



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 05:59 PM UTC

PDB ID : 6AZJ / pdb_00006azj
Title : Crystal Structure of human NAMPT in complex with NVP-LQN520
Authors : Weihofen, W.A.; Thigale, S.
Deposited on : 2017-09-11
Resolution : 2.53 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

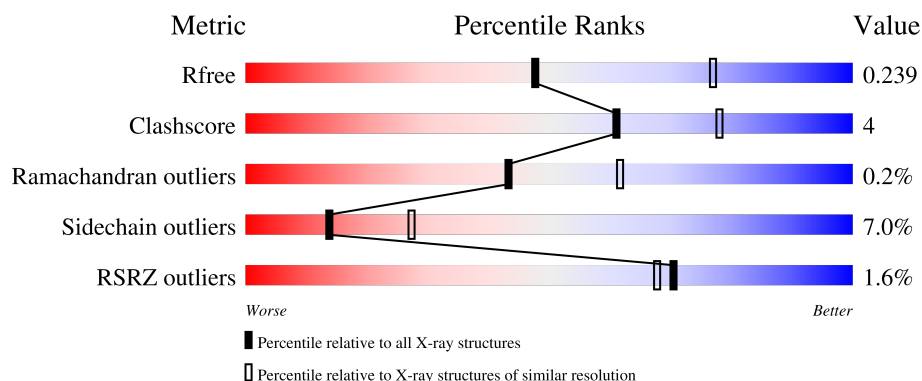
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	495	75% 17% • 6%
1	B	495	2% 75% 17% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7790 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3738	2405	618	708	7			
1	B	462	Total	C	N	O	S	0	0	0
			3701	2383	611	700	7			

There are 34 discrepancies between the modelled and reference sequences:

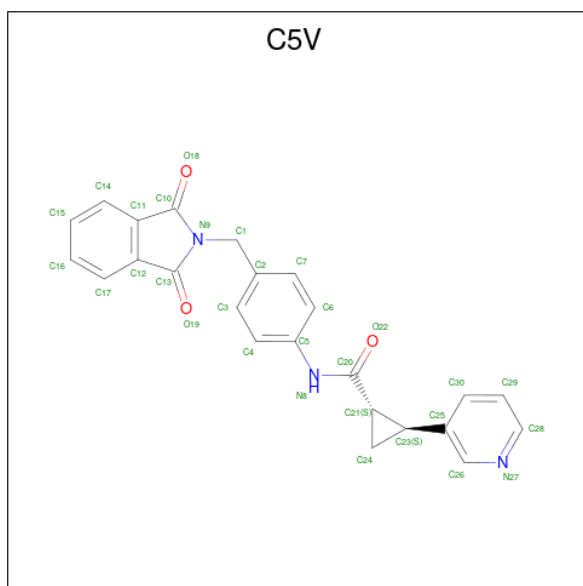
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P43490
A	-8	HIS	-	expression tag	UNP P43490
A	-7	HIS	-	expression tag	UNP P43490
A	-6	HIS	-	expression tag	UNP P43490
A	-5	HIS	-	expression tag	UNP P43490
A	-4	HIS	-	expression tag	UNP P43490
A	-3	HIS	-	expression tag	UNP P43490
A	-2	SER	-	expression tag	UNP P43490
A	-1	ALA	-	expression tag	UNP P43490
A	0	ALA	-	expression tag	UNP P43490
A	1	GLU	-	expression tag	UNP P43490
A	2	ASN	-	expression tag	UNP P43490
A	3	LEU	-	expression tag	UNP P43490
A	4	TYR	-	expression tag	UNP P43490
A	5	PHE	-	expression tag	UNP P43490
A	6	GLN	-	expression tag	UNP P43490
A	7	GLY	-	expression tag	UNP P43490
B	-9	ALA	-	expression tag	UNP P43490
B	-8	HIS	-	expression tag	UNP P43490
B	-7	HIS	-	expression tag	UNP P43490
B	-6	HIS	-	expression tag	UNP P43490
B	-5	HIS	-	expression tag	UNP P43490
B	-4	HIS	-	expression tag	UNP P43490
B	-3	HIS	-	expression tag	UNP P43490
B	-2	SER	-	expression tag	UNP P43490

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ALA	-	expression tag	UNP P43490
B	0	ALA	-	expression tag	UNP P43490
B	1	GLU	-	expression tag	UNP P43490
B	2	ASN	-	expression tag	UNP P43490
B	3	LEU	-	expression tag	UNP P43490
B	4	TYR	-	expression tag	UNP P43490
B	5	PHE	-	expression tag	UNP P43490
B	6	GLN	-	expression tag	UNP P43490
B	7	GLY	-	expression tag	UNP P43490

