wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 07:02 AM EDT

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 (i) 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 (i)) were used in the production of this report:

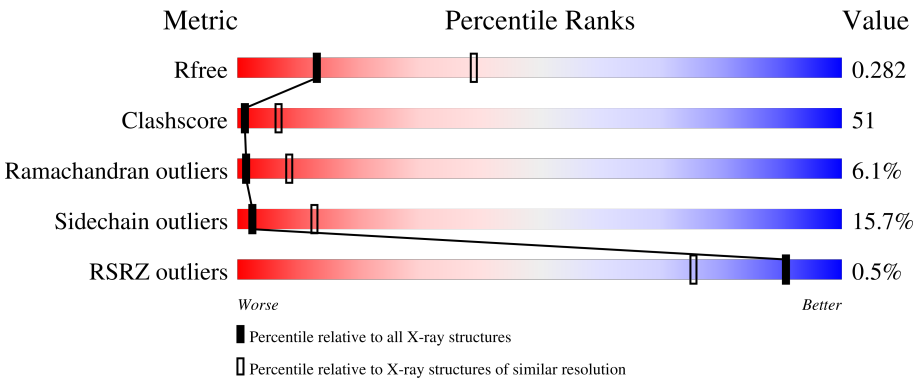
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 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 <=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	% 31% 50% 12% • 6%
1	B	491	34% 45% 14% • 6%

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)

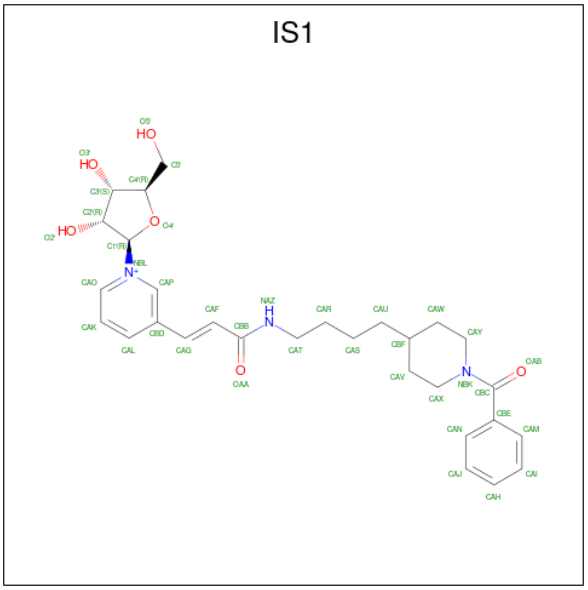
There are 2 unique types of molecules in this entry. The entry contains 7476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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: $C_{29}H_{38}N_3O_6$).



