



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:08 AM EDT

PDB ID : 3LU7
Title : Human serum albumin in complex with compound 2
Authors : Buttar, D.; Colclough, N.; Gerhardt, S.; MacFaul, P.A.; Phillips, S.D.; Plowright, A.; Whittamore, P.; Tam, K.; Maskos, K.; Steinbacher, S.; Steuber, H.
Deposited on : 2010-02-17
Resolution : 2.80 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

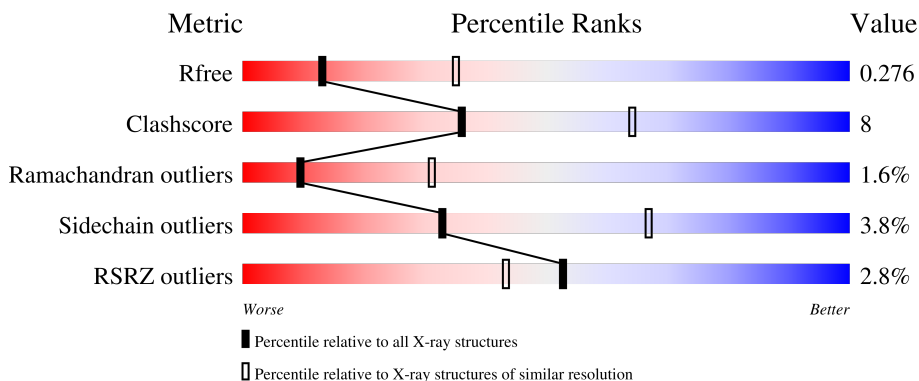
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	585	
1	B	585	

2 Entry composition [i](#)

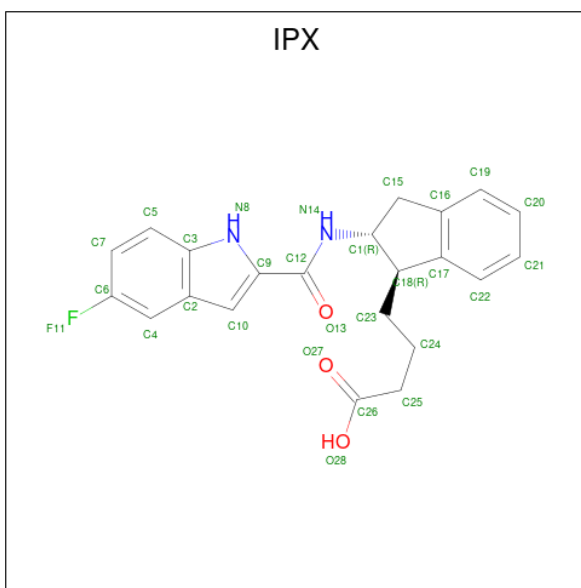
There are 4 unique types of molecules in this entry. The entry contains 9291 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	20	0	0
			4599	2903	776	879	41			
1	B	579	Total	C	N	O	S	17	0	0
			4608	2909	778	880	41			

- Molecule 2 is 4-[(1R,2R)-2-[[5-fluoro-1H-indol-2-yl]carbonyl]amino]-2,3-dihydro-1H-inden-1-yl]butanoic acid (three-letter code: IPX) (formula: C₂₂H₂₁FN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	Total	C	F	N	O	0	0
			28	22	1	2	3		
2	B	1	Total	C	F	N	O	0	0
			28	22	1	2	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

