/24	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	587	IMX	C12-N14	2.36	1.39	1.34
2	A	587	IMX	C7-C6	2.26	1.41	1.37
2	B	587	IMX	C12-N14	2.25	1.39	1.34
2	A	586	IMX	C9-C12	-2.18	1.45	1.50
2	A	586	IMX	C12-N14	2.15	1.38	1.34
2	B	586	IMX	C4-C2	-2.12	1.37	1.42
2	B	587	IMX	C4-C2	-2.10	1.37	1.42
2	A	586	IMX	C4-C2	-2.01	1.37	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	587	IMX	C9-C12-N14	4.97	124.43	115.20
2	B	587	IMX	C9-C12-N14	4.70	123.94	115.20
2	A	587	IMX	C7-C6-C4	-3.35	119.54	123.23
2	B	587	IMX	C7-C6-C4	-2.81	120.13	123.23
2	A	587	IMX	C4-C2-C3	2.49	123.34	119.87
2	A	586	IMX	C4-C2-C3	2.48	123.33	119.87
2	A	586	IMX	C9-C12-N14	2.36	119.59	115.20
2	B	587	IMX	C9-N8-C3	2.35	109.35	104.45
2	A	587	IMX	O13-C12-C9	-2.35	115.97	121.08
2	A	587	IMX	C9-C10-C2	2.34	109.48	106.55
2	A	587	IMX	C7-C5-C3	-2.30	117.95	120.84
2	A	587	IMX	C5-C7-C6	2.29	121.36	118.74
2	B	587	IMX	O13-C12-C9	-2.24	116.20	121.08
2	A	586	IMX	C7-C5-C3	-2.16	118.12	120.84
2	B	587	IMX	C1-N14-C12	-2.12	119.16	123.01
2	A	587	IMX	C9-N8-C3	2.08	108.80	104.45
2	B	586	IMX	C7-C5-C3	-2.02	118.30	120.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	587	IMX	C15-C1-N14-C12
2	A	587	IMX	O13-C12-C9-C10
2	A	587	IMX	C1-C18-C23-C24
2	A	587	IMX	C17-C18-C23-C24
2	B	586	IMX	C15-C1-N14-C12
2	B	587	IMX	C15-C1-N14-C12
2	B	587	IMX	C1-C18-C23-C24

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Mol	Chain	Res	Type	Atoms
2	A	586	IMX	C15-C1-N14-C12
2	B	587	IMX	C18-C1-N14-C12
2	B	586	IMX	C1-C18-C23-C24
2	A	586	IMX	C1-C18-C23-C24
2	B	587	IMX	C17-C18-C23-C24
2	A	586	IMX	C18-C1-N14-C12

