



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:16 PM UTC

PDB ID : 9HDN / pdb_00009hdn
Title : SARS-CoV-2 Main Protease in complex with (1R)-3-oxo-N-[2-oxo-2-(N-phenylanilino)ethyl]indane-1-carboxamide
Authors : Hanouille, X.; Charton, J.; Deprez, B.
Deposited on : 2024-11-12
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

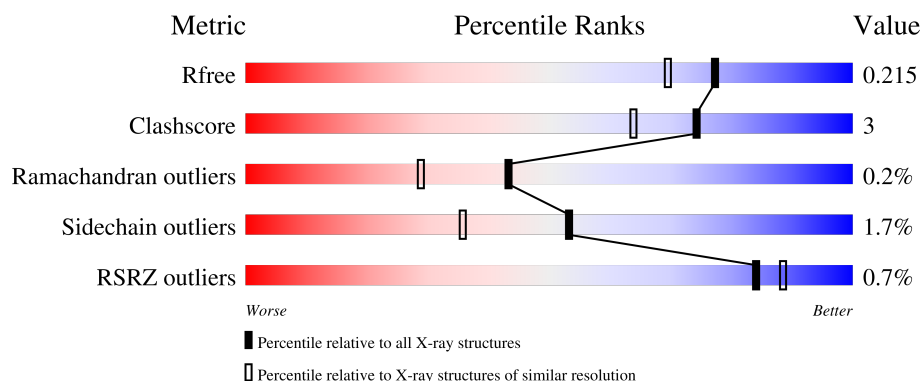
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	306	 86% 12% .
1	B	306	 87% 9% . .
1	C	306	 83% 14% . .
1	D	306	 84% 14% .

2 Entry composition [i](#)

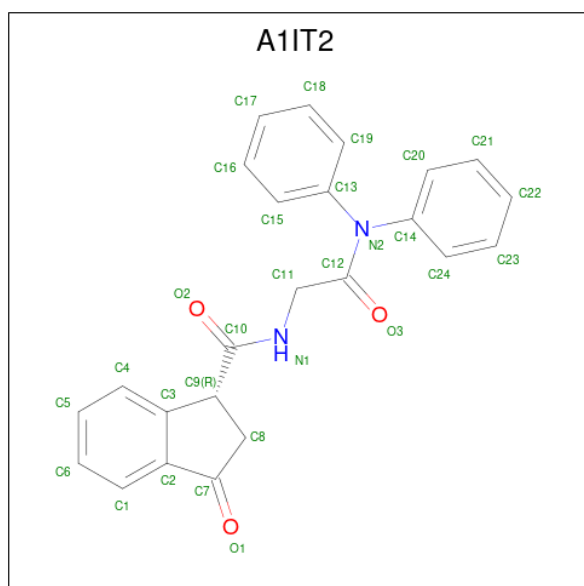
There are 3 unique types of molecules in this entry. The entry contains 19804 atoms, of which 9403 are hydrogens and 0 are deuteriums.

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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	H	N	O	S	78	6	0
			4785	1526	2370	412	452	25			
1	B	301	Total	C	H	N	O	S	78	3	0
			4644	1484	2298	396	443	23			
1	C	301	Total	C	H	N	O	S	78	4	0
			4677	1492	2319	400	443	23			
1	D	306	Total	C	H	N	O	S	76	3	0
			4720	1510	2336	403	448	23			

- Molecule 2 is (1 {R})- {N}-[2-(diphenylamino)-2-oxidanylidene-ethyl]-3-oxidanylidene-1,2-dihydroindene-1-carboxamide (CCD ID: A1IT2) (formula: C₂₄H₂₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			49	24	20	2	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 49	C 24	H 20	N 2	O 3	0	0
2	C	1	Total 49	C 24	H 20	N 2	O 3	0	0
2	D	1	Total 49	C 24	H 20	N 2	O 3	0	0

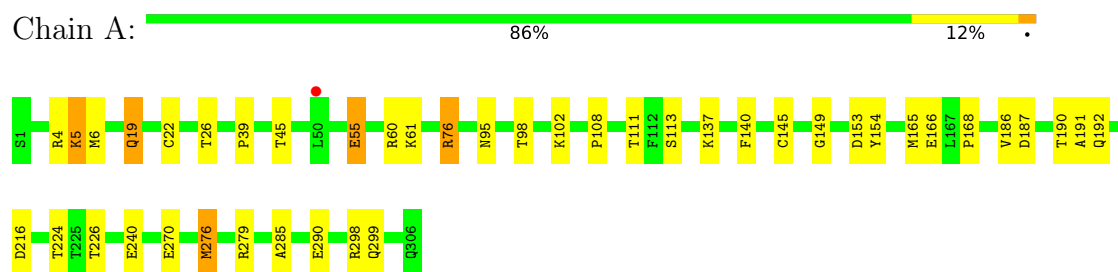
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	223	Total 223	O 223	0	0
3	B	200	Total 200	O 200	0	0
3	C	199	Total 199	O 199	0	0
3	D	160	Total 160	O 160	0	0

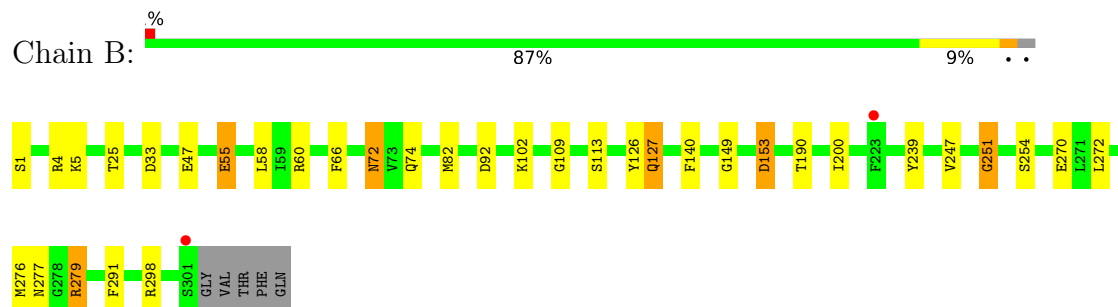
3 Residue-property plots [i](#)

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.