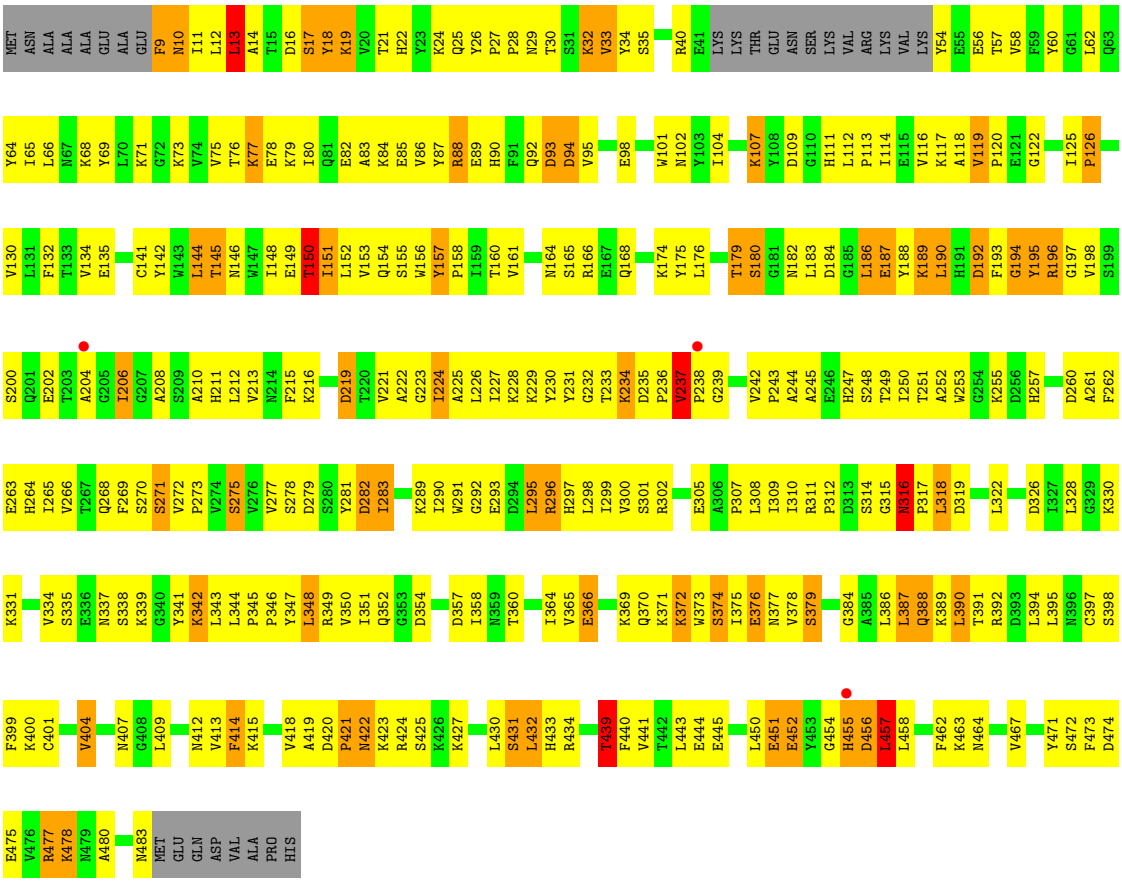
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	38	29	3	6	0	0
2	B	1	38	29	3	6	0	0

3 Residue-property plots (i)

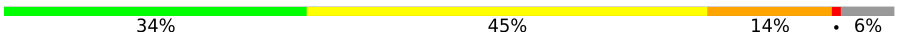
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

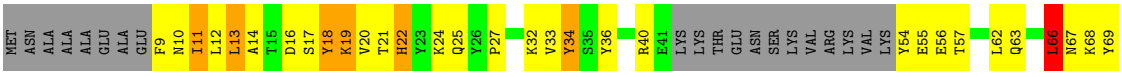
• Molecule 1: Nicotinamide phosphoribosyltransferase

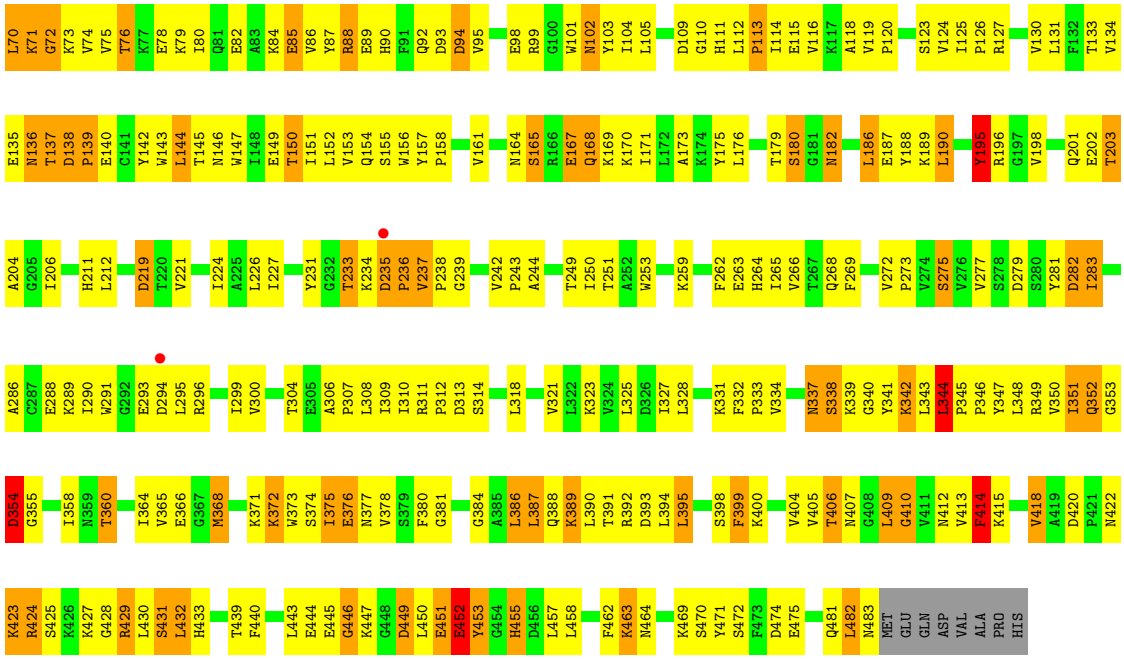
Chain A:



• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B: 




L70 K71 G72 K73 V74 V75 T76 K77 E78 K79 I80 Q81 E82 A83 K84 E85 V86 Y87 R88 E89 H90 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 N136 T137 D138 P139 E140 C141 Y142 W143 L144 T145 N146 W147 I148 E149 T150 I151 L152 V153 Q154 S155 W156 Y157 P158 V161 N164 S165 R166 E167 Q168 K169 K170 I171 L172 A173 K174 Y175 L176 T179 S180 G181 N182 L186 E187 Y188 K189 L190 Y195 R196 G197 V198 Q201 E202 T203
A204 G205 I206 H211 L212 D219 T220 V221 I224 A225 L226 I227 Y231 G232 T233 K234 D235 P236 V237 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 W291 G292 E293 D294 L295 R296 I299 V300 T304 E305 A306 P307 L308 I309 I310 R311 P312 D313 S314 L318 V321 L322 K323 V324 L325 D326 I327 L328 K331 F332 P333 V334 N337 S338 K339 G340 Y341 K342 L343 L344 P345 P346 Y347 L348 R349 V350 I351 Q352 G353
D354 G355 I358 N359 T360 I364 V365 E366 G367 M368 K371 K372 W373 S374 I375 E376 N377 V378 S379 F380 G381 G384 A385 L386 L387 Q388 K389 L390 T391 R392 D393 L394 L395 S398 F399 K400 V404 V405 T406 N407 G408 L409 G410 V411 N412 V413 F414 K415 V418 A419 D420 P421 N422
K423 R424 S425 K426 K427 G428 R429 L430 S431 L432 H433 T439 F440 L443 E444 E445 G446 K447 G448 D449 L450 E451 E452 Y453 G454 H455 D456 L457 L458 F462 K463 N464 K469 S470 Y471 S472 F473 D474 E475 Q481 L482 N483 MET GLU GLN ASP VAL ALA PRO HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	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 $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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

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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 (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	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	B	409	LEU
1	B	431	SER
1	A	388	GLN
1	A	387	LEU
1	B	449	ASP

Sometimes 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	422	ASN
1	B	455	HIS
1	A	396	ASN
1	A	388	GLN
1	B	459	HIS

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)

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

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	B	502	-	-	6/27/53/53	0/4/4/4
2	IS1	A	501	-	-	2/27/53/53	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(^{o})	Ideal(^{o})
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.

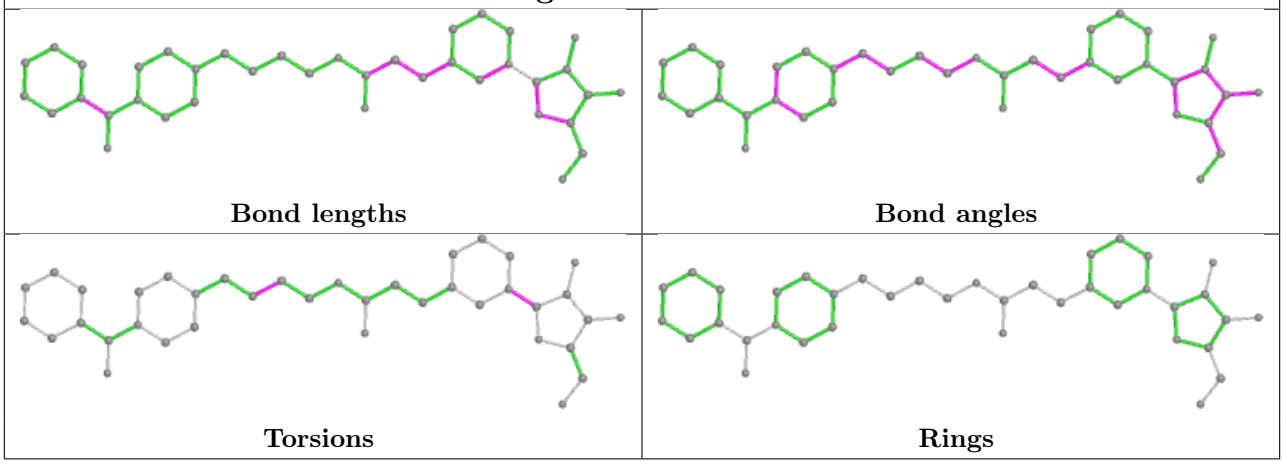
2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	IS1	8	0
2	A	501	IS1	15	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 then 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 IS1 B 502

Ligand IS1 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	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 monosaccharides in this entry.

