



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:14 am BST

PDB ID : 3G8E
Title : Crystal Structure of Rattus norvegicus Visfatin/PBEF/Nampt in Complex with an FK866-based inhibitor
Authors : Kang, G.B.; Bae, M.H.; Kim, M.K.; Im, I.; Kim, Y.C.; Eom, S.H.
Deposited on : 2009-02-12
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

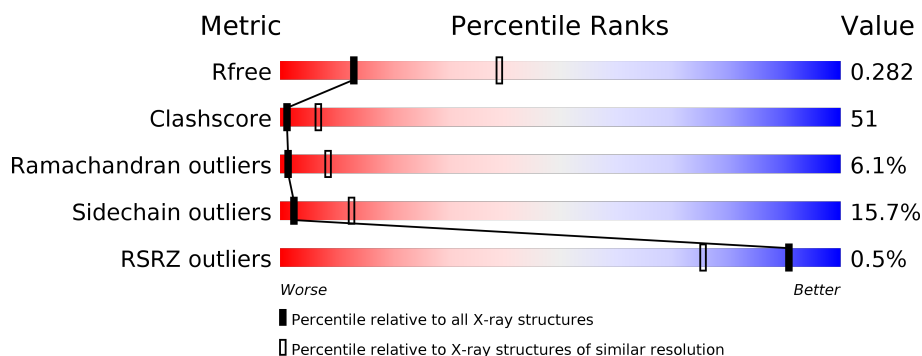
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	491	<div> <div></div> <div> <div></div> <div>31%</div> <div>50%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	491	<div> <div></div> <div> <div></div> <div>34%</div> <div>45%</div> <div>14%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IS1	A	501	-	-	-	X
2	IS1	B	502	-	-	-	X

2 Entry composition [i](#)

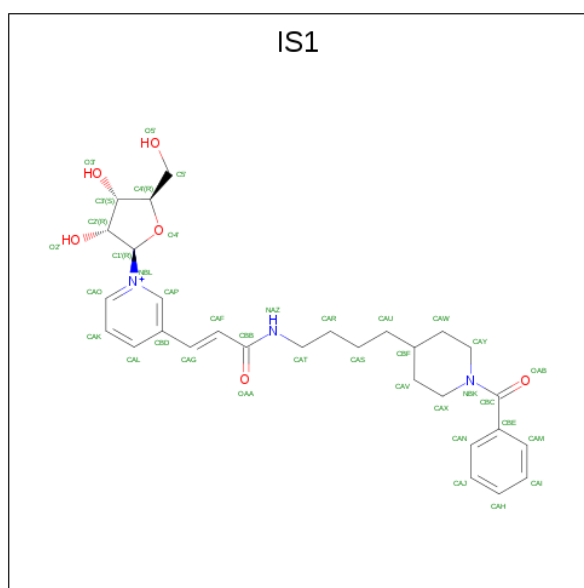
There are 2 unique types of molecules in this entry. The entry contains 7476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is 3-[(1E)-3-oxo-3-({4-[1-(phenylcarbonyl)piperidin-4-yl]butyl}amino)prop-1-en-1-yl]-1-beta-D-ribofuranosylpyridinium (three-letter code: IS1) (formula: C₂₉H₃₈N₃O₆).