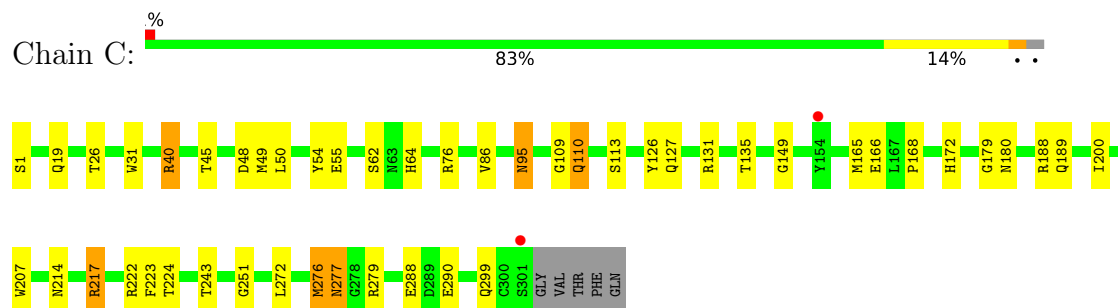
- Molecule 1: 3C-like proteinase nsp5



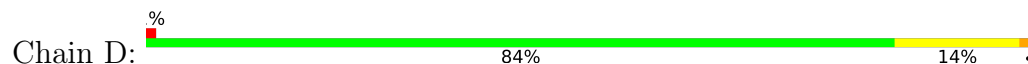
- Molecule 1: 3C-like proteinase nsp5

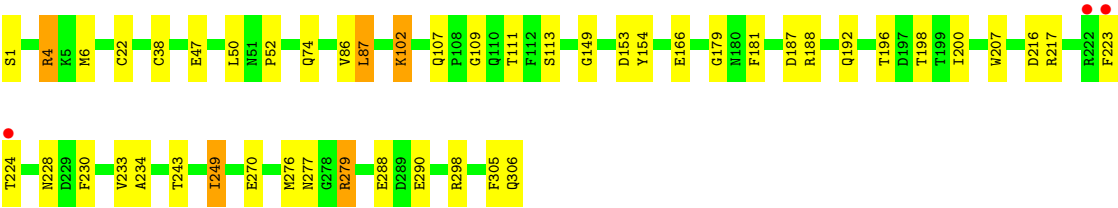


- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.32Å 124.24Å 71.23Å 90.00° 101.02° 90.00°	Depositor
Resolution (Å)	46.48 – 1.77 46.48 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.48-1.77) 97.6 (46.48-1.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.167 , 0.214 0.167 , 0.215	Depositor DCC
R_{free} test set	5408 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19804	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IT2

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	1.03	2/2468 (0.1%)	1.48	26/3352 (0.8%)
1	B	1.04	1/2398 (0.0%)	1.48	16/3259 (0.5%)
1	C	0.97	4/2410 (0.2%)	1.47	24/3275 (0.7%)
1	D	0.97	1/2437 (0.0%)	1.45	24/3313 (0.7%)
All	All	1.00	8/9713 (0.1%)	1.47	90/13199 (0.7%)

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	0	3
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	GLU	CD-OE2	8.68	1.41	1.25
1	C	290	GLU	CD-OE2	6.45	1.37	1.25
1	D	249	ILE	CB-CG1	-5.68	1.42	1.53
1	C	172	HIS	CG-CD2	-5.63	1.29	1.35
1	C	188	ARG	NE-CZ	5.29	1.38	1.33
1	A	39	PRO	CA-CB	-5.08	1.47	1.53
1	B	33	ASP	C-O	-5.04	1.19	1.24
1	C	40	ARG	CZ-NH2	-5.00	1.26	1.33