- Molecule 2 is (1S,2S)-N-{4-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]phenyl}-2-(pyridin-3-yl)cyclopropane-1-carboxamide (CCD ID: C5V) (formula: C₂₄H₁₉N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	3	3		
2	B	1	Total	C	N	O	0	0
			30	24	3	3		

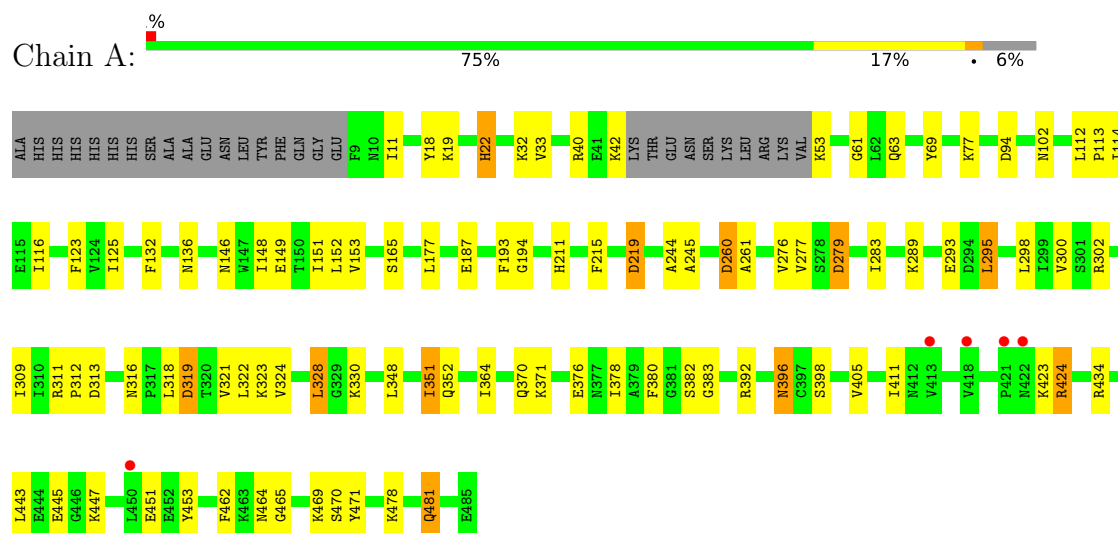
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		
3	B	144	Total	O	0	0
			144	144		

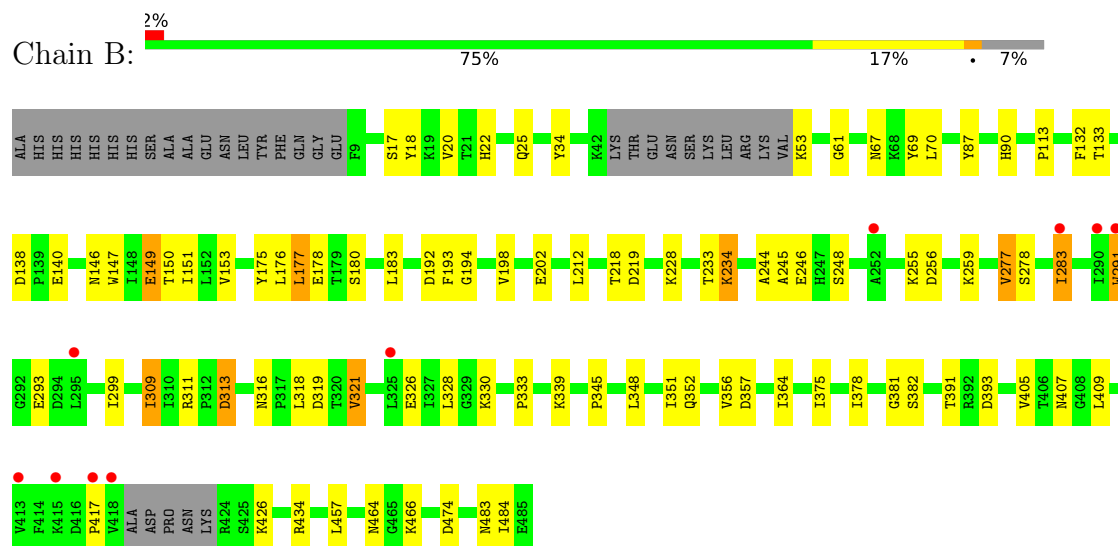
3 Residue-property plots

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: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.23Å 157.72Å 192.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.09 – 2.53 96.09 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.09-2.53) 99.9 (96.09-2.53)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.171 , 0.229 0.177 , 0.239	Depositor DCC
R_{free} test set	1824 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7790	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: C5V