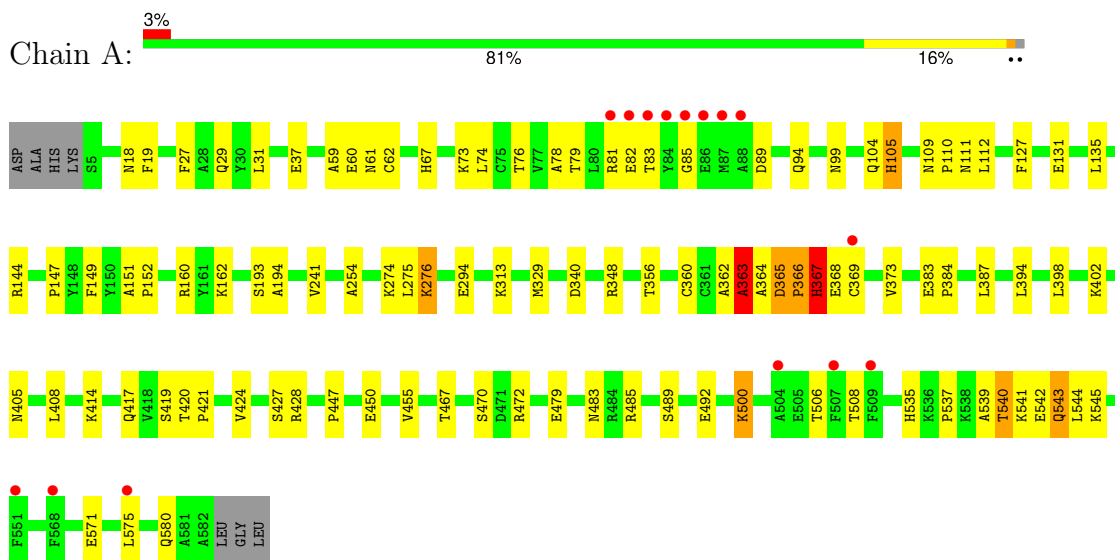
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		

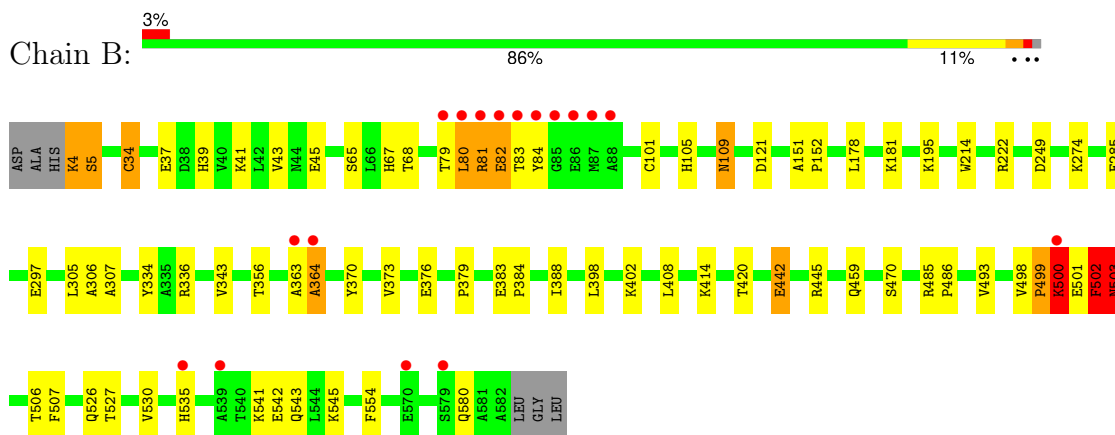
3 Residue-property plots [i](#)

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: Serum albumin



- Molecule 1: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.54Å 59.19Å 95.60Å 75.30° 87.86° 75.51°	Depositor
Resolution (Å)	55.44 – 2.80 55.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.7 (55.44-2.80) 92.7 (55.44-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.276 0.226 , 0.276	Depositor DCC
R_{free} test set	1392 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9291	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: IPX, PO4

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	0.47	0/4688	0.59	2/6324 (0.0%)
1	B	0.45	0/4697	0.57	1/6335 (0.0%)
All	All	0.46	0/9385	0.58	3/12659 (0.0%)

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	A	1	2
1	B	0	3
All	All	1	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	363	ALA	CB-CA-C	8.02	122.12	110.10
1	A	363	ALA	N-CA-C	6.23	127.82	111.00
1	B	502	PHE	N-CA-CB	-5.26	101.13	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	ALA	Peptide
1	A	363	ALA	Peptide
1	B	500	LYS	Peptide
1	B	502	PHE	Peptide
1	B	503	ASN	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	72	0
1	B	4608	0	4531	73	0
2	A	28	0	21	0	0
2	B	28	0	20	1	0
3	A	15	0	0	0	0
3	B	10	0	0	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
All	All	9291	0	9090	146	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 8.