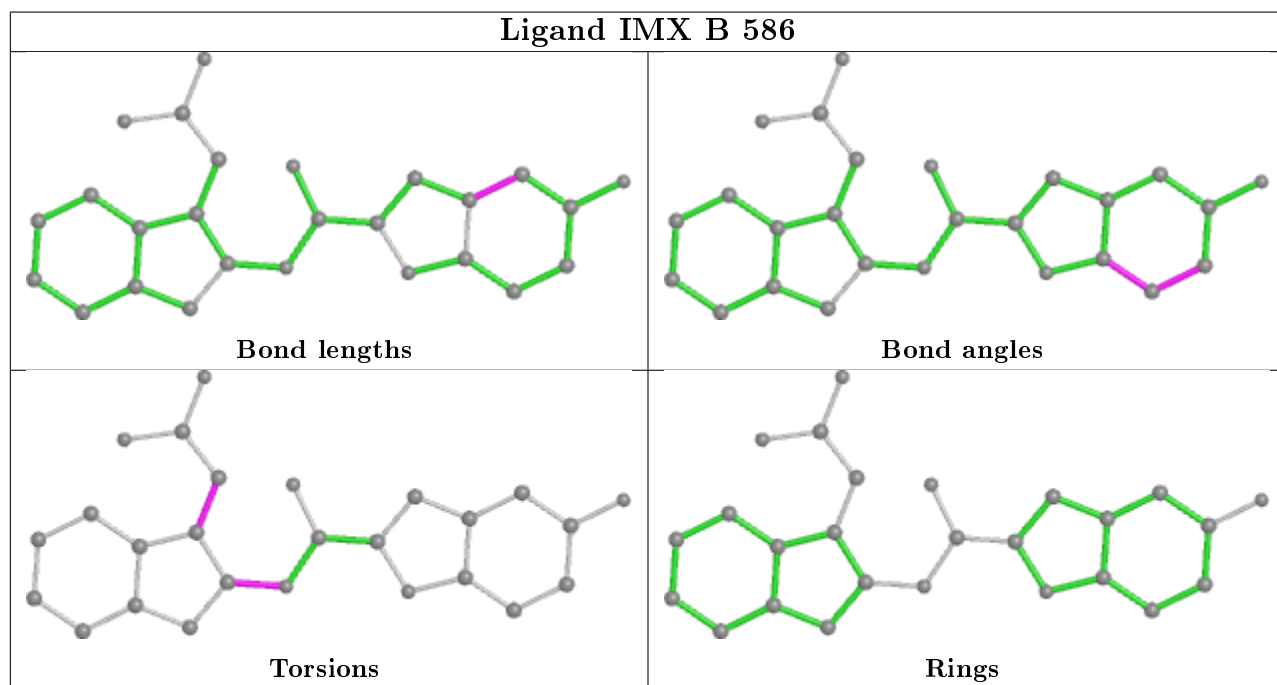
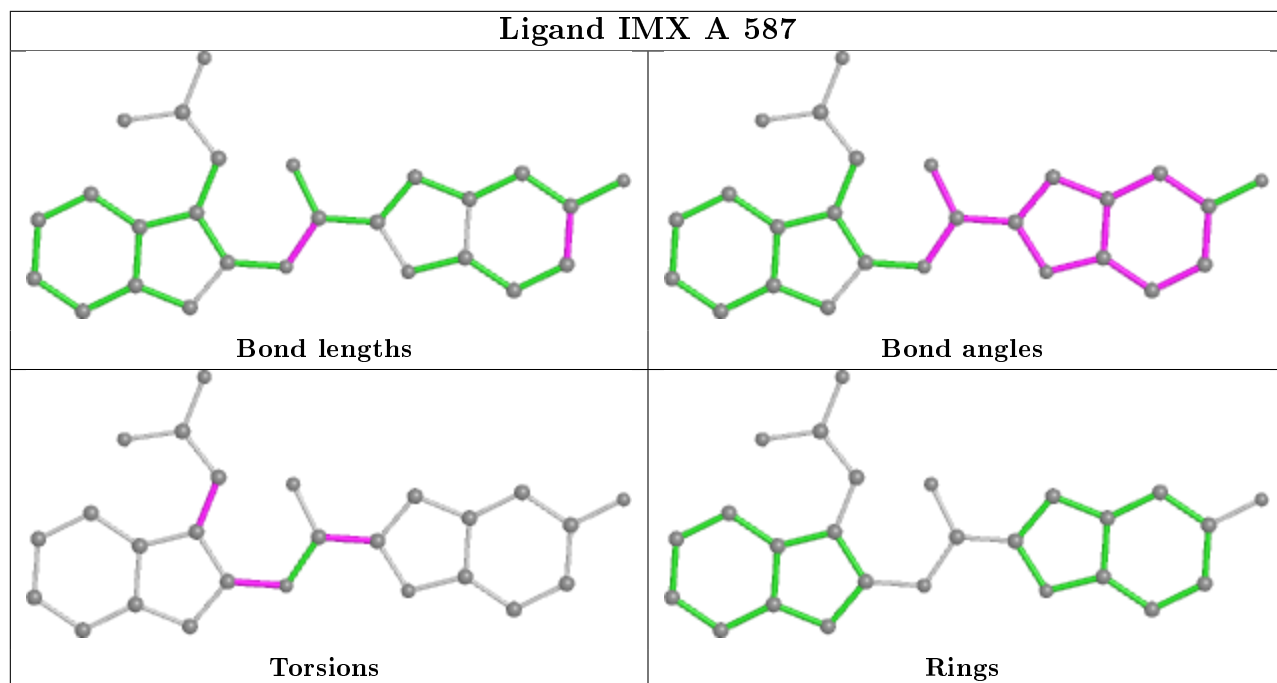
There are no ring outliers.