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	0.87	1/3826 (0.0%)	1.37	24/5183 (0.5%)
1	B	0.87	0/3787	1.39	35/5128 (0.7%)
All	All	0.87	1/7613 (0.0%)	1.38	59/10311 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	SER	CA-C	5.12	1.59	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	GLY	N-CA-C	8.35	123.67	114.40
1	A	193	PHE	CA-CB-CG	7.77	121.57	113.80
1	A	260	ASP	CA-CB-CG	7.28	119.88	112.60
1	A	22	HIS	N-CA-C	6.40	119.07	111.71
1	B	234	LYS	N-CA-C	-6.39	103.83	111.69
1	A	276	VAL	CA-C-N	6.38	129.06	120.50
1	A	276	VAL	C-N-CA	6.38	129.06	120.50
1	B	278	SER	N-CA-C	6.38	120.55	113.21
1	B	313	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	192	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	132	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	255	LYS	CA-C-N	5.97	129.38	120.31
1	B	255	LYS	C-N-CA	5.97	129.38	120.31
1	B	22	HIS	N-CA-C	5.96	118.56	111.71
1	A	481	GLN	CB-CA-C	-5.95	98.59	110.42
1	B	357	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	391	THR	CA-C-N	5.64	128.40	120.28
1	B	391	THR	C-N-CA	5.64	128.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	VAL	CB-CA-C	5.58	117.71	111.80
1	A	378	ILE	N-CA-C	5.55	117.33	108.89
1	B	70	LEU	N-CA-C	5.51	120.13	113.41
1	B	228	LYS	CA-C-N	5.45	128.03	120.29
1	B	228	LYS	C-N-CA	5.45	128.03	120.29
1	A	219	ASP	N-CA-C	-5.43	105.31	113.89
1	B	291	TRP	CA-C-N	5.40	126.93	120.13
1	B	291	TRP	C-N-CA	5.40	126.93	120.13
1	B	61	GLY	N-CA-C	5.36	121.13	114.37
1	B	405	VAL	N-CA-CB	5.35	118.41	111.67
1	A	302	ARG	N-CA-C	5.33	117.59	110.35
1	A	451	GLU	CA-C-N	5.32	127.41	120.28
1	A	451	GLU	C-N-CA	5.32	127.41	120.28
1	B	132	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	279	ASP	N-CA-C	5.26	119.33	113.02
1	B	483	ASN	CA-C-N	5.25	129.26	120.64
1	B	483	ASN	C-N-CA	5.25	129.26	120.64
1	B	378	ILE	CA-C-N	5.24	130.82	121.75
1	B	378	ILE	C-N-CA	5.24	130.82	121.75
1	A	61	GLY	N-CA-C	5.20	120.92	114.37
1	B	149	GLU	CA-C-N	5.14	127.94	120.79
1	B	149	GLU	C-N-CA	5.14	127.94	120.79
1	B	474	ASP	CA-C-N	5.12	127.10	120.44
1	B	474	ASP	C-N-CA	5.12	127.10	120.44
1	B	407	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	69	TYR	N-CA-C	5.11	120.16	113.88
1	A	424	ARG	CB-CA-C	5.08	120.52	110.42
1	B	67	ASN	N-CA-C	5.07	116.62	111.14
1	A	376	GLU	CA-C-N	5.07	128.02	120.31
1	A	376	GLU	C-N-CA	5.07	128.02	120.31
1	B	87	TYR	CA-C-N	5.07	127.33	120.38
1	B	87	TYR	C-N-CA	5.07	127.33	120.38
1	A	261	ALA	CA-C-N	5.07	127.03	120.44
1	A	261	ALA	C-N-CA	5.07	127.03	120.44
1	A	392	ARG	CA-C-N	5.06	129.18	120.72
1	A	392	ARG	C-N-CA	5.06	129.18	120.72
1	B	426	LYS	N-CA-C	-5.05	103.05	110.52
1	A	380	PHE	CA-C-N	5.04	125.08	121.65
1	A	380	PHE	C-N-CA	5.04	125.08	121.65
1	B	198	VAL	CA-C-N	5.04	129.14	120.72
1	B	198	VAL	C-N-CA	5.04	129.14	120.72

There are no chirality outliers.

There are no planarity outliers.

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	3738	0	3718	37	0
1	B	3701	0	3682	30	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	147	0	0	2	0
3	B	144	0	0	1	0
All	All	7790	0	7400	63	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 4.