All (146) 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:81:ARG:CB	1:A:85:GLY:HA2	1.74	1.16
1:A:81:ARG:HB2	1:A:85:GLY:HA2	1.08	1.07
1:A:81:ARG:HA	1:A:85:GLY:H	1.19	1.07
1:A:365:ASP:H	1:A:366:PRO:HD3	1.20	1.06
1:B:502:PHE:HE2	1:B:580:GLN:HG3	1.21	1.04
1:B:4:LYS:N	1:B:4:LYS:HD2	1.73	1.03
1:B:503:ASN:HB3	1:B:506:THR:HB	1.36	1.02
1:B:503:ASN:HD22	1:B:506:THR:CG2	1.79	0.95
1:B:503:ASN:CB	1:B:506:THR:HB	1.98	0.93
1:B:503:ASN:HB2	1:B:507:PHE:CD1	2.03	0.92
1:B:503:ASN:HB2	1:B:507:PHE:HD1	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASN:HD22	1:B:506:THR:CB	1.83	0.91
1:A:365:ASP:H	1:A:366:PRO:CD	1.81	0.91
1:A:365:ASP:N	1:A:366:PRO:CD	2.36	0.87
1:B:503:ASN:HB3	1:B:506:THR:CB	2.05	0.86
1:A:81:ARG:HB2	1:A:85:GLY:CA	2.02	0.86
1:A:365:ASP:N	1:A:366:PRO:HD3	1.91	0.86
1:B:503:ASN:HD22	1:B:506:THR:HB	1.39	0.86
1:B:4:LYS:N	1:B:4:LYS:CD	2.40	0.85
1:A:81:ARG:HA	1:A:85:GLY:N	1.90	0.84
1:B:502:PHE:CE2	1:B:580:GLN:HG3	2.12	0.83
1:B:4:LYS:O	1:B:5:SER:HB3	1.83	0.79
1:B:79:THR:O	1:B:80:LEU:HG	1.83	0.78
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.66	0.77
1:B:503:ASN:ND2	1:B:506:THR:HB	2.00	0.76
1:A:313:LYS:HA	1:A:367:HIS:CE1	2.22	0.75
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.05	0.72
1:B:502:PHE:HE2	1:B:580:GLN:CG	1.99	0.72
1:B:80:LEU:HB2	1:B:84:TYR:CE2	2.25	0.72
1:B:502:PHE:HD1	1:B:503:ASN:O	1.72	0.72
1:B:80:LEU:HB2	1:B:84:TYR:HE2	1.55	0.71
1:B:503:ASN:HD22	1:B:506:THR:HG21	1.56	0.70
1:A:402:LYS:HA	1:A:405:ASN:HD22	1.56	0.69
1:B:4:LYS:O	1:B:5:SER:CB	2.43	0.67
1:A:366:PRO:C	1:A:368:GLU:H	1.99	0.65
1:B:80:LEU:O	1:B:82:GLU:N	2.30	0.65
1:A:365:ASP:O	1:A:368:GLU:N	2.30	0.65
1:A:366:PRO:O	1:A:368:GLU:N	2.30	0.64
1:A:81:ARG:CA	1:A:85:GLY:HA2	2.27	0.64
1:A:365:ASP:O	1:A:367:HIS:N	2.30	0.64
1:B:503:ASN:ND2	1:B:506:THR:HG21	2.11	0.64
1:A:365:ASP:O	1:A:366:PRO:C	2.37	0.64
1:A:356:THR:HG21	1:A:373:VAL:HG22	1.79	0.63
1:B:80:LEU:O	1:B:83:THR:N	2.31	0.62
1:A:364:ALA:H	1:A:366:PRO:HD3	1.64	0.62
1:B:81:ARG:O	1:B:83:THR:N	2.35	0.59
1:A:152:PRO:HG3	1:A:254:ALA:HA	1.85	0.59
1:B:503:ASN:ND2	1:B:506:THR:CB	2.58	0.58
2:B:586:IPX:N14	3:B:587:PO4:O4	2.26	0.58
1:A:424:VAL:O	1:A:428:ARG:HG3	2.04	0.57
1:A:81:ARG:C	1:A:83:THR:H	2.08	0.57