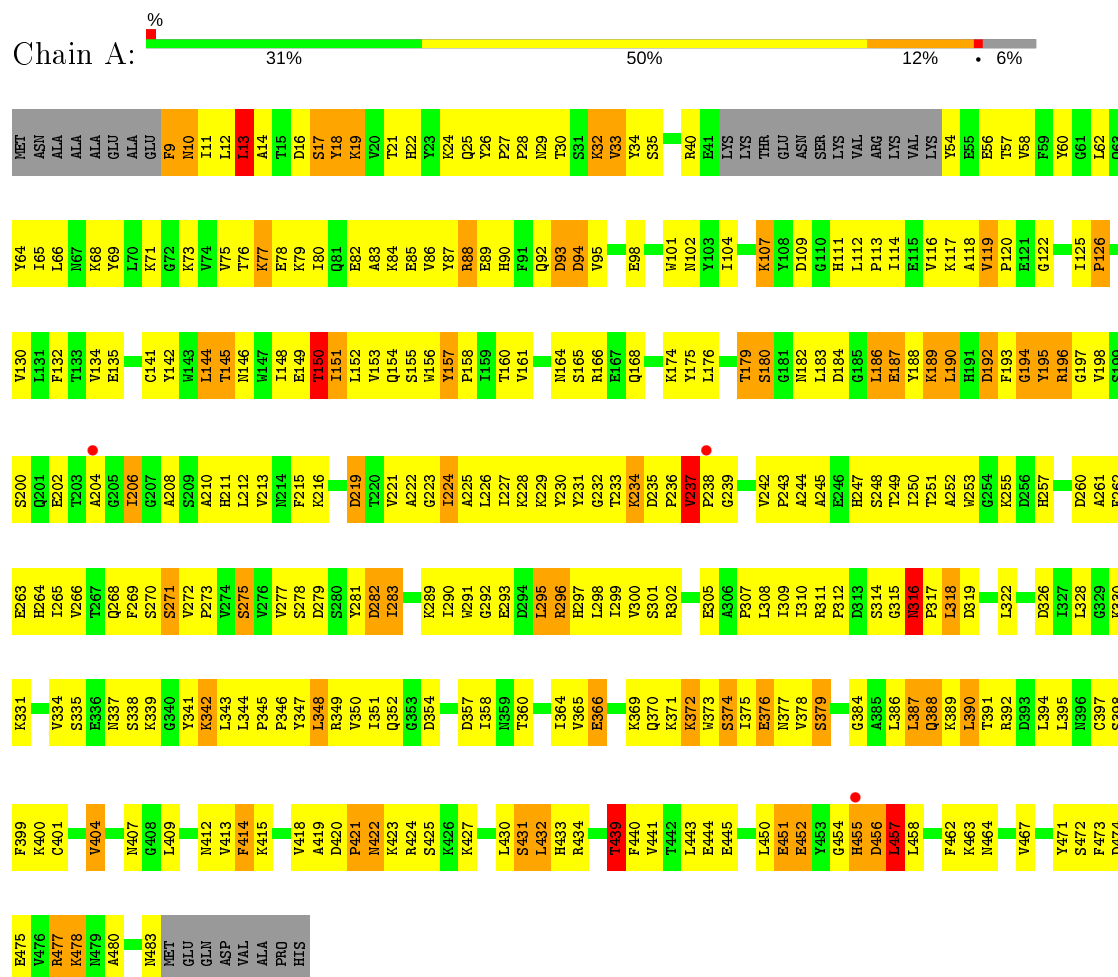


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	29	3	6		
2	B	1	Total	C	N	O	0	0
			38	29	3	6		

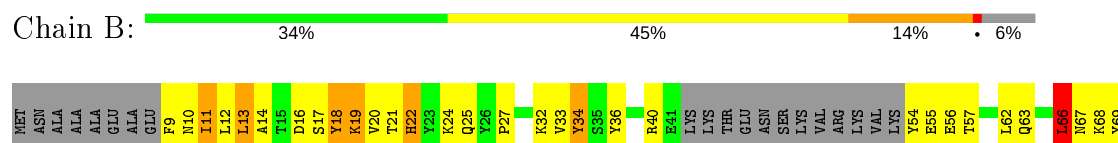
3 Residue-property plots

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: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase



K423	K424	S425	K426	K427	K428	K429	L430	S431	L432	K433		T439	F440		L443	E444	E445	O446	K447	G448	D449	L450	E451	E452	Y453	G454	L455	D456	L457	L458		F462	K463	K464		K469	S470	K471	S472	F473	D474	E475		Q481	L482	K483	MET	GLU	GLN	ASP	VAL	ALA	PRO	HIS					
D354	G355		I358	N359	T360		I364	V365	E366	G367	N368		K371	K372	K373	S374	I375	E376	N377	V378	S379	F380	G381		G384	A385	L386	L387	Q388	K389	L390	I391	R392	D393	L394	L395		S398	F399	K400		V404	V405	T406	N407	G408	L409	G410	V411	N412	V413	F414	K415		V418	K419	D420	P421	N422
A204	G205	I206		H211	L212		D219	T220	V221		I224	A225	L226	I227		Y231	G232	T233	K234	D235	P236	Y237	P238	G239		V242	P243	A244		T249	I250	T251	A252	W253		K259		F262	E263	H264	I265	V266	T267	Q268	F269		V272	P273	V274	S275	V276	V277	S278	D279	S280	Y281	D282	I283	
A286	C287	E288	K289	I290	K291	E292	E293	D294	L295	R296		I299	V300		T304	A306	P307	L308	I309	I310	R311	P312	D313	S314		L318		V321	L322	K323	V324	L325	D326	I327	L328		K331	F332	P333	V334		K337	S338	K339	G340	Y341	K342	L343	L344	F345	P346	Y347	L348	R349	V350	I351	Q352	G353	
L70	K71	G72	K73	V74	V75	T76	K77	E78	K79	I80	Q81	E82	A83	K84	E85	V86	Y87	R88	E89	S89	F91	Q92	D93	D94	V95		E98	R99	G100	W101	N102	Y103	I104	L105		D109	G110	H111	L112	P113	I114	E115	V116	K117	A118	V119	P120		S123	V124	I125	P126	R127		V130	L131	F132	T133	V134
E135	M136	T137	D138	P139	E140	G141	Y142	W143	L144	T145	N146	W147	L148	E149	T150	L151	L152	V153	Q154	S155	W156	Y157	P158		V161		M164	S165	R166	E167	Q168	K169	K170	I171	L172	A173	K174	L175		T179	S180	G181	N182		L186	E187	Y188	K189	L190		Y195	R196	G197	V198		Q201	E202	T203	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 107.41Å 120.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 40.04 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 99.0 (40.04-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.299 0.265 , 0.282	Depositor DCC
R_{free} test set	1136 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7476	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6152e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: IS1

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	0.53	2/3788 (0.1%)	0.81	4/5136 (0.1%)
1	B	0.45	0/3788	0.78	3/5136 (0.1%)
All	All	0.49	2/7576 (0.0%)	0.80	7/10272 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	LEU	CG-CD1	-7.57	1.23	1.51
1	A	432	LEU	C-O	-6.38	1.11	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	348	LEU	CA-CB-CG	5.68	128.38	115.30
1	B	66	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	455	HIS	N-CA-C	5.50	125.84	111.00
1	A	270	SER	N-CA-C	-5.41	96.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3700	0	3665	397	0
1	B	3700	0	3665	390	0
2	A	38	0	37	15	0
2	B	38	0	37	8	0
All	All	7476	0	7404	753	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 51.

The worst 5 of 753 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:432:LEU:O	1:A:457:LEU:CD1	1.90	1.19
1:A:19:LYS:HG3	1:A:22:HIS:CD2	1.80	1.15
1:A:432:LEU:O	1:A:457:LEU:HD13	1.46	1.12
1:A:148:ILE:HD13	1:A:152:LEU:HD12	1.32	1.11
1:B:179:THR:HG21	1:B:374:SER:HA	1.13	1.08

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	459/491 (94%)	372 (81%)	58 (13%)	29 (6%)	1 7
1	B	459/491 (94%)	371 (81%)	61 (13%)	27 (6%)	1 9
All	All	918/982 (94%)	743 (81%)	119 (13%)	56 (6%)	1 8

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271	SER
1	A	282	ASP
1	B	71	LYS
1	B	72	GLY

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	408/431 (95%)	345 (85%)	63 (15%)	2	13
1	B	408/431 (95%)	343 (84%)	65 (16%)	2	12
All	All	816/862 (95%)	688 (84%)	128 (16%)	2	13

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	SER
1	B	85	GLU
1	B	429	ARG
1	A	451	GLU
1	B	18	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN
1	B	111	HIS
1	B	455	HIS
1	B	102	ASN
1	B	129	ASN

5.3.3 RNA ⓘ

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](#)