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASP	CA-CB-CG	9.50	122.10	112.60
1	A	290	GLU	CB-CG-CD	9.15	128.15	112.60
1	D	22	CYS	CB-CA-C	9.04	124.07	111.23
1	A	22	CYS	CB-CA-C	8.56	123.32	110.14
1	D	230	PHE	CA-CB-CG	-8.08	105.72	113.80
1	C	299	GLN	N-CA-CB	-7.50	99.07	110.33
1	C	251	GLY	O-C-N	-7.47	118.38	121.07
1	A	111	THR	CA-CB-OG1	-7.28	98.69	109.60
1	A	290	GLU	CG-CD-OE2	7.26	135.11	118.40
1	A	153	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	187	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	4	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	D	298	ARG	N-CA-CB	-7.11	99.63	110.16
1	D	74	GLN	CB-CA-C	7.08	121.40	109.80
1	B	47	GLU	CB-CG-CD	7.01	124.53	112.60
1	D	290	GLU	CB-CG-CD	6.94	124.40	112.60
1	B	72	ASN	CA-CB-CG	-6.94	105.66	112.60
1	D	223	PHE	N-CA-CB	6.93	120.95	110.42
1	D	216	ASP	CB-CA-C	-6.89	99.75	110.78
1	B	60	ARG	CD-NE-CZ	6.67	133.74	124.40
1	C	224	THR	CA-CB-OG1	-6.56	99.76	109.60
1	C	50	LEU	CA-C-N	-6.47	116.35	122.37
1	C	50	LEU	C-N-CA	-6.47	116.35	122.37
1	A	111	THR	OG1-CB-CG2	6.47	122.23	109.30
1	B	140	PHE	CA-CB-CG	6.47	120.27	113.80
1	C	172	HIS	CA-CB-CG	-6.46	107.34	113.80
1	B	127	GLN	N-CA-CB	-6.38	100.43	110.06
1	B	60	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	D	4	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	A	224	THR	CA-CB-OG1	-6.25	100.23	109.60
1	D	187	ASP	CA-CB-CG	6.17	118.78	112.60
1	A	19	GLN	N-CA-CB	-6.13	100.82	110.69
1	D	4	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	C	49	MET	CG-SD-CE	6.00	114.10	100.90
1	D	87	LEU	N-CA-CB	-6.00	100.51	110.23
1	C	48	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	108	PRO	N-CA-CB	-5.90	98.06	103.31
1	A	76	ARG	CA-CB-CG	-5.89	102.33	114.10
1	D	102	LYS	CB-CG-CD	5.85	124.75	111.30
1	C	222	ARG	CD-NE-CZ	5.83	132.56	124.40
1	C	55	GLU	N-CA-CB	5.80	118.42	110.01
1	A	298	ARG	N-CA-CB	-5.74	101.69	110.12
1	C	290	GLU	CB-CG-CD	5.73	122.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LYS	CB-CG-CD	5.70	124.42	111.30
1	A	290	GLU	CG-CD-OE1	-5.69	105.32	118.40
1	A	226	THR	CA-CB-OG1	-5.68	101.09	109.60
1	C	277	ASN	CB-CA-C	-5.67	104.26	111.86
1	D	107	GLN	CB-CA-C	-5.65	100.44	109.08
1	D	306	GLN	CB-CA-C	5.65	120.83	110.10
1	B	251	GLY	CA-C-N	5.62	125.73	119.32
1	B	251	GLY	C-N-CA	5.62	125.73	119.32
1	A	45	THR	CA-CB-OG1	-5.61	101.19	109.60
1	C	276	MET	CG-SD-CE	-5.59	88.60	100.90
1	D	243	THR	CA-CB-OG1	-5.58	101.24	109.60
1	C	168	PRO	N-CA-C	5.56	121.07	113.84
1	C	55	GLU	CB-CA-C	-5.49	102.26	110.88
1	B	153	ASP	CB-CA-C	5.46	118.54	110.14
1	D	196	THR	N-CA-CB	5.38	117.92	109.69
1	B	25	THR	CA-C-O	-5.38	114.83	120.80
1	C	223	PHE	CA-C-N	-5.37	113.89	122.53
1	C	223	PHE	C-N-CA	-5.37	113.89	122.53
1	D	305	PHE	CA-CB-CG	-5.33	108.47	113.80
1	D	198	THR	CA-CB-OG1	-5.30	101.64	109.60
1	A	137	LYS	N-CA-CB	5.29	117.71	110.57
1	D	111	THR	CA-CB-OG1	-5.28	101.68	109.60
1	B	55	GLU	N-CA-CB	5.26	117.86	110.12
1	B	277	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	270	GLU	N-CA-CB	5.26	117.95	110.16
1	C	214	ASN	CA-CB-CG	-5.23	107.37	112.60
1	D	192	GLN	CB-CA-C	5.20	120.11	109.76
1	A	55	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	168	PRO	N-CA-C	5.19	120.58	113.84
1	D	38	CYS	N-CA-C	5.18	114.10	108.14
1	D	224	THR	OG1-CB-CG2	5.18	119.66	109.30
1	A	270	GLU	CB-CA-C	-5.18	102.05	110.85
1	D	153	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	66	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	135	THR	CA-CB-OG1	5.15	117.32	109.60
1	B	102	LYS	CB-CA-C	-5.12	99.44	110.45
1	C	110	GLN	CB-CG-CD	5.10	121.27	112.60
1	A	240	GLU	CB-CA-C	-5.10	101.47	109.52
1	A	102	LYS	N-CA-CB	5.09	120.99	111.52
1	B	153	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	140	PHE	CA-CB-CG	5.07	118.87	113.80
1	D	181	PHE	N-CA-CB	5.07	117.49	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	THR	OG1-CB-CG2	5.06	119.42	109.30
1	C	243	THR	CA-CB-OG1	-5.06	102.02	109.60
1	C	127	GLN	CG-CD-NE2	-5.03	108.86	116.40
1	C	95	ASN	O-C-N	-5.02	116.51	121.18
1	B	247	VAL	O-C-N	5.00	126.72	121.87

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279[A]	ARG	Sidechain
1	A	60	ARG	Sidechain
1	A	76	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	4	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	217	ARG	Sidechain
1	D	279	ARG	Sidechain
1	D	4	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	2415	2370	2358	15	0
1	B	2346	2298	2286	14	0
1	C	2358	2319	2308	24	0
1	D	2384	2336	2324	13	0
2	A	29	20	0	0	0
2	B	29	20	0	0	0
2	C	29	20	0	0	0
2	D	29	20	0	0	0
3	A	223	0	0	2	0
3	B	200	0	0	3	1
3	C	199	0	0	4	1
3	D	160	0	0	0	0
All	All	10401	9403	9276	58	1

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 3.