1:A:366:PRO:HA	1:A:369:CYS:SG	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:C	1:A:83:THR:N	2.59	0.56
1:A:366:PRO:C	1:A:368:GLU:N	2.59	0.56
1:A:313:LYS:HA	1:A:367:HIS:NE2	2.20	0.56
1:B:81:ARG:C	1:B:83:THR:N	2.59	0.56
1:A:500:LYS:O	1:A:535:HIS:ND1	2.34	0.56
1:B:65:SER:OG	1:B:68:THR:OG1	2.24	0.55
1:B:109:ASN:C	1:B:109:ASN:HD22	2.10	0.55
1:B:376:GLU:O	1:B:379:PRO:HD2	2.06	0.55
1:B:80:LEU:O	1:B:81:ARG:C	2.42	0.55
1:B:39:HIS:O	1:B:43:VAL:HG23	2.07	0.55
1:A:81:ARG:O	1:A:83:THR:N	2.40	0.54
1:B:101:CYS:O	1:B:105:HIS:ND1	2.39	0.54
1:B:34:CYS:HG	1:B:84:TYR:HH	1.56	0.53
1:A:60:GLU:O	1:A:61:ASN:HB2	2.10	0.52
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.92	0.52
1:B:503:ASN:CG	1:B:506:THR:HB	2.30	0.52
1:B:274:LYS:NZ	1:B:297:GLU:OE2	2.41	0.51
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.93	0.51
1:A:450:GLU:OE2	1:A:485:ARG:NE	2.43	0.51
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.93	0.50
1:B:498:VAL:CG2	1:B:499:PRO:HD2	2.42	0.50
1:B:81:ARG:C	1:B:83:THR:H	2.14	0.50
1:B:356:THR:HG21	1:B:373:VAL:CG2	2.41	0.50
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.42	0.50
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.94	0.50
1:A:365:ASP:OD2	1:A:368:GLU:OE1	2.30	0.50
1:A:472:ARG:NH1	1:A:492:GLU:O	2.45	0.50
1:B:306:ALA:O	1:B:307:ALA:C	2.50	0.49
1:B:503:ASN:ND2	1:B:506:THR:CG2	2.58	0.49
1:B:363:ALA:O	1:B:364:ALA:C	2.51	0.49
1:A:81:ARG:CA	1:A:85:GLY:CA	2.90	0.49
1:A:541:LYS:HB2	1:A:543:GLN:HE21	1.77	0.49
1:A:81:ARG:HA	1:A:85:GLY:CA	2.41	0.49
1:A:73:LYS:O	1:A:76:THR:OG1	2.28	0.49
1:A:417:GLN:HB2	1:A:470:SER:HB3	1.94	0.49
1:A:540:THR:HG22	1:A:544:LEU:HD11	1.94	0.48
1:A:348:ARG:HG2	1:A:483:ASN:HD21	1.78	0.48
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.53	0.48
1:B:502:PHE:CD1	1:B:503:ASN:O	2.61	0.48
1:A:402:LYS:HA	1:A:405:ASN:ND2	2.27	0.48
1:B:498:VAL:HG23	1:B:499:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:O	1:B:80:LEU:CG	2.60	0.48
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.43	0.47
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.96	0.47
1:B:80:LEU:C	1:B:82:GLU:N	2.68	0.47
1:B:420:THR:CG2	1:B:527:THR:HG23	2.45	0.47
1:A:81:ARG:CA	1:A:85:GLY:N	2.70	0.47
1:A:539:ALA:O	1:A:540:THR:HG23	2.14	0.47
1:B:384:PRO:O	1:B:388:ILE:HG12	2.14	0.46