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	IS1	A	501	-	40,41,41	1.56	7 (17%)	51,55,55	2.42	10 (19%)
2	IS1	B	502	-	40,41,41	1.46	7 (17%)	51,55,55	2.17	9 (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	IS1	A	501	-	-	2/27/53/53	0/4/4/4
2	IS1	B	502	-	-	6/27/53/53	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IS1	O4'-C4'	-5.15	1.33	1.45
2	B	502	IS1	CAF-CBB	-4.55	1.38	1.48
2	B	502	IS1	CAP-NBL	4.41	1.40	1.35
2	A	501	IS1	CAF-CBB	-4.13	1.39	1.48
2	A	501	IS1	CAP-NBL	4.01	1.39	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	501	IS1	O3'-C3'-C2'	7.47	135.98	111.82
2	B	502	IS1	O3'-C3'-C4'	7.29	132.12	111.05
2	B	502	IS1	O2'-C2'-C1'	6.57	135.10	110.85
2	B	502	IS1	O4'-C4'-C5'	6.47	123.19	109.21
2	A	501	IS1	C3'-C2'-C1'	-6.42	91.31	100.98

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

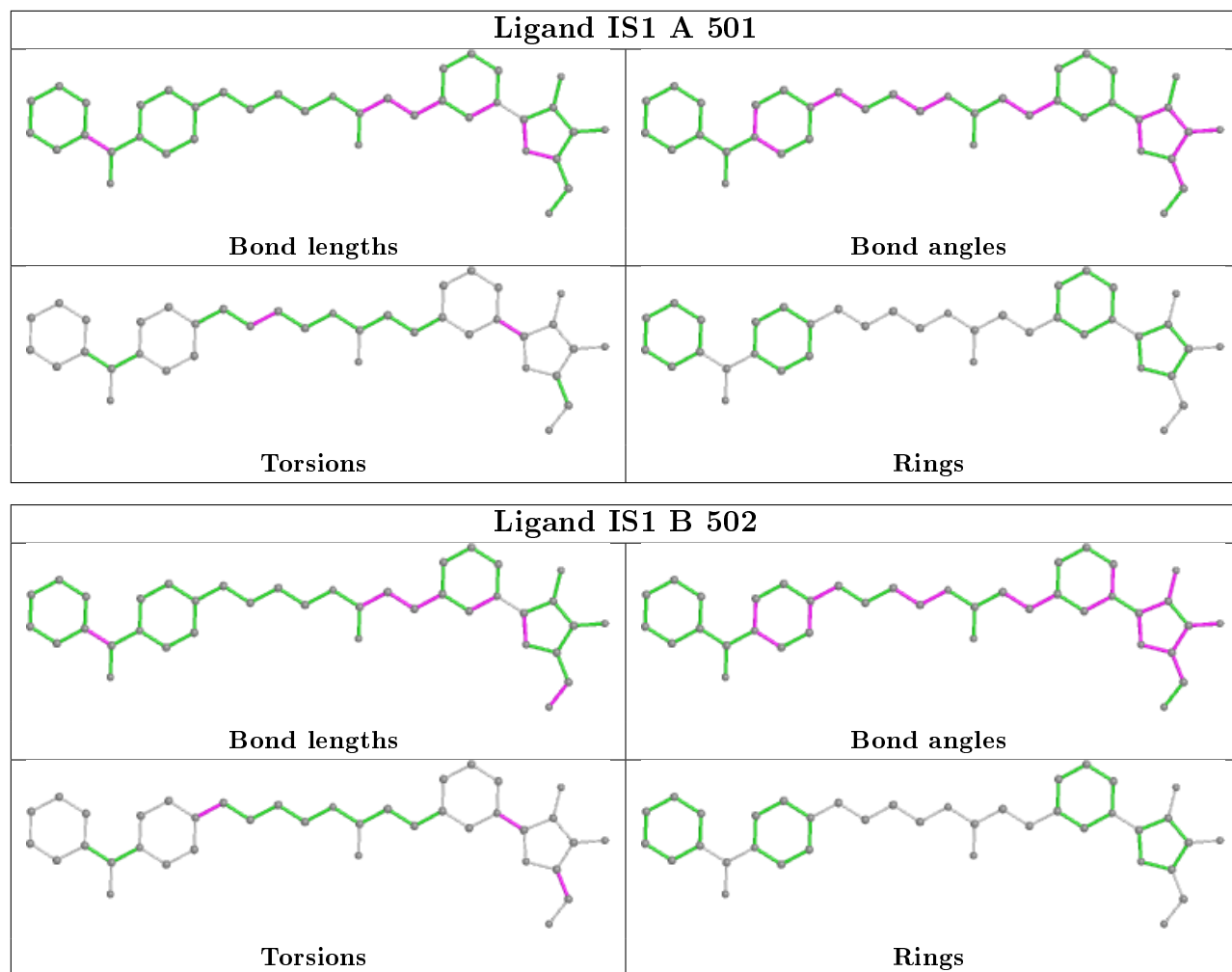
Mol	Chain	Res	Type	Atoms
2	A	501	IS1	C2'-C1'-NBL-CAP
2	B	502	IS1	C2'-C1'-NBL-CAO
2	B	502	IS1	C3'-C4'-C5'-O5'
2	A	501	IS1	CAT-CAR-CAS-CAU
2	B	502	IS1	CAS-CAU-CBF-CAV