All (58) 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:B:298:ARG:NH2	3:B:501:HOH:O	1.87	1.00
1:A:186:VAL:H	1:A:192:GLN:HE22	1.28	0.81
1:A:276:MET:HE2	1:A:285:ALA:HA	1.71	0.71
1:D:228[B]:ASN:ND2	1:D:228[B]:ASN:H	1.90	0.69
1:A:145:CYS:SG	3:A:625:HOH:O	2.34	0.69
1:C:76:ARG:HG3	1:C:76:ARG:HH21	1.60	0.66
1:C:180:ASN:ND2	3:C:501:HOH:O	2.17	0.65
1:A:19:GLN:HE21	1:A:26:THR:HG21	1.63	0.63
1:C:19:GLN:HE21	1:C:26:THR:HG21	1.66	0.60
1:B:58:LEU:HD22	1:B:82:MET:HE3	1.84	0.60
1:C:189:GLN:OE1	3:C:502:HOH:O	2.17	0.58
1:B:92:ASP:OD1	1:B:92:ASP:C	2.45	0.57
1:A:61:LYS:HE3	3:A:583:HOH:O	2.08	0.54
1:C:288:GLU:OE2	3:C:503:HOH:O	2.18	0.53
1:D:47:GLU:HA	1:D:50:LEU:HD23	1.93	0.51
1:C:126:TYR:HD2	1:D:6[A]:MET:HG3	1.75	0.51
1:A:6[B]:MET:HG2	1:B:126:TYR:CD2	2.46	0.51
1:C:86:VAL:HG23	1:C:179:GLY:HA2	1.92	0.51
1:A:191:ALA:CB	1:C:110:GLN:HE22	2.25	0.50
1:B:251:GLY:O	1:B:254:SER:HB3	2.13	0.49
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.93	0.48
1:C:189:GLN:HG3	3:C:502:HOH:O	2.13	0.48
1:D:86[A]:VAL:HG13	1:D:179:GLY:HA2	1.95	0.48
1:C:207:TRP:CE2	1:C:288:GLU:HB3	2.48	0.48
1:D:233:VAL:O	1:D:234:ALA:C	2.56	0.47
1:A:113:SER:O	1:A:149:GLY:HA2	2.14	0.47
1:C:31:TRP:CD2	1:C:95:ASN:HB2	2.50	0.47
1:C:113:SER:O	1:C:149:GLY:HA2	2.15	0.46
1:A:6[B]:MET:HG2	1:B:126:TYR:HD2	1.80	0.46
1:C:276:MET:HE2	1:C:279:ARG:O	2.17	0.45
1:C:62:SER:OG	1:C:64:HIS:CE1	2.70	0.45
1:A:190:THR:HG22	1:A:192:GLN:H	1.82	0.45
1:C:165[A]:MET:HB3	1:C:165[A]:MET:HE2	1.71	0.45
1:B:127:GLN:HG2	3:B:603:HOH:O	2.17	0.44
1:C:1[B]:SER:N	1:D:166:GLU:OE2	2.44	0.44
1:C:277:ASN:HD22	1:C:279:ARG:NH1	2.15	0.44
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:HB2	1:C:110:GLN:HE22	1.82	0.44
1:C:76:ARG:HG3	1:C:76:ARG:NH2	2.30	0.44
1:B:276:MET:HB3	1:B:276:MET:HE2	1.77	0.44
1:D:52:PRO:HD2	1:D:188:ARG:NH1	2.33	0.44
1:B:270[A]:GLU:HG2	3:B:547:HOH:O	2.17	0.44
1:A:61:LYS:HA	1:A:61:LYS:HD3	1.82	0.44
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.68	0.43
1:D:113:SER:O	1:D:149:GLY:HA2	2.18	0.43
1:A:166:GLU:OE2	1:B:1[B]:SER:N	2.43	0.43
1:C:31:TRP:CE2	1:C:95:ASN:HB2	2.54	0.43
1:B:113:SER:O	1:B:149:GLY:HA2	2.19	0.43
1:C:109:GLY:HA2	1:C:200:ILE:HD13	2.00	0.42
1:D:228[B]:ASN:H	1:D:228[B]:ASN:HD22	1.66	0.42
1:C:166:GLU:OE2	1:D:1:SER:HB2	2.20	0.42
1:D:207:TRP:CE2	1:D:288:GLU:HB3	2.54	0.42
1:D:109:GLY:HA2	1:D:200:ILE:HD13	2.01	0.41
1:C:40:ARG:HG3	1:C:54:TYR:CE1	2.56	0.41
1:D:249:ILE:HD13	1:D:249:ILE:HG21	1.80	0.41
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.56	0.41
1:B:5:LYS:HD3	1:B:291:PHE:CZ	2.56	0.41
1:A:6[A]:MET:HE3	1:A:299:GLN:CD	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:615:HOH:O	3:C:599:HOH:O[2_646]	1.99	0.21

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	310/306 (101%)	301 (97%)	8 (3%)	1 (0%)	36	22
1	B	301/306 (98%)	295 (98%)	6 (2%)	0	100	100
1	C	302/306 (99%)	293 (97%)	9 (3%)	0	100	100
1	D	307/306 (100%)	298 (97%)	8 (3%)	1 (0%)	36	22
All	All	1220/1224 (100%)	1187 (97%)	31 (2%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	D	154	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/263 (102%)	265 (98%)	4 (2%)	57	41
1	B	261/263 (99%)	255 (98%)	6 (2%)	44	25
1	C	263/263 (100%)	262 (100%)	1 (0%)	84	78
1	D	265/263 (101%)	258 (97%)	7 (3%)	40	20
All	All	1058/1052 (101%)	1040 (98%)	18 (2%)	53	36

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	55	GLU
1	A	165	MET
1	A	276	MET
1	B	55	GLU
1	B	72	ASN
1	B	74	GLN
1	B	153	ASP
1	B	190	THR

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Mol	Chain	Res	Type
1	B	279	ARG
1	C	217	ARG
1	D	87	LEU
1	D	102	LYS
1	D	217	ARG
1	D	270	GLU
1	D	276	MET
1	D	277	ASN
1	D	279	ARG

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

Mol	Chain	Res	Type
1	A	19	GLN
1	A	164	HIS
1	A	180	ASN
1	A	192	GLN
1	A	238	ASN
1	A	274	ASN
1	A	306	GLN
1	B	19	GLN
1	B	74	GLN
1	B	119	ASN
1	B	277	ASN
1	C	19	GLN
1	C	64	HIS
1	C	110	GLN
1	C	203	ASN
1	C	273	GLN
1	C	274	ASN
1	C	277	ASN
1	D	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1IT2	C	401	-	32,32,32	0.79	1 (3%)	39,44,44	1.35	4 (10%)
2	A1IT2	D	401	-	32,32,32	0.76	1 (3%)	39,44,44	0.94	3 (7%)
2	A1IT2	A	401	-	32,32,32	0.76	1 (3%)	39,44,44	1.53	5 (12%)
2	A1IT2	B	401	-	32,32,32	0.88	1 (3%)	39,44,44	1.20	4 (10%)