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.98	0.46
1:B:541:LYS:N	1:B:543:GLN:HE21	2.14	0.46
1:A:467:THR:O	1:A:467:THR:OG1	2.33	0.46
1:B:178:LEU:O	1:B:181:LYS:N	2.44	0.45
1:B:420:THR:HG21	1:B:527:THR:HG23	1.97	0.45
1:B:500:LYS:H	1:B:500:LYS:HG3	1.44	0.45
1:A:27:PHE:CD1	1:A:74:LEU:HD21	2.52	0.45
1:A:340:ASP:O	1:A:447:PRO:HD3	2.16	0.45
1:B:503:ASN:CG	1:B:507:PHE:HE1	2.20	0.45
1:B:503:ASN:HB2	1:B:507:PHE:CE1	2.50	0.44
1:A:542:GLU:O	1:A:545:LYS:N	2.50	0.44
1:A:104:GLN:HB3	1:A:105:HIS:ND1	2.33	0.44
1:A:408:LEU:HD21	1:A:424:VAL:HA	2.00	0.44
1:B:356:THR:HG21	1:B:373:VAL:HG22	2.00	0.44
1:A:27:PHE:CG	1:A:74:LEU:HD21	2.54	0.43
1:A:571:GLU:O	1:A:575:LEU:HG	2.18	0.43
1:B:305:LEU:O	1:B:306:ALA:C	2.56	0.43
1:A:67:HIS:CE1	1:A:99:ASN:OD1	2.71	0.43
1:A:274:LYS:HD2	1:A:294:GLU:HG3	2.00	0.43
1:A:313:LYS:HA	1:A:367:HIS:HE2	1.83	0.43
1:A:127:PHE:O	1:A:131:GLU:HB3	2.19	0.43
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.99	0.43
1:A:81:ARG:CB	1:A:85:GLY:CA	2.69	0.43
1:B:41:LYS:NZ	1:B:45:GLU:OE2	2.52	0.43
1:A:420:THR:N	1:A:421:PRO:HD2	2.35	0.42
1:A:275:LEU:O	1:A:276:LYS:C	2.58	0.42
1:A:112:LEU:HD21	1:A:144:ARG:NH2	2.35	0.41
1:A:408:LEU:HD23	1:A:427:SER:CB	2.50	0.41
1:B:363:ALA:O	1:B:364:ALA:O	2.37	0.41
1:B:501:GLU:HA	1:B:501:GLU:OE2	2.20	0.41
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.35	0.41
1:B:398:LEU:HB3	1:B:402:LYS:HB2	2.03	0.41
1:A:394:LEU:HD11	1:A:398:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:O	1:A:19:PHE:C	2.59	0.41
1:B:67:HIS:NE2	1:B:249:ASP:OD1	2.54	0.41
1:B:373:VAL:O	1:B:376:GLU:HB2	2.20	0.41
1:B:542:GLU:O	1:B:545:LYS:N	2.54	0.41
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.02	0.41
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.03	0.41
1:A:110:PRO:O	1:A:112:LEU:N	2.53	0.40
1:A:135:LEU:HD21	1:A:162:LYS:HB2	2.03	0.40
1:A:398:LEU:O	1:A:402:LYS:HB2	2.21	0.40
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.56	0.40
1:A:360:CYS:O	1:A:366:PRO:HG3	2.22	0.40
1:B:503:ASN:OD1	1:B:535:HIS:CE1	2.75	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%)	528 (92%)	38 (7%)	10 (2%)	9	29
1	B	577/585 (99%)	520 (90%)	49 (8%)	8 (1%)	11	34
All	All	1153/1170 (98%)	1048 (91%)	87 (8%)	18 (2%)	9	31