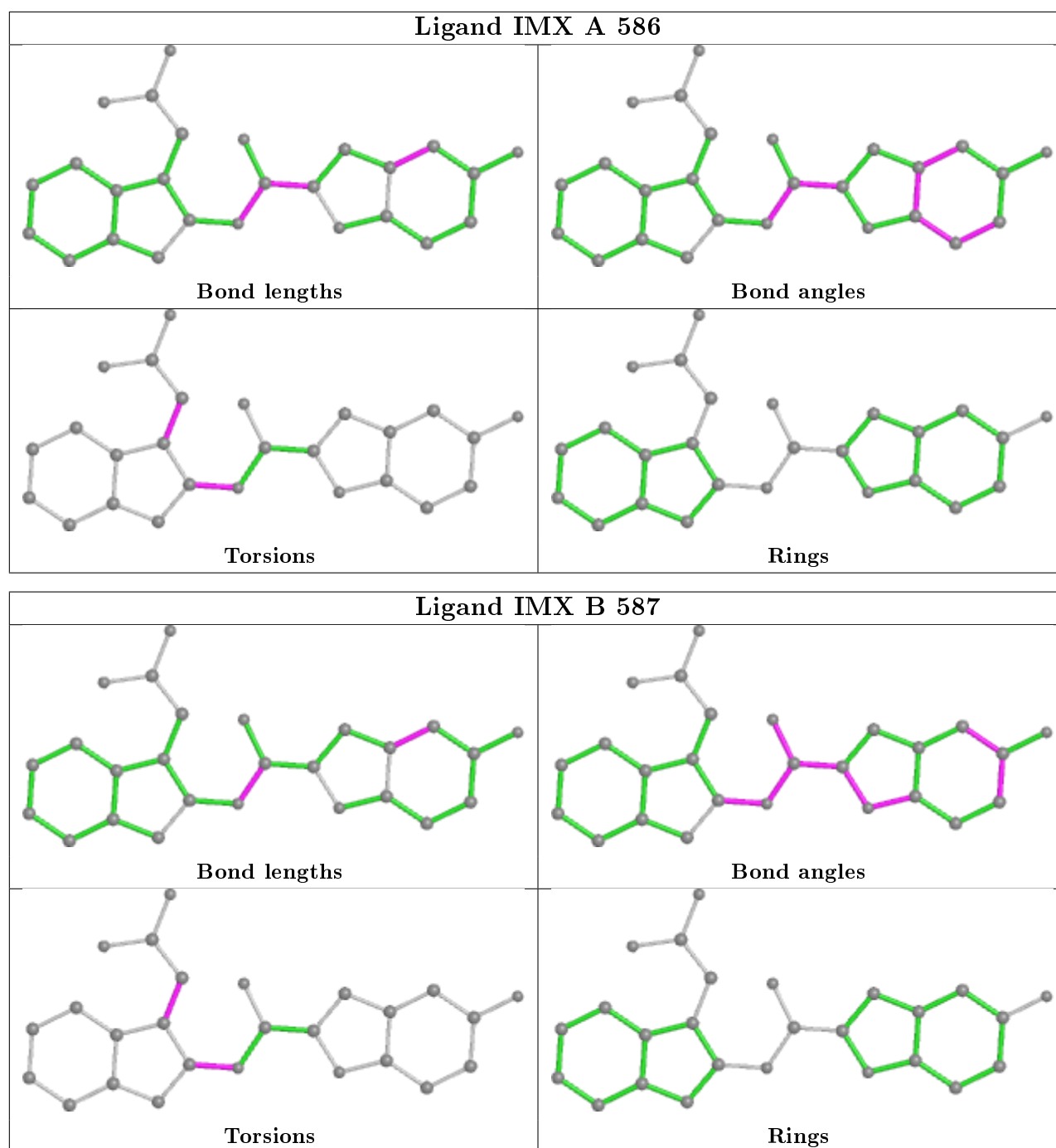
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	587	IMX	1	0
2	B	586	IMX	2	0
2	A	586	IMX	1	0
2	B	587	IMX	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	578/585 (98%)	0.43	46 (7%) <b>12</b>   <b>10</b>	35, 73, 123, 143	7 (1%)
1	B	578/585 (98%)	0.38	44 (7%) <b>13</b>   <b>12</b>	40, 70, 120, 179	7 (1%)
All	All	1156/1170 (98%)	0.41	90 (7%) <b>13</b>   <b>11</b>	35, 72, 122, 179	14 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	8.5
1	B	582	ALA	7.5
1	A	575	LEU	6.5
1	A	87	MET	6.3
1	A	564	LYS	5.6
1	A	397	GLN	5.4
1	A	300	ALA	5.4
1	A	501	GLU	5.3
1	A	372	LYS	5.2
1	A	375	ASP	5.0
1	A	368	GLU	5.0
1	B	82	GLU	4.8
1	A	562	ASP	4.8
1	B	322	ALA	4.8
1	A	572	GLY	4.8
1	B	83	THR	4.6
1	A	582	ALA	4.4
1	A	539	ALA	4.4
1	A	563	ASP	4.1
1	A	85	GLY	3.9
1	A	510	HIS	3.9
1	A	579	SER	3.8
1	B	86	GLU	3.8
1	B	80	LEU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	561	ALA	3.7
1	A	551	PHE	3.7
1	B	504	ALA	3.7
1	A	506	THR	3.6
1	A	503	ASN	3.6
1	B	513	ILE	3.5
1	B	79	THR	3.5
1	A	443	ALA	3.5
1	B	130	ASN	3.5
1	B	434	GLY	3.5
1	A	122	VAL	3.4
1	B	87	MET	3.4
1	A	400	GLU	3.4
1	B	571	GLU	3.4
1	B	88	ALA	3.4
1	A	490	ALA	3.3
1	B	398	LEU	3.2
1	A	556	GLU	3.2
1	B	111	ASN	3.1
1	A	366	PRO	3.0
1	B	536	LYS	3.0
1	A	79	THR	3.0
1	A	187	ASP	2.9
1	B	471	ASP	2.9
1	B	505	GLU	2.9
1	A	540	THR	2.9
1	B	538	LYS	2.9
1	A	444	LYS	2.9
1	B	500	LYS	2.8
1	B	132	GLU	2.8
1	B	84	TYR	2.7
1	A	83	THR	2.7
1	B	55	ALA	2.6
1	B	501	GLU	2.6
1	A	398	LEU	2.6
1	A	321	GLU	2.6
1	B	315	VAL	2.6
1	B	541	LYS	2.6
1	A	479	GLU	2.5
1	B	122	VAL	2.5
1	A	313	LYS	2.5
1	B	365	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	375	ASP	2.4
1	A	576	VAL	2.4
1	A	322	ALA	2.3
1	A	82	GLU	2.3
1	A	580	GLN	2.3
1	A	84	TYR	2.3
1	A	512	ASP	2.3
1	B	447	PRO	2.2
1	B	556	GLU	2.2
1	A	401	TYR	2.2
1	B	579	SER	2.2
1	B	580	GLN	2.1
1	B	374	PHE	2.1
1	A	448	CYS	2.1
1	B	118	PRO	2.1
1	A	386	ASN	2.1
1	B	115	LEU	2.1
1	A	369	CYS	2.1
1	A	92	ALA	2.1
1	B	399	GLY	2.1
1	B	382	GLU	2.0
1	B	310	VAL	2.0
1	B	494	ASP	2.0
1	B	574	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](#)