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IS1	15	0
2	B	502	IS1	8	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 [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	463/491 (94%)	-0.07	3 (0%)	89 72	7, 33, 56, 78	0
1	B	463/491 (94%)	-0.10	2 (0%)	92 79	10, 32, 55, 79	0
All	All	926/982 (94%)	-0.08	5 (0%)	91 75	7, 33, 56, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	ASP	2.8
1	A	455	HIS	2.4
1	A	238	PRO	2.2
1	A	204	ALA	2.1
1	B	294	ASP	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](#)

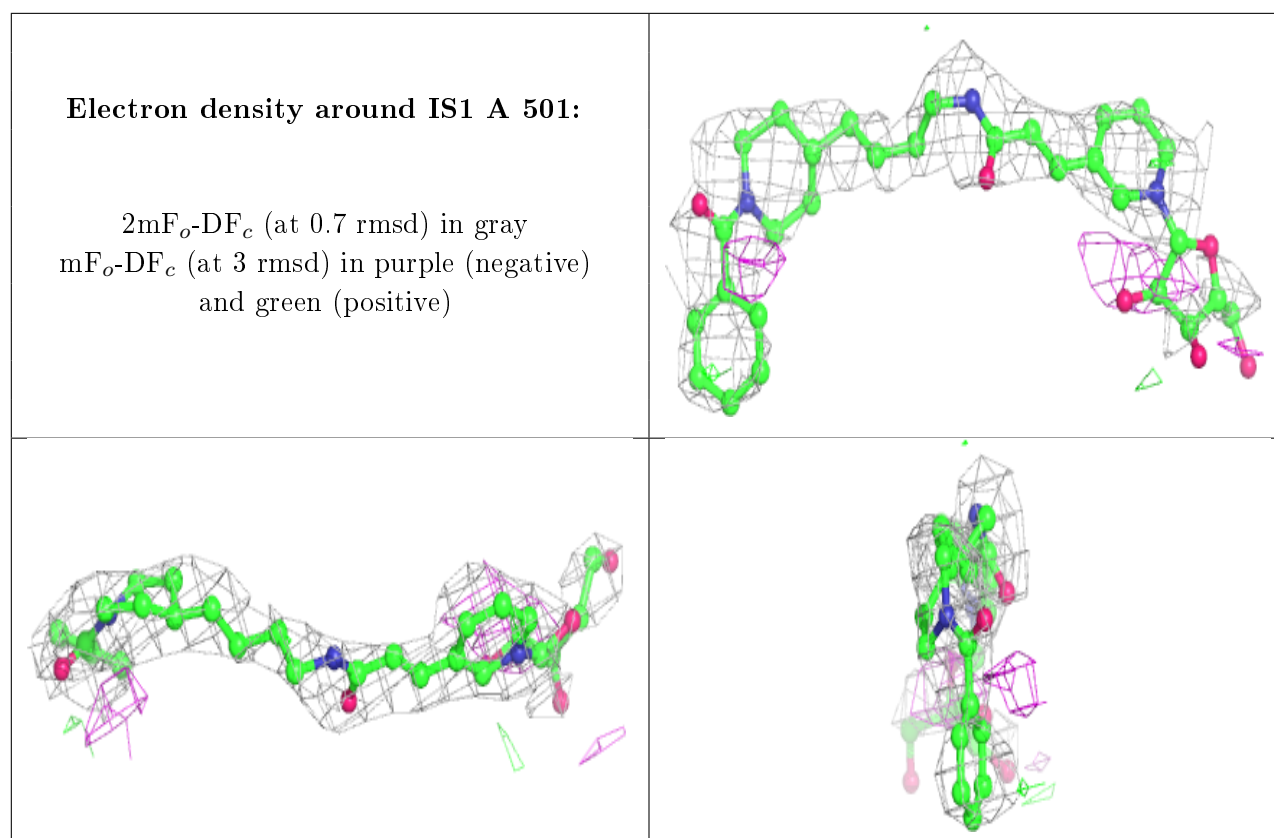
There are no carbohydrates in this entry.