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	A	366	PRO
1	B	364	ALA
1	A	82	GLU
1	A	363	ALA
1	A	367	HIS

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Mol	Chain	Res	Type
1	A	543	GLN
1	B	81	ARG
1	B	82	GLU
1	B	442	GLU
1	A	111	ASN
1	A	276	LYS
1	B	5	SER
1	B	80	LEU
1	A	537	PRO
1	B	499	PRO
1	A	241	VAL
1	B	493	VAL

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%)	486 (96%)	20 (4%)	31 65
1	B	507/511 (99%)	489 (96%)	18 (4%)	35 69
All	All	1013/1022 (99%)	975 (96%)	38 (4%)	33 67

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	79	THR
1	A	89	ASP
1	A	94	GLN
1	A	105	HIS
1	A	109	ASN
1	A	149	PHE
1	A	160	ARG
1	A	193	SER
1	A	329	MET
1	A	367	HIS

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Mol	Chain	Res	Type
1	A	414	LYS
1	A	419	SER
1	A	479	GLU
1	A	489	SER
1	A	500	LYS
1	A	506	THR
1	A	508	THR
1	A	540	THR
1	A	580	GLN
1	B	4	LYS
1	B	34	CYS
1	B	37	GLU
1	B	109	ASN
1	B	121	ASP
1	B	195	LYS
1	B	222	ARG
1	B	285	GLU
1	B	334	TYR
1	B	336	ARG
1	B	370	TYR
1	B	414	LYS
1	B	459	GLN
1	B	470	SER
1	B	500	LYS
1	B	502	PHE
1	B	503	ASN
1	B	554	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	67	HIS
1	A	109	ASN
1	A	196	GLN
1	A	338	HIS
1	A	385	GLN
1	A	405	ASN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
1	B	33	GLN

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Mol	Chain	Res	Type
1	B	104	GLN
1	B	109	ASN
1	B	130	ASN
1	B	170	GLN
1	B	196	GLN
1	B	247	HIS
1	B	483	ASN
1	B	543	GLN
1	B	580	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
3	PO4	A	588	-	4,4,4	0.91	0	6,6,6	0.51	0
2	IPX	A	586	-	29,31,31	1.27	2 (6%)	35,44,44	1.25	4 (11%)
3	PO4	B	587	-	4,4,4	0.87	0	6,6,6	0.45	0
2	IPX	B	586	-	29,31,31	1.29	4 (13%)	35,44,44	1.56	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	587	-	4,4,4	0.84	0	6,6,6	0.64	0
3	PO4	B	588	-	4,4,4	0.90	0	6,6,6	0.33	0
3	PO4	A	589	-	4,4,4	0.83	0	6,6,6	0.66	0

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	IPX	A	586	-	-	6/11/26/26	0/4/4/4
2	IPX	B	586	-	-	6/11/26/26	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	586	IPX	C15-C1	2.92	1.55	1.53
2	A	586	IPX	C15-C1	2.70	1.55	1.53
2	B	586	IPX	C4-C6	2.28	1.39	1.36
2	A	586	IPX	C4-C6	2.25	1.39	1.36
2	B	586	IPX	C7-C6	2.06	1.41	1.37
2	B	586	IPX	C12-N14	2.02	1.38	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	586	IPX	C9-C12-N14	3.62	122.15	115.19
2	B	586	IPX	C7-C6-C4	-3.56	119.17	123.32
2	B	586	IPX	F11-C6-C7	2.40	122.39	118.55
2	A	586	IPX	C7-C5-C3	-2.33	118.02	120.80
2	A	586	IPX	C7-C6-C4	-2.21	120.74	123.32
2	A	586	IPX	O28-C26-C25	2.15	120.81	114.00
2	B	586	IPX	O28-C26-C25	2.15	120.80	114.00
2	B	586	IPX	C9-N8-C3	2.09	108.82	104.45
2	A	586	IPX	C9-N8-C3	2.02	108.66	104.45
2	B	586	IPX	C9-C10-C2	2.00	109.06	106.55

There are no chirality outliers.

All (12) torsion outliers are listed below:

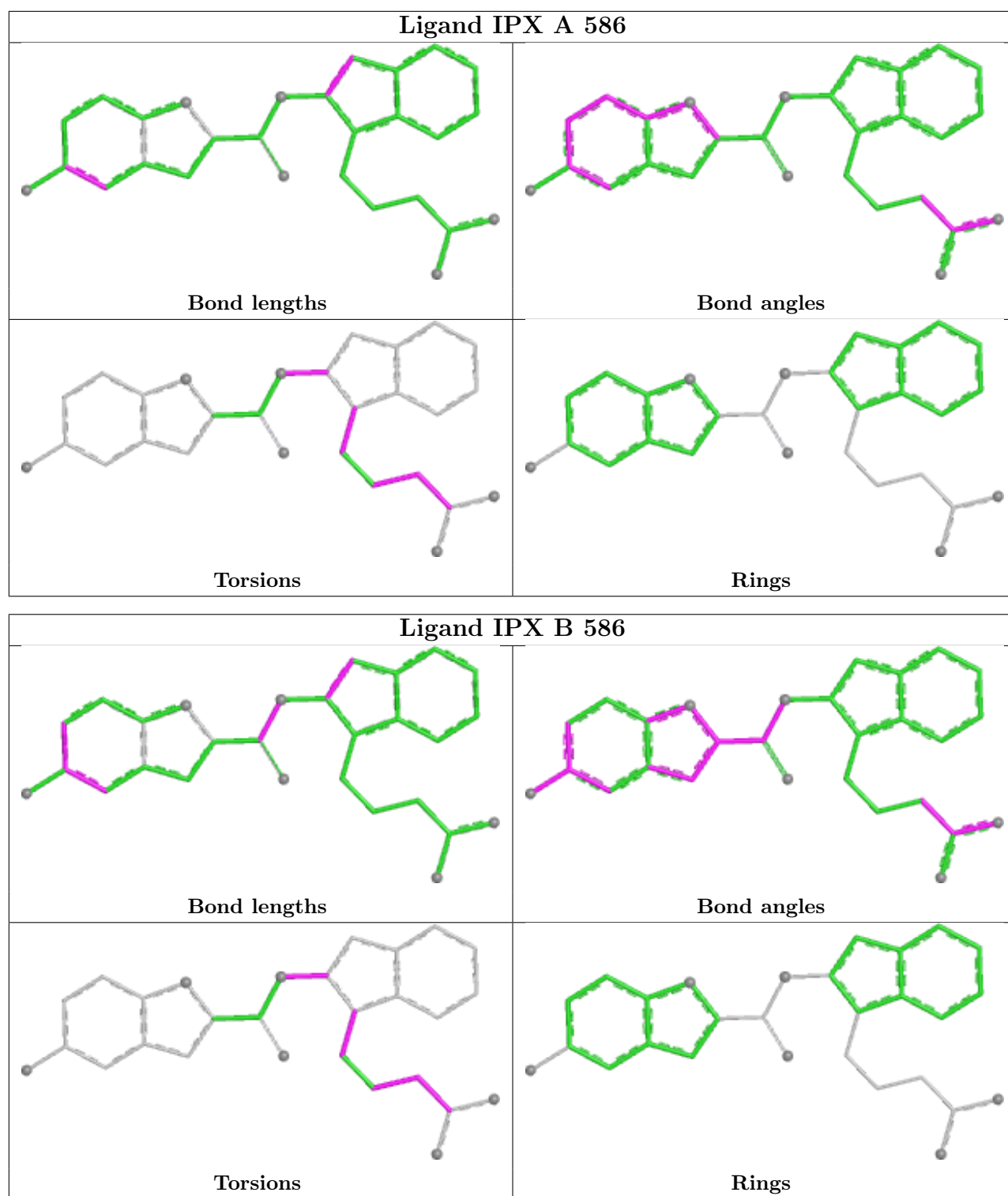
Mol	Chain	Res	Type	Atoms
2	A	586	IPX	C15-C1-N14-C12
2	A	586	IPX	C17-C18-C23-C24
2	B	586	IPX	C17-C18-C23-C24
2	B	586	IPX	C15-C1-N14-C12
2	A	586	IPX	C1-C18-C23-C24
2	B	586	IPX	C1-C18-C23-C24
2	A	586	IPX	C23-C24-C25-C26
2	B	586	IPX	C24-C25-C26-O28
2	B	586	IPX	C24-C25-C26-O27
2	A	586	IPX	C24-C25-C26-O28
2	A	586	IPX	C24-C25-C26-O27
2	B	586	IPX	C23-C24-C25-C26

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	587	PO4	1	0
2	B	586	IPX	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

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	578/585 (98%)	-0.22	15 (2%) 56 46	36, 64, 110, 126	21 (3%)
1	B	579/585 (98%)	-0.21	17 (2%) 51 41	20, 67, 101, 122	26 (4%)
All	All	1157/1170 (98%)	-0.21	32 (2%) 53 43	20, 66, 107, 126	47 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	THR	8.3
1	A	87	MET	7.5
1	B	87	MET	6.4
1	B	86	GLU	5.5
1	A	88	ALA	5.3
1	B	85	GLY	5.1
1	B	84	TYR	4.6
1	B	79	THR	4.4
1	B	82	GLU	4.4
1	B	570	GLU	3.8
1	A	82	GLU	3.7
1	B	364	ALA	3.4
1	B	88	ALA	3.3
1	A	84	TYR	3.3
1	A	509	PHE	3.1
1	A	86	GLU	3.1
1	B	80	LEU	3.1
1	A	83	THR	3.1
1	A	575	LEU	3.0
1	A	85	GLY	2.7
1	B	81	ARG	2.6
1	A	551	PHE	2.6
1	A	81	ARG	2.5
1	B	535	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	2.4
1	B	539	ALA	2.4
1	B	579	SER	2.3
1	A	504	ALA	2.3
1	A	507	PHE	2.3
1	A	369	CYS	2.2
1	A	568	PHE	2.1
1	B	500	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 monosaccharides in this entry.