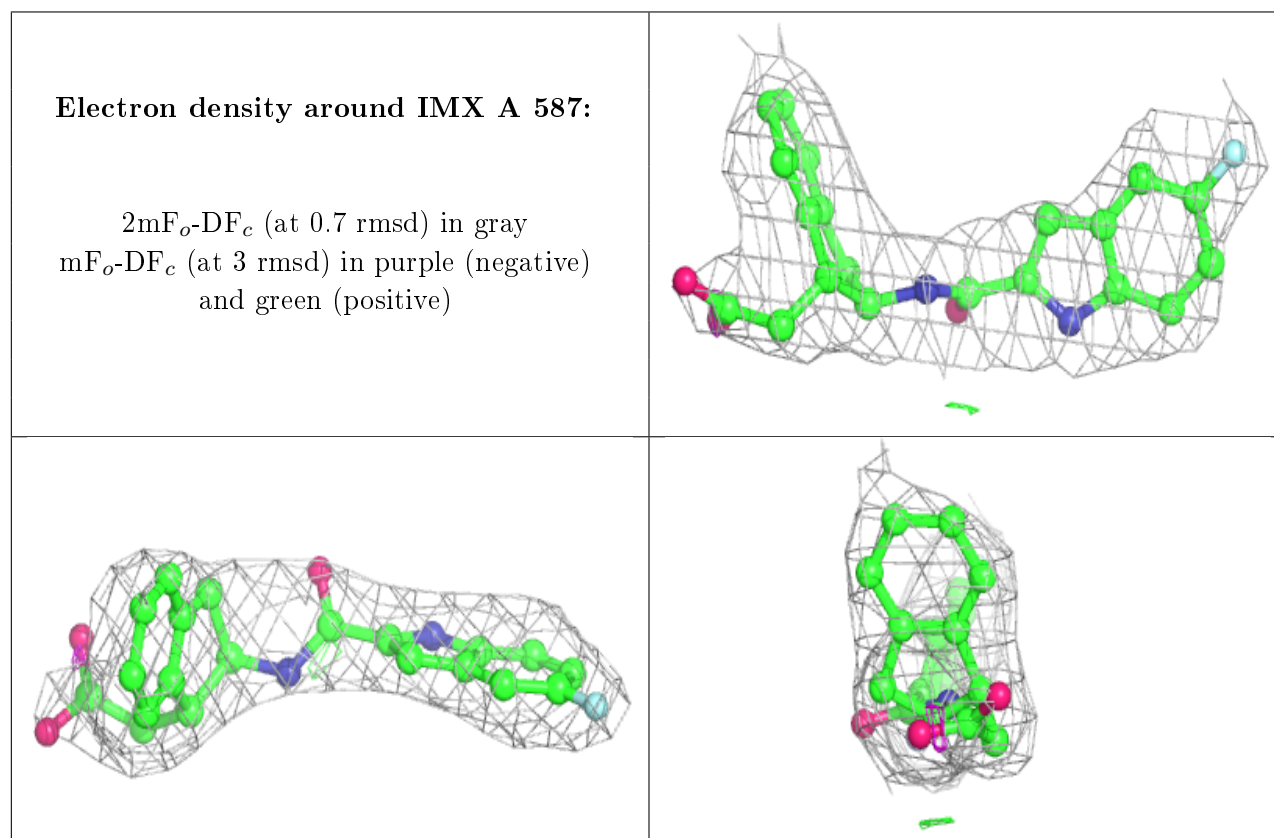
There are no carbohydrates in this entry.