All (63) 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:113:PRO:HA	1:A:464:ASN:HD22	1.40	0.86
1:A:316:ASN:HB3	1:A:319:ASP:HB2	1.67	0.75
1:B:291:TRP:HE3	1:B:299:ILE:HD11	1.60	0.67
1:B:193:PHE:CE2	1:B:381:GLY:HA3	2.32	0.65
1:A:244:ALA:HB3	1:B:18:TYR:HB2	1.80	0.62
1:A:316:ASN:HD22	1:A:319:ASP:H	1.50	0.60
1:B:321:VAL:HG23	1:B:352:GLN:HE21	1.66	0.59
1:B:277:VAL:HA	1:B:311:ARG:HB2	1.83	0.59
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.69	0.58
1:A:63:GLN:HE22	1:A:471:TYR:H	1.52	0.58
1:B:328:LEU:HD22	1:B:348:LEU:HD21	1.87	0.56
1:A:328:LEU:HG	1:A:348:LEU:HD21	1.88	0.56
1:A:445:GLU:HB2	1:A:447:LYS:HE2	1.89	0.55
1:A:311:ARG:HG2	1:A:351:ILE:HG23	1.89	0.55
1:A:33:VAL:H	1:A:136:ASN:HD21	1.54	0.54
1:B:356:VAL:O	1:B:382:SER:OG	2.24	0.54
1:A:149:GLU:O	1:A:153:VAL:HG23	2.08	0.53
1:B:177:LEU:HD22	1:B:183:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HD11	1:A:453:TYR:HD2	1.72	0.53
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.75	0.51
1:B:69:TYR:OH	1:B:202:GLU:OE2	2.29	0.51
1:B:283:ILE:HG12	1:B:313:ASP:HB3	1.93	0.51
1:A:113:PRO:HA	1:A:464:ASN:ND2	2.19	0.50
1:B:212:LEU:HD11	1:B:218:THR:HG21	1.93	0.49
1:A:453:TYR:HA	3:A:646:HOH:O	2.13	0.48
1:A:148:ILE:HD12	1:A:152:LEU:HD11	1.94	0.48
1:A:312:PRO:HD3	1:A:351:ILE:O	2.14	0.47
1:A:194:GLY:HA2	1:A:383:GLY:HA2	1.95	0.47
1:A:40:ARG:HB2	1:A:396:ASN:HB3	1.97	0.47
1:A:112:LEU:O	1:A:464:ASN:HA	2.14	0.47
1:A:245:ALA:HA	1:B:25:GLN:HE22	1.80	0.47
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.97	0.47
1:A:18:TYR:HB2	1:B:244:ALA:HB3	1.97	0.46
1:A:22:HIS:CE1	1:B:246:GLU:HG2	2.51	0.46
1:A:283:ILE:HD11	1:A:324:VAL:HG22	1.97	0.46
1:B:245:ALA:O	1:B:277:VAL:HG12	2.16	0.46
1:A:19:LYS:HD3	1:A:146:ASN:O	2.16	0.46
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.98	0.45
1:A:289:LYS:O	1:A:293:GLU:HB2	2.17	0.45
1:B:311:ARG:HG2	1:B:351:ILE:HG23	1.99	0.45
1:B:34:TYR:OH	1:B:133:THR:HG21	2.18	0.44
1:B:150:THR:HB	3:B:628:HOH:O	2.17	0.44
1:A:116:ILE:HB	1:A:462:PHE:HB3	2.00	0.44
1:A:295:LEU:HG	1:A:298:LEU:HD12	1.99	0.44
1:B:149:GLU:O	1:B:153:VAL:HG23	2.18	0.44
1:B:316:ASN:HB3	1:B:319:ASP:HB2	1.98	0.44
1:B:20:VAL:HA	1:B:147:TRP:CZ3	2.53	0.43
1:B:17:SER:OG	1:B:90:HIS:NE2	2.48	0.43
1:B:176:LEU:HD23	1:B:183:LEU:HA	1.99	0.43
1:B:309:ILE:HG22	1:B:351:ILE:HG22	2.00	0.43
1:B:318:LEU:HD13	1:B:364:ILE:HA	2.00	0.43
1:A:465:GLY:HA2	3:A:628:HOH:O	2.19	0.42
1:A:63:GLN:HE22	1:A:471:TYR:N	2.17	0.42
1:B:291:TRP:CE3	1:B:299:ILE:HD11	2.48	0.42
1:A:123:PHE:HB3	1:A:125:ILE:HD11	2.02	0.41
1:B:333:PRO:HD2	1:B:345:PRO:HG3	2.01	0.41
1:A:211:HIS:CE1	1:A:215:PHE:CD2	3.08	0.41
1:A:279:ASP:HB3	1:A:313:ASP:HA	2.03	0.41
1:B:138:ASP:OD1	1:B:140:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HD13	1:A:112:LEU:HD11	2.02	0.41
1:A:136:ASN:ND2	1:A:136:ASN:H	2.19	0.41
1:A:318:LEU:HD13	1:A:364:ILE:HA	2.03	0.41
1:A:32:LYS:HB3	1:A:405:VAL:HB	2.03	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	463/495 (94%)	441 (95%)	22 (5%)	0	100	100
1	B	456/495 (92%)	434 (95%)	20 (4%)	2 (0%)	30	47
All	All	919/990 (93%)	875 (95%)	42 (5%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	LYS
1	B	417	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/435 (94%)	378 (92%)	33 (8%)	11	22
1	B	407/435 (94%)	383 (94%)	24 (6%)	18	35
All	All	818/870 (94%)	761 (93%)	57 (7%)	14	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	53	LYS
1	A	77	LYS
1	A	94	ASP
1	A	102	ASN
1	A	114	ILE
1	A	151	ILE
1	A	177	LEU
1	A	187	GLU
1	A	219	ASP
1	A	260	ASP
1	A	277	VAL
1	A	295	LEU
1	A	300	VAL
1	A	319	ASP
1	A	322	LEU
1	A	323	LYS
1	A	328	LEU
1	A	330	LYS
1	A	351	ILE
1	A	370	GLN
1	A	371	LYS
1	A	382	SER
1	A	396	ASN
1	A	398	SER
1	A	411	ILE
1	A	423	LYS
1	A	424	ARG
1	A	434	ARG
1	A	469	LYS
1	A	470	SER
1	A	478	LYS