6.4 Ligands [i](#)

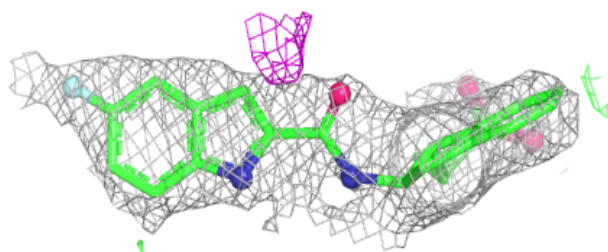
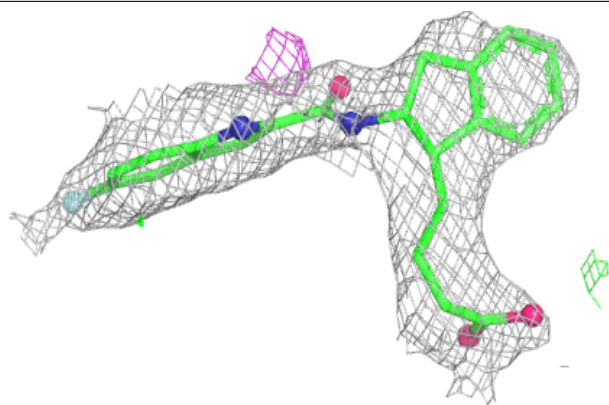
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IPX	A	586	28/28	0.87	0.26	60,76,81,83	0
2	IPX	B	586	28/28	0.90	0.24	70,74,79,86	0
3	PO4	A	588	5/5	0.90	0.16	88,89,91,96	0
3	PO4	A	587	5/5	0.91	0.14	71,73,79,79	0
3	PO4	A	589	5/5	0.94	0.11	67,68,71,74	0
3	PO4	B	587	5/5	0.95	0.12	60,64,68,70	0
3	PO4	B	588	5/5	0.95	0.10	83,85,90,92	0

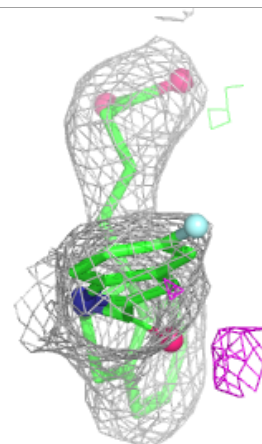
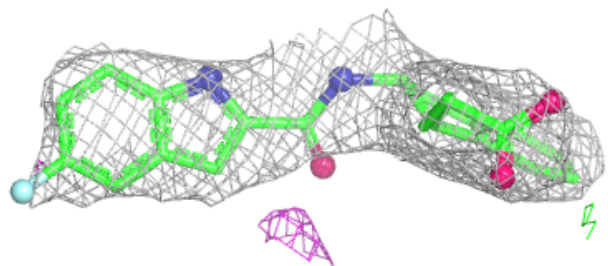
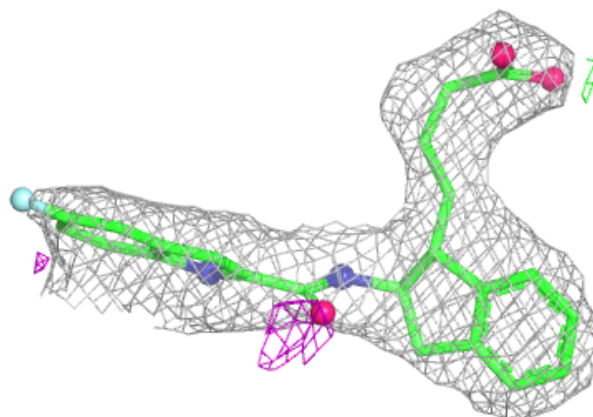
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IPX 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)

**Electron density around IPX B 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.