## 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.

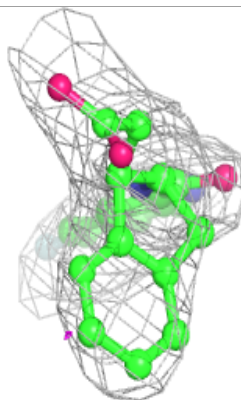
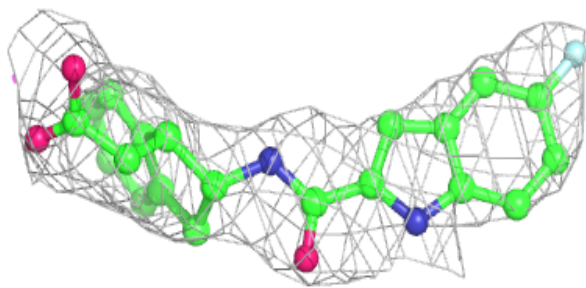
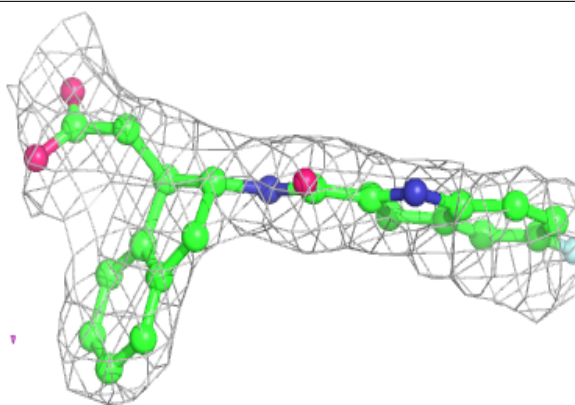
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IMX	A	587	26/26	0.88	0.21	61,77,82,82	0
2	IMX	B	587	26/26	0.89	0.23	58,73,86,91	0
2	IMX	A	586	26/26	0.91	0.20	55,65,69,89	0
2	IMX	B	586	26/26	0.93	0.15	43,58,62,73	0

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.

