



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2024 – 04:39 pm BST

PDB ID : 8OQ2  
Title : Binding of NADP to a formate dehydrogenase from *Starkeya novella*.  
Authors : Partipilo, M.; Whittaker, J.J.; Pontillo, N.; Guskov, A.; Slotboom, D.J.  
Deposited on : 2023-04-10  
Resolution : 1.91 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

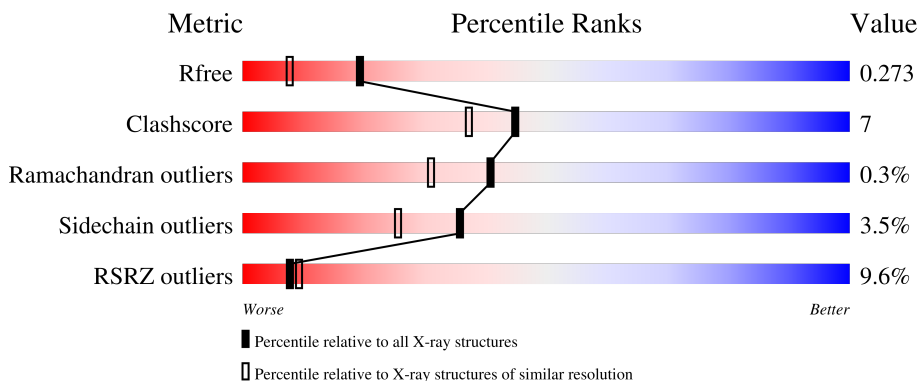
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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.



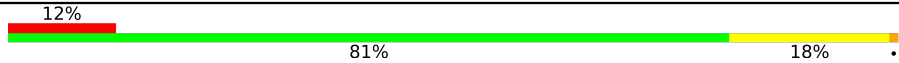
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	381	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">9%      86%      13%      .</p>
1	B	381	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">8%      80%      19%</p>
1	C	381	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">7%      83%      17%      .</p>
1	D	381	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">9%      86%      13%      .</p>
1	E	381	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">12%      83%      15%      .</p>

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Mol	Chain	Length	Quality of chain
1	F	381	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a large green segment in the middle labeled '81%', and a yellow segment on the right labeled '18%'. A small black dot is located at the far right end of the bar.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18219 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2966	1884	519	551	12	9	1	0
1	B	381	2958	1879	516	551	12	21	0	0
1	C	381	2958	1879	516	551	12	0	0	0
1	D	381	2958	1879	516	551	12	17	0	0
1	E	380	2952	1876	515	549	12	74	0	0
1	F	381	2958	1879	516	551	12	21	0	0

There are 30 discrepancies between the modelled and reference sequences:

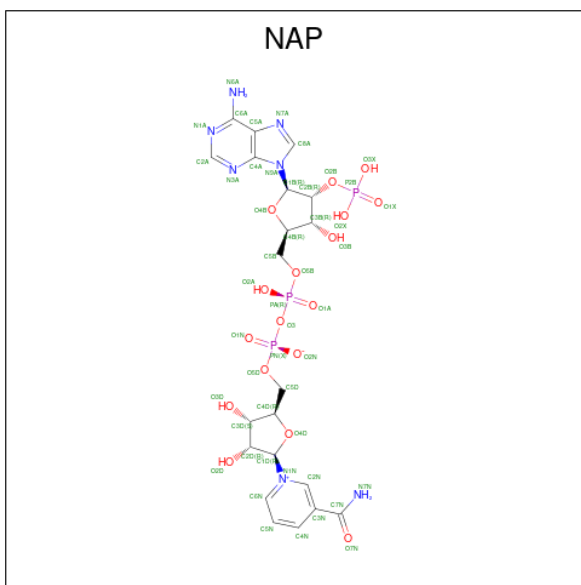
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP D7A8L2
A	200	GLY	ALA	engineered mutation	UNP D7A8L2
A	223	GLN	ASP	engineered mutation	UNP D7A8L2
A	381	LYS	HIS	engineered mutation	UNP D7A8L2
A	382	VAL	SER	engineered mutation	UNP D7A8L2
B	2	SER	-	expression tag	UNP D7A8L2
B	200	GLY	ALA	engineered mutation	UNP D7A8L2
B	223	GLN	ASP	engineered mutation	UNP D7A8L2
B	381	LYS	HIS	engineered mutation	UNP D7A8L2
B	382	VAL	SER	engineered mutation	UNP D7A8L2
C	2	SER	-	expression tag	UNP D7A8L2
C	200	GLY	ALA	engineered mutation	UNP D7A8L2
C	223	GLN	ASP	engineered mutation	UNP D7A8L2
C	381	LYS	HIS	engineered mutation	UNP D7A8L2
C	382	VAL	SER	engineered mutation	UNP D7A8L2
D	2	SER	-	expression tag	UNP D7A8L2
D	200	GLY	ALA	engineered mutation	UNP D7A8L2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	223	GLN	ASP	engineered mutation	UNP D7A8L2
D	381	LYS	HIS	engineered mutation	UNP D7A8L2
D	382	VAL	SER	engineered mutation	UNP D7A8L2
E	2	SER	-	expression tag	UNP D7A8L2
E	200	GLY	ALA	engineered mutation	UNP D7A8L2
E	223	GLN	ASP	engineered mutation	UNP D7A8L2
E	381	LYS	HIS	engineered mutation	UNP D7A8L2
E	382	VAL	SER	engineered mutation	UNP D7A8L2
F	2	SER	-	expression tag	UNP D7A8L2
F	200	GLY	ALA	engineered mutation	UNP D7A8L2
F	223	GLN	ASP	engineered mutation	UNP D7A8L2
F	381	LYS	HIS	engineered mutation	UNP D7A8L2
F	382	VAL	SER	engineered mutation	UNP D7A8L2

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



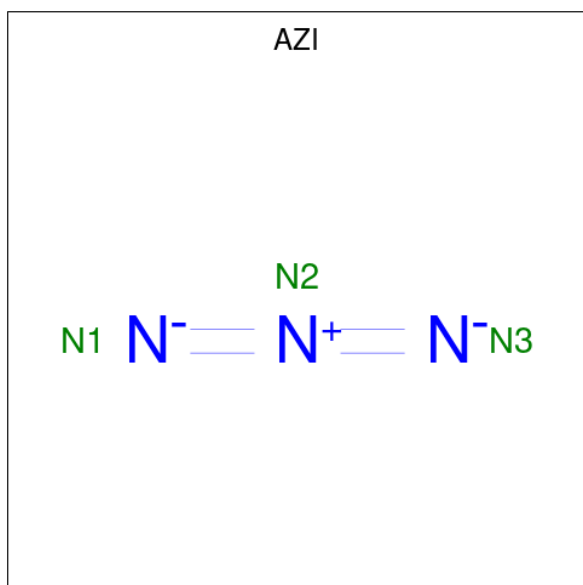
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	48	21	7	17	3	0	0
2	F	1	48	21	7	17	3	0	0

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		
3	C	1	Total	N	0	0
			3	3		
3	C	1	Total	N	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0

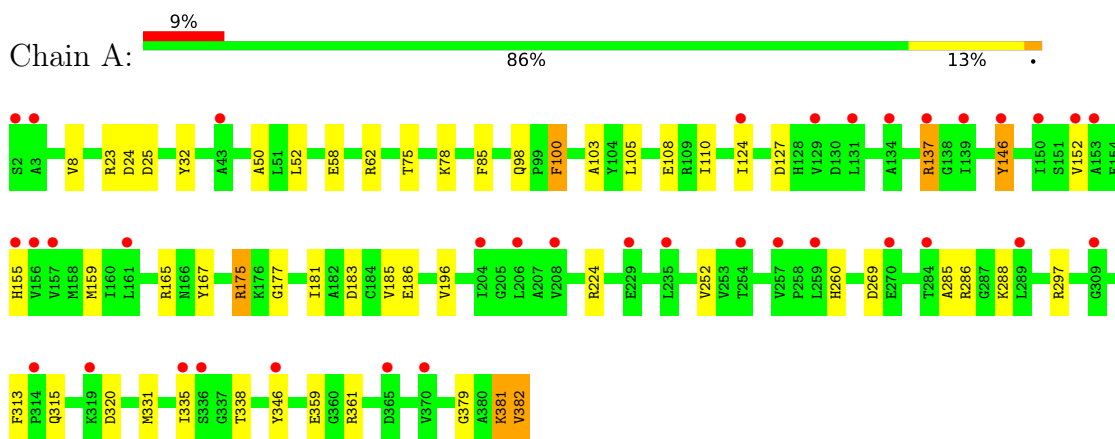
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	36	Total O 36 36	0	0
4	B	30	Total O 30 30	0	0
4	C	21	Total O 21 21	0	0
4	D	13	Total O 13 13	0	0
4	E	15	Total O 15 15	0	0
4	F	24	Total O 24 24	0	0