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Mol	Chain	Res	Type
1	A	481	GLN
1	B	53	LYS
1	B	146	ASN
1	B	151	ILE
1	B	177	LEU
1	B	178	GLU
1	B	180	SER
1	B	219	ASP
1	B	233	THR
1	B	234	LYS
1	B	248	SER
1	B	256	ASP
1	B	259	LYS
1	B	283	ILE
1	B	293	GLU
1	B	309	ILE
1	B	321	VAL
1	B	326	GLU
1	B	339	LYS
1	B	393	ASP
1	B	409	LEU
1	B	434	ARG
1	B	457	LEU
1	B	466	LYS
1	B	484	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	129	ASN
1	A	136	ASN
1	A	154	GLN
1	A	164	ASN
1	A	201	GLN
1	A	316	ASN
1	A	362	GLN
1	A	396	ASN
1	A	412	ASN
1	A	422	ASN
1	A	433	HIS
1	A	464	ASN

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Mol	Chain	Res	Type
1	B	25	GLN
1	B	102	ASN
1	B	146	ASN
1	B	154	GLN
1	B	164	ASN
1	B	201	GLN
1	B	247	HIS
1	B	257	HIS
1	B	285	ASN
1	B	407	ASN
1	B	412	ASN
1	B	433	HIS
1	B	455	GLN
1	B	464	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 [i](#)

2 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	C5V	B	501	-	34,34,34	1.40	3 (8%)	49,49,49	1.91	15 (30%)
2	C5V	A	501	-	34,34,34	1.55	5 (14%)	49,49,49	1.71	11 (22%)

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	C5V	B	501	-	-	6/16/37/37	0/5/5/5
2	C5V	A	501	-	-	2/16/37/37	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	C5V	C13-N9	-3.77	1.35	1.39
2	B	501	C5V	C10-N9	-3.04	1.36	1.39
2	A	501	C5V	C10-N9	-3.03	1.36	1.39
2	B	501	C5V	C13-N9	-2.75	1.36	1.39
2	A	501	C5V	C24-C23	2.59	1.54	1.50
2	B	501	C5V	C24-C23	2.39	1.54	1.50
2	A	501	C5V	C26-C25	2.16	1.42	1.39
2	A	501	C5V	C24-C21	2.10	1.55	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C5V	C12-C13-N9	4.93	109.53	105.88
2	B	501	C5V	C11-C10-N9	4.50	109.21	105.88
2	B	501	C5V	C12-C13-N9	4.40	109.14	105.88
2	A	501	C5V	C11-C10-N9	3.97	108.81	105.88
2	B	501	C5V	C24-C21-C20	3.86	124.54	117.83
2	A	501	C5V	C24-C21-C20	3.32	123.59	117.83
2	A	501	C5V	C11-C12-C13	-3.15	105.50	108.26
2	B	501	C5V	O18-C10-N9	3.11	127.94	124.79
2	B	501	C5V	C28-N27-C26	3.02	122.14	116.85
2	B	501	C5V	O22-C20-C21	-3.01	118.06	121.67
2	B	501	C5V	O18-C10-C11	-3.01	122.83	128.66
2	A	501	C5V	C12-C11-C10	-2.94	105.69	108.26
2	B	501	C5V	O19-C13-N9	2.93	127.76	124.79
2	B	501	C5V	O19-C13-C12	-2.87	123.09	128.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C5V	C12-C11-C10	-2.79	105.82	108.26
2	B	501	C5V	C11-C12-C13	-2.74	105.86	108.26
2	A	501	C5V	C28-N27-C26	2.62	121.45	116.85
2	B	501	C5V	C25-C26-N27	-2.54	120.09	124.05
2	A	501	C5V	O19-C13-C12	-2.48	123.85	128.66
2	B	501	C5V	C10-N9-C13	-2.40	109.97	112.02
2	B	501	C5V	C25-C23-C21	-2.27	116.25	120.67
2	A	501	C5V	O18-C10-C11	-2.23	124.34	128.66
2	A	501	C5V	C10-N9-C13	-2.17	110.17	112.02
2	A	501	C5V	C23-C21-C20	-2.16	111.49	116.81
2	B	501	C5V	C5-N8-C20	-2.10	122.59	127.37
2	A	501	C5V	C14-C11-C10	2.00	132.95	129.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