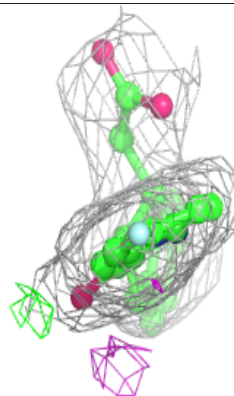
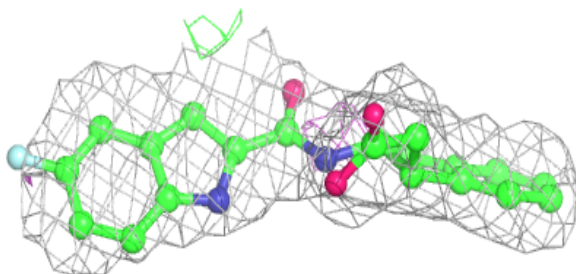
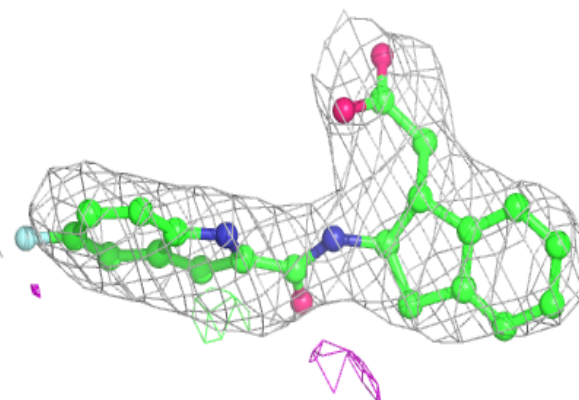


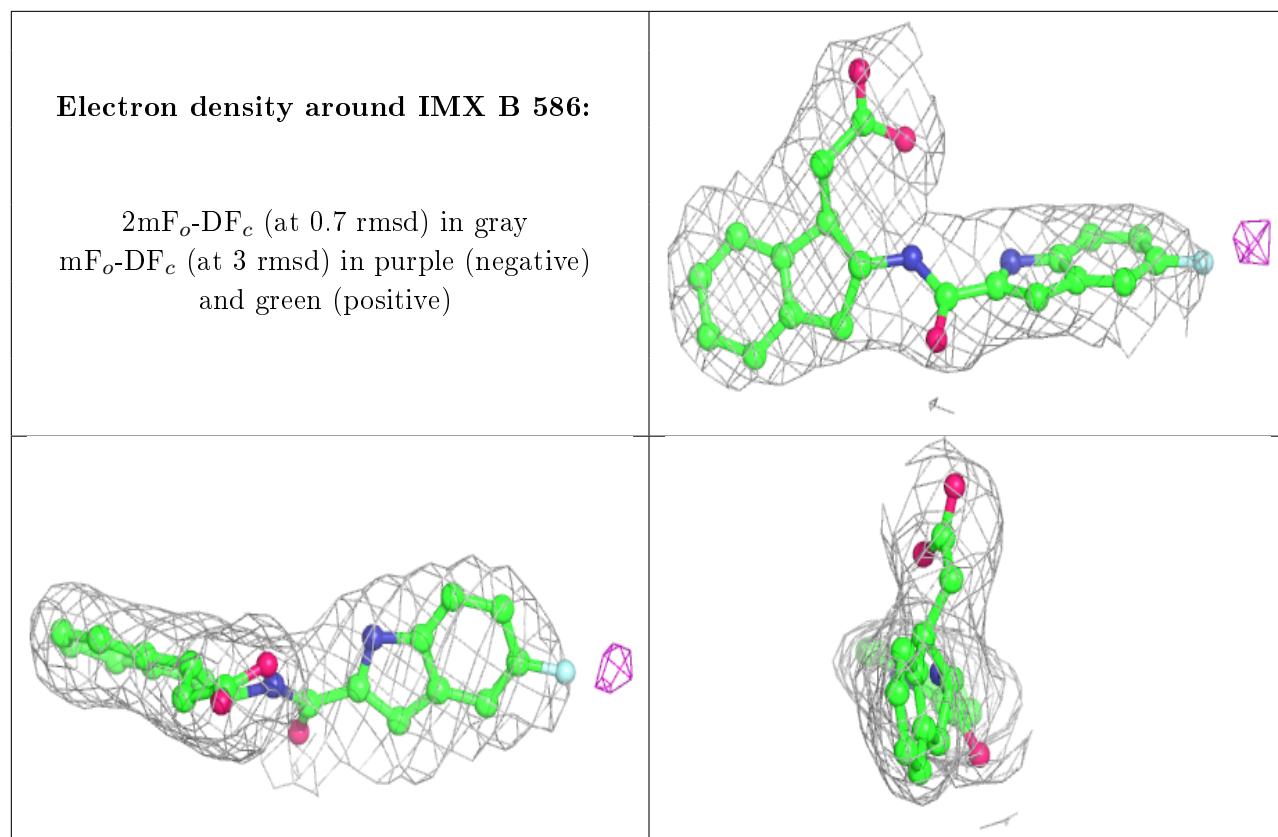
**Electron density around IMX B 587:**

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

**Electron density around IMX A 586:**

$2mF_o-DF_c$  (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.