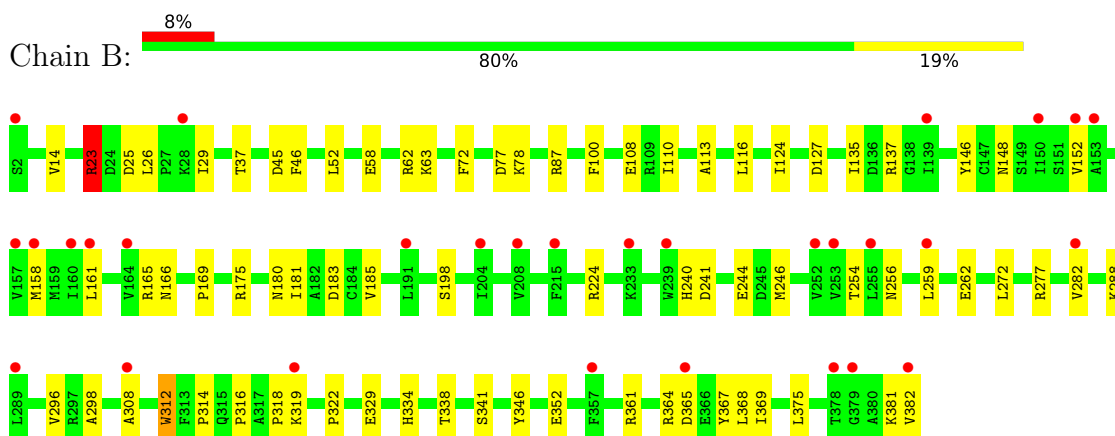
### 3 Residue-property plots [i](#)

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.