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	A1IT2	C	401	-	-	3/21/33/33	0/4/4/4
2	A1IT2	D	401	-	-	3/21/33/33	0/4/4/4
2	A1IT2	A	401	-	-	2/21/33/33	0/4/4/4
2	A1IT2	B	401	-	-	3/21/33/33	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	A1IT2	C6-C5	2.28	1.43	1.38
2	D	401	A1IT2	C13-N2	2.16	1.47	1.44
2	B	401	A1IT2	C22-C21	2.06	1.42	1.38
2	A	401	A1IT2	C9-C10	2.04	1.55	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1IT2	O2-C10-C9	5.84	127.63	122.31
2	C	401	A1IT2	C8-C9-C3	5.01	105.43	103.44
2	A	401	A1IT2	C13-N2-C12	-4.41	114.23	121.58
2	B	401	A1IT2	C14-N2-C12	-3.52	115.72	121.58
2	B	401	A1IT2	C13-N2-C12	3.03	126.64	121.58
2	A	401	A1IT2	C14-N2-C12	2.89	126.41	121.58
2	B	401	A1IT2	C8-C7-C2	-2.82	105.45	107.79
2	D	401	A1IT2	C13-N2-C12	-2.75	116.99	121.58
2	C	401	A1IT2	C13-N2-C12	-2.65	117.16	121.58
2	C	401	A1IT2	C5-C4-C3	-2.39	118.13	120.99
2	C	401	A1IT2	O2-C10-N1	2.20	127.63	122.98
2	A	401	A1IT2	O2-C10-N1	-2.19	118.34	122.98
2	D	401	A1IT2	C14-N2-C13	2.16	122.55	117.88
2	A	401	A1IT2	C12-C11-N1	-2.13	105.64	110.90
2	D	401	A1IT2	O2-C10-C9	2.04	124.17	122.31
2	B	401	A1IT2	O1-C7-C2	2.03	129.64	126.56

There are no chirality outliers.

All (11) torsion outliers are listed below:

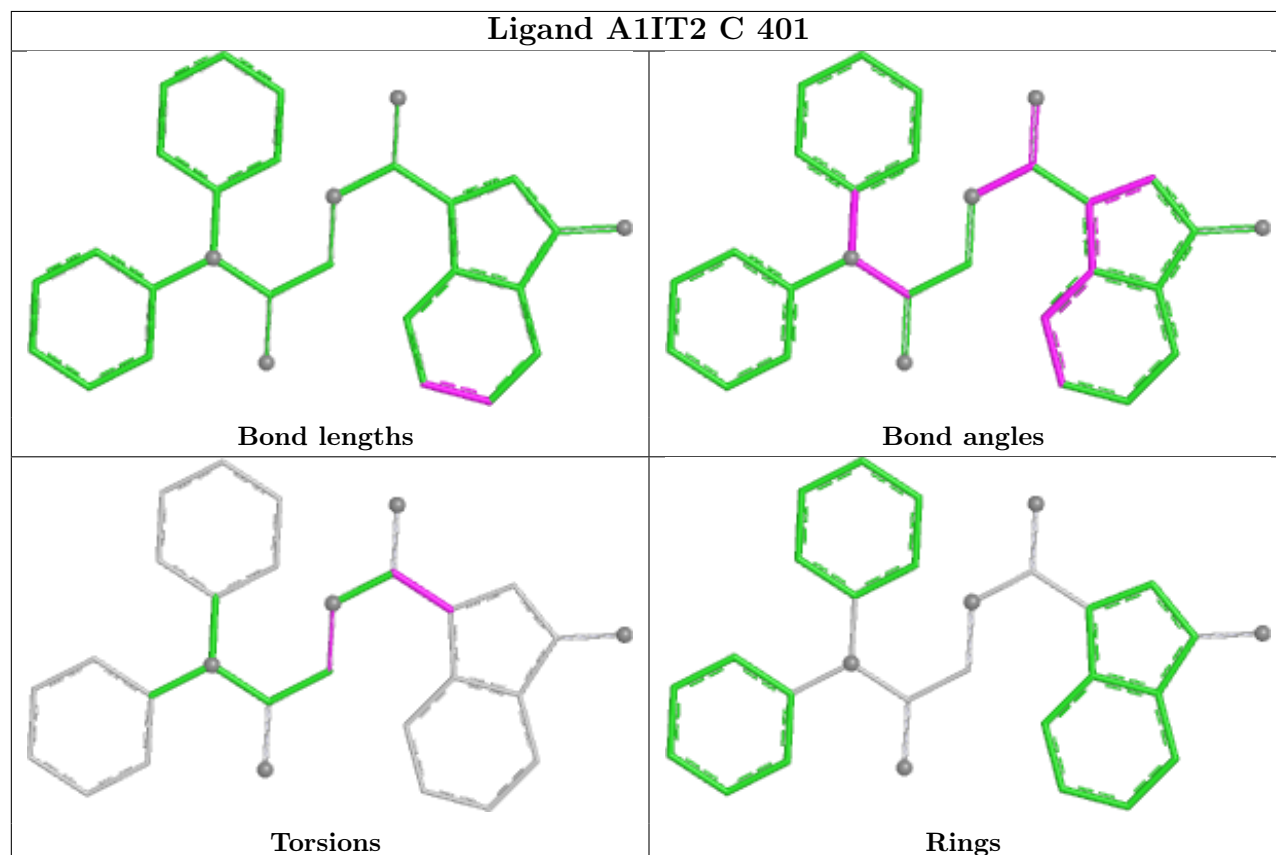
Mol	Chain	Res	Type	Atoms
2	B	401	A1IT2	N1-C10-C9-C8
2	B	401	A1IT2	O2-C10-C9-C8
2	C	401	A1IT2	N1-C10-C9-C8
2	A	401	A1IT2	N1-C10-C9-C8
2	A	401	A1IT2	O2-C10-C9-C8
2	C	401	A1IT2	O2-C10-C9-C8
2	D	401	A1IT2	N1-C10-C9-C8
2	D	401	A1IT2	O2-C10-C9-C8
2	D	401	A1IT2	C12-C11-N1-C10
2	B	401	A1IT2	C12-C11-N1-C10
2	C	401	A1IT2	C12-C11-N1-C10

There are no ring outliers.