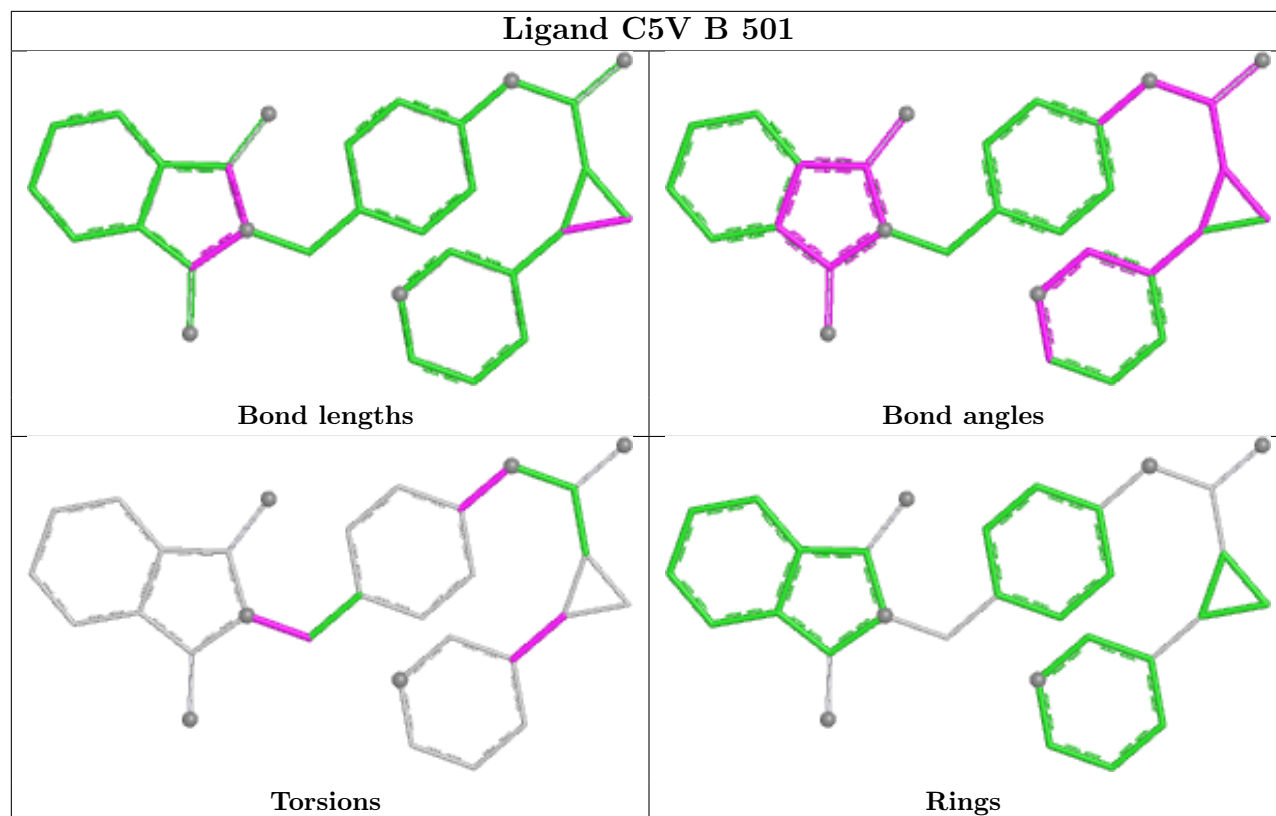
Mol	Chain	Res	Type	Atoms
2	B	501	C5V	C21-C23-C25-C26
2	B	501	C5V	C21-C23-C25-C30
2	B	501	C5V	C24-C23-C25-C26
2	B	501	C5V	C6-C5-N8-C20
2	A	501	C5V	C24-C23-C25-C26
2	A	501	C5V	C24-C23-C25-C30
2	B	501	C5V	C24-C23-C25-C30
2	B	501	C5V	C2-C1-N9-C13

There are no ring outliers.