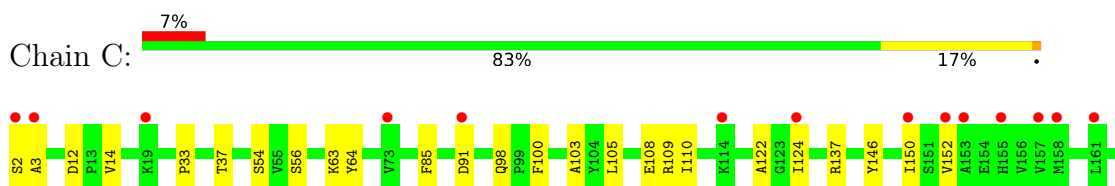
- Molecule 1: Formate dehydrogenase



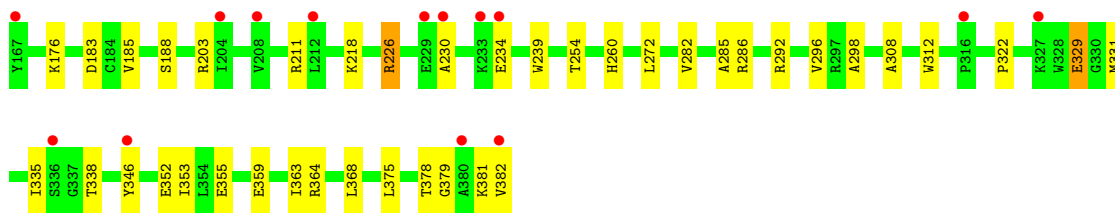
- Molecule 1: Formate dehydrogenase



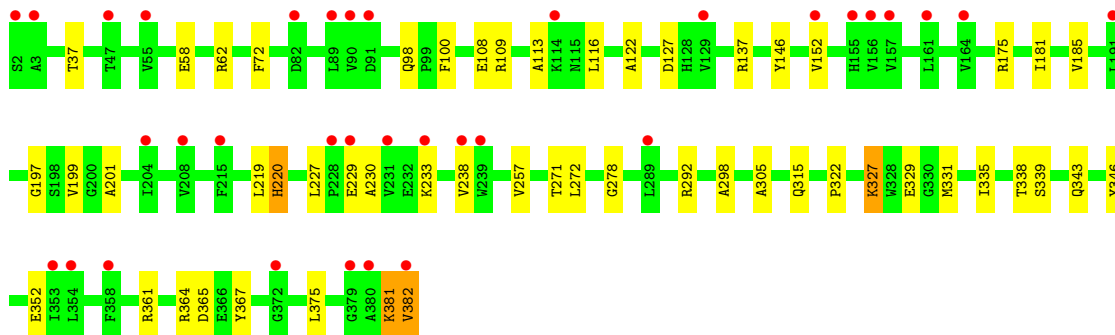
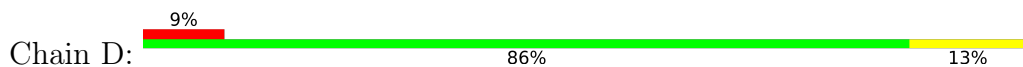
- Molecule 1: Formate dehydrogenase



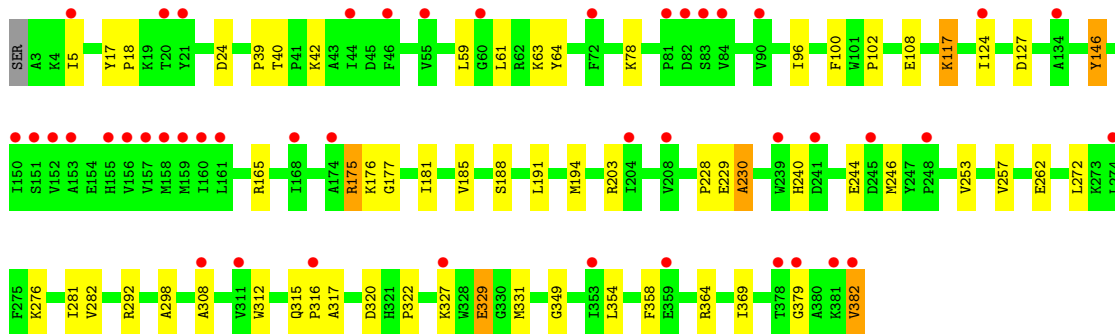
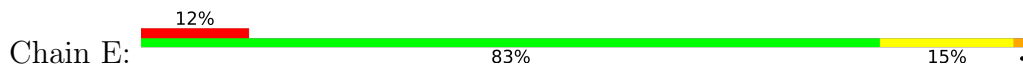




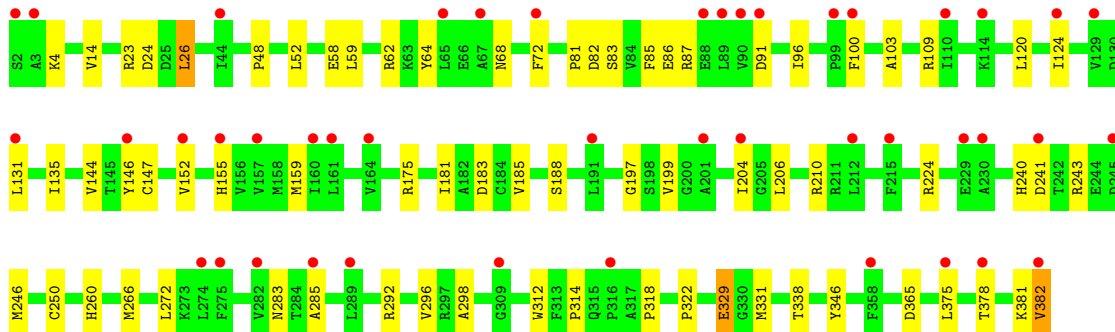