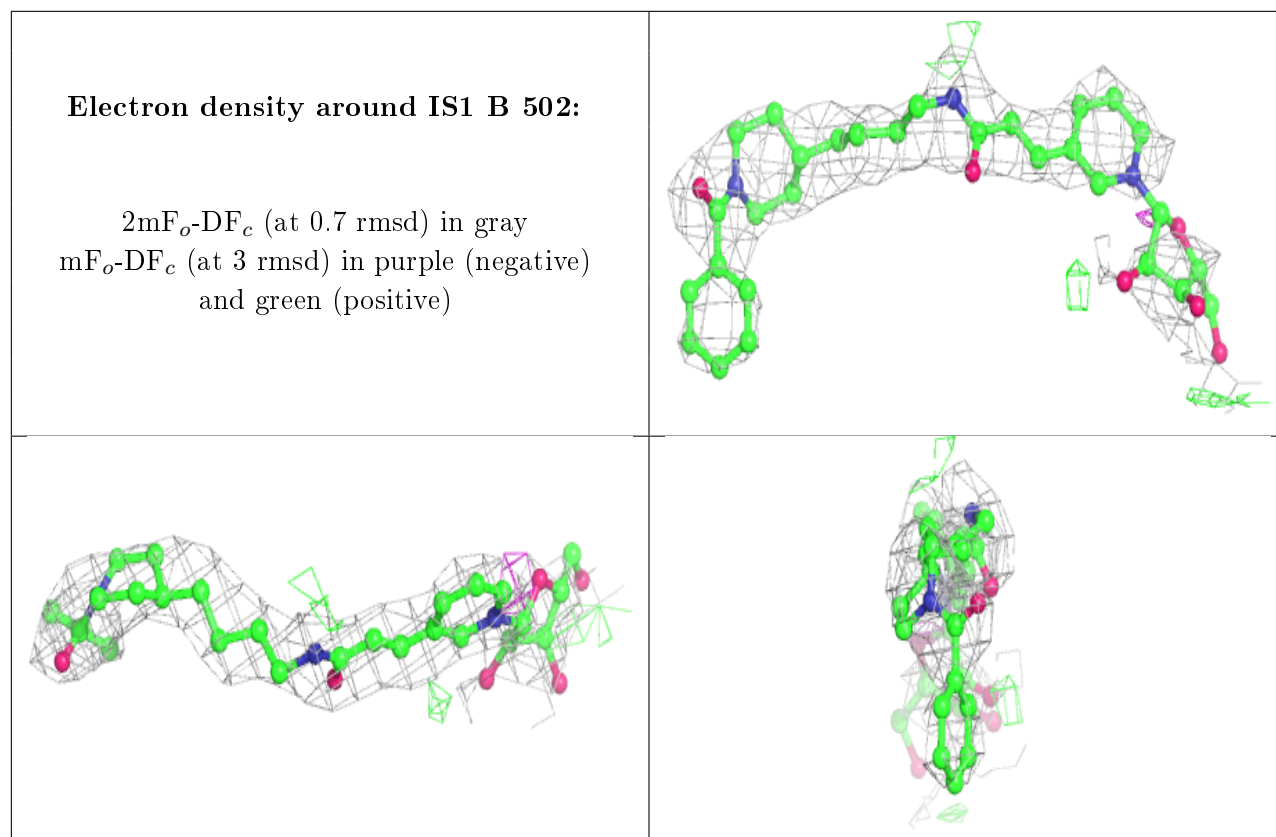
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
2	IS1	A	501	38/38	0.74	0.41	54,64,87,89	0
2	IS1	B	502	38/38	0.75	0.40	56,62,78,83	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.