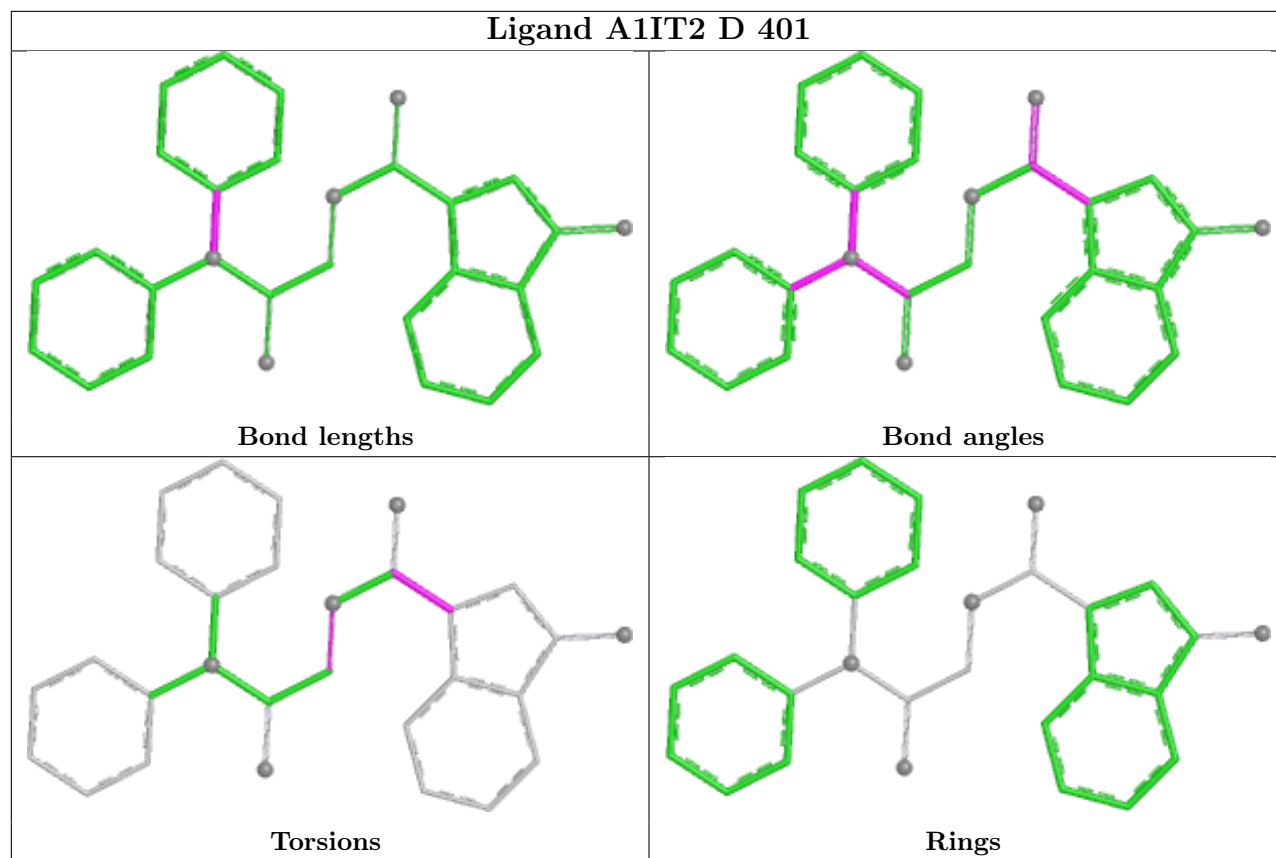
No monomer is involved in short contacts.

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

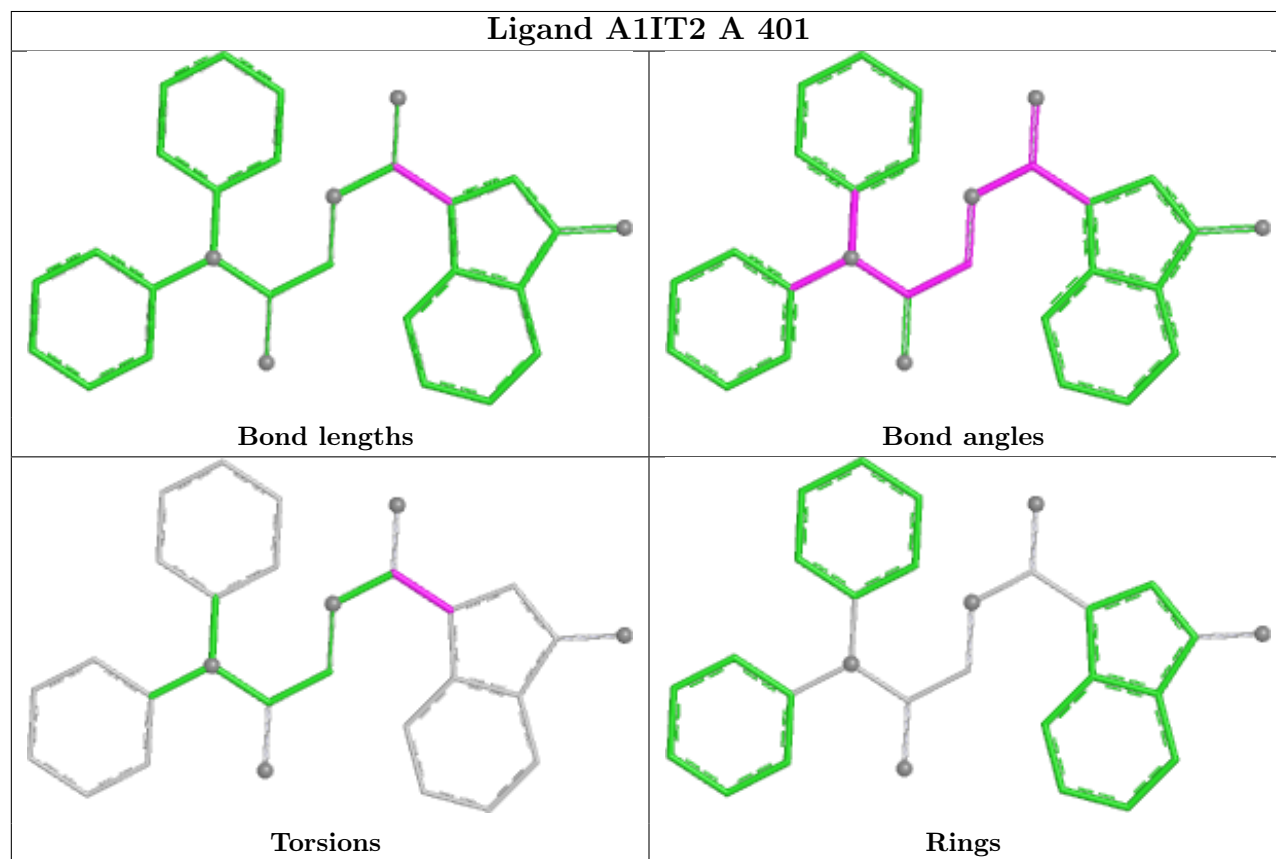
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