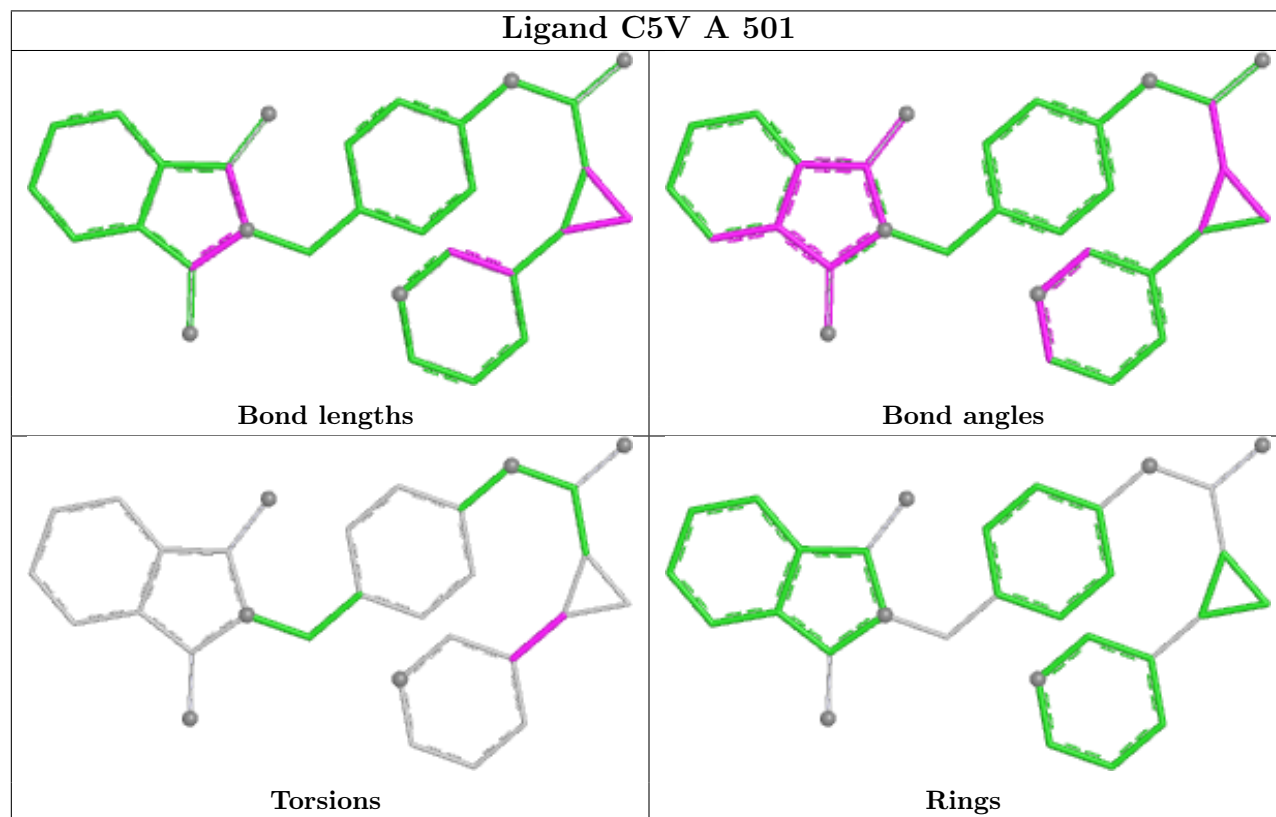
No monomer is involved in short contacts.

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 C5V B 501



Ligand C5V A 501



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	467/495 (94%)	-0.10	5 (1%) 78 76	21, 45, 75, 115	0
1	B	462/495 (93%)	-0.01	10 (2%) 62 59	21, 47, 88, 157	0
All	All	929/990 (93%)	-0.06	15 (1%) 70 68	21, 45, 86, 157	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	VAL	6.2
1	B	413	VAL	3.4
1	B	417	PRO	3.3
1	A	413	VAL	3.0
1	B	291	TRP	2.6
1	B	415	LYS	2.6
1	A	418	VAL	2.6
1	B	283	ILE	2.4
1	B	290	ILE	2.3
1	B	295	LEU	2.2
1	A	422	ASN	2.2
1	A	450	LEU	2.2
1	B	252	ALA	2.1
1	A	421	PRO	2.1
1	B	325	LEU	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 ⓘ