6.4 Ligands (i)

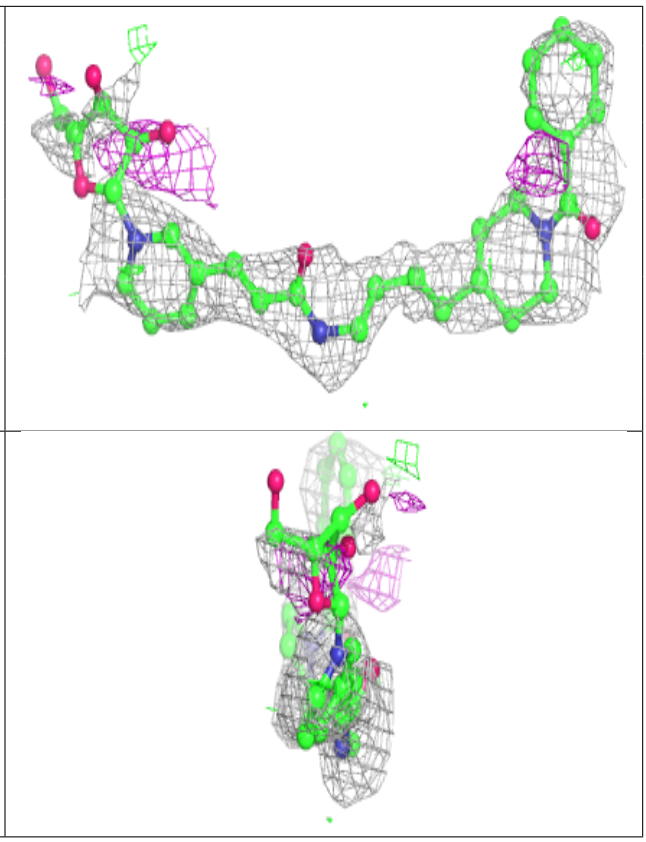
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

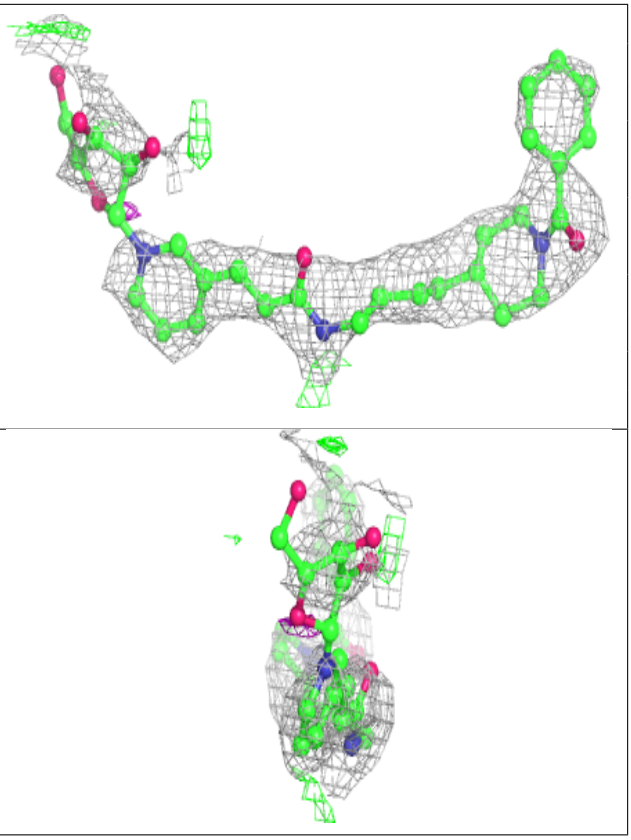
Electron density around IS1 A 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around IS1 B 502:

$2mF_o$-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.