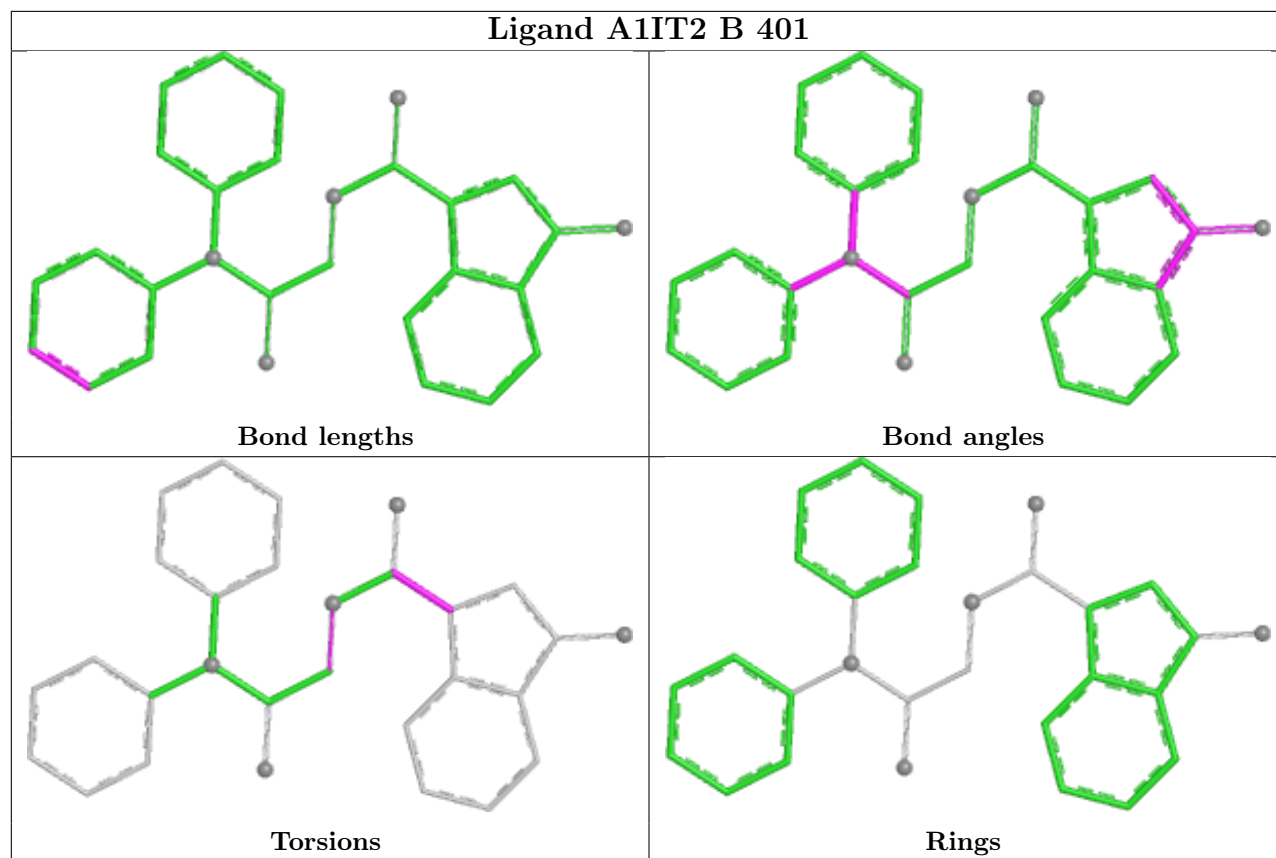


Ligand A1IT2 D 401



Ligand A1IT2 A 401





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	306/306 (100%)	-0.43	1 (0%) 90 93	8, 23, 43, 67	6 (1%)
1	B	301/306 (98%)	-0.39	2 (0%) 84 88	10, 24, 44, 63	3 (0%)
1	C	301/306 (98%)	-0.35	2 (0%) 84 88	11, 25, 46, 66	4 (1%)
1	D	306/306 (100%)	-0.20	3 (0%) 79 85	12, 27, 49, 68	3 (0%)
All	All	1214/1224 (99%)	-0.34	8 (0%) 84 88	8, 25, 46, 68	16 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	PHE	3.2
1	A	50	LEU	3.2
1	C	301	SER	3.1
1	B	301	SER	2.9
1	B	223	PHE	2.6
1	D	224	THR	2.3
1	C	154	TYR	2.2
1	D	222	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