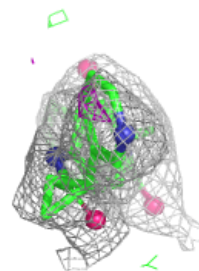
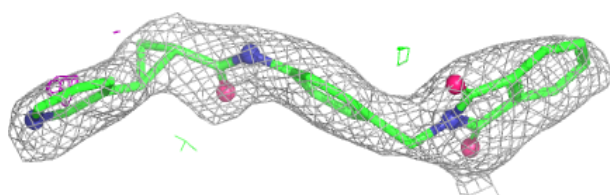
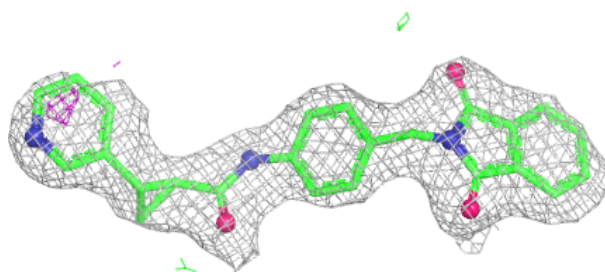
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

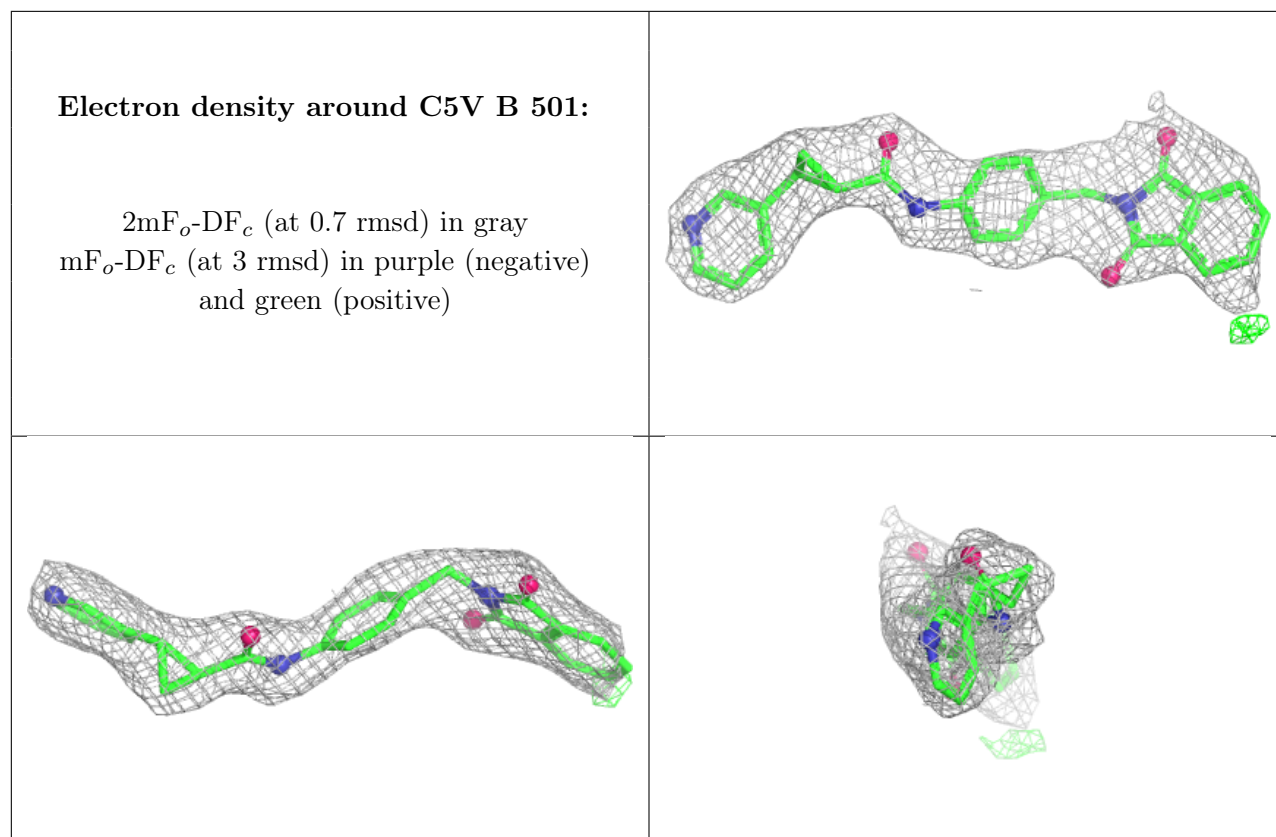
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C5V	A	501	30/30	0.88	0.11	45,52,65,66	0
2	C5V	B	501	30/30	0.89	0.12	50,57,67,70	0

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 C5V A 501:

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.