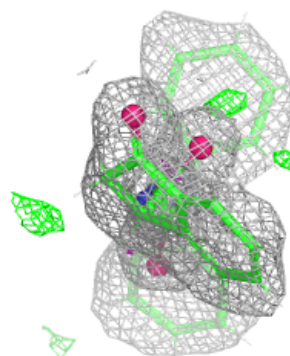
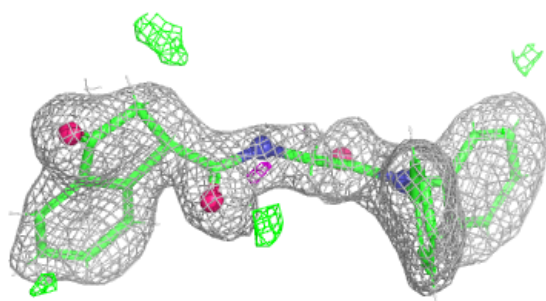
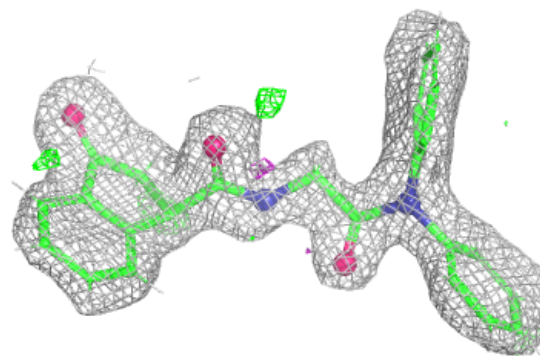
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1IT2	D	401	29/29	0.89	0.10	32,41,51,52	0
2	A1IT2	A	401	29/29	0.94	0.08	22,31,41,45	0
2	A1IT2	C	401	29/29	0.97	0.05	14,20,24,25	0
2	A1IT2	B	401	29/29	0.98	0.04	14,17,21,22	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.

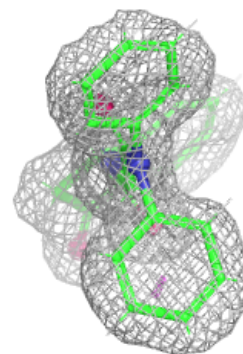
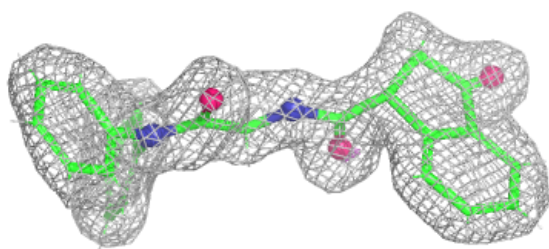
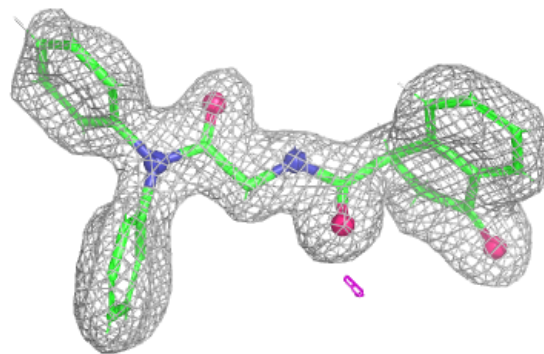
Electron density around A1IT2 D 401:

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

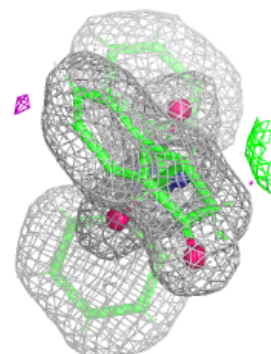
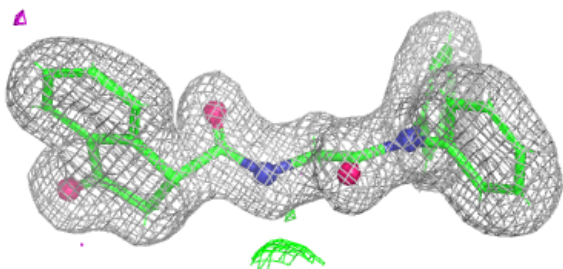
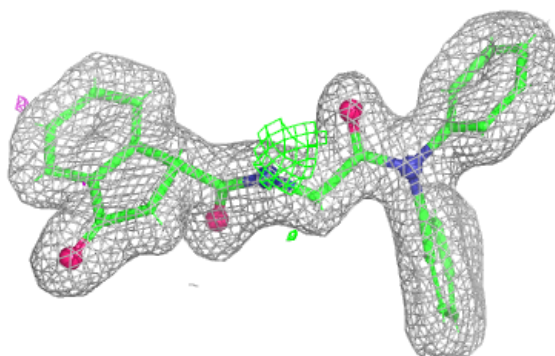


Electron density around A1IT2 A 401:

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

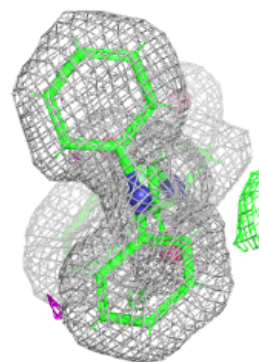
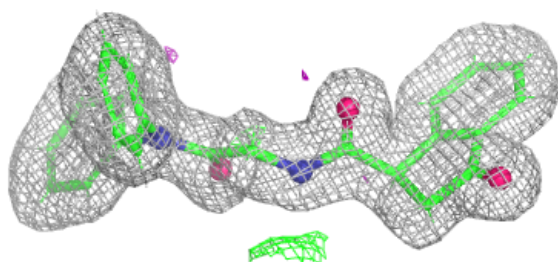
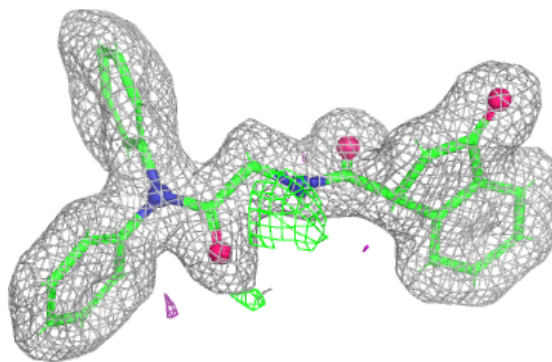
**Electron density around A1IT2 C 401:**

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



Electron density around A1IT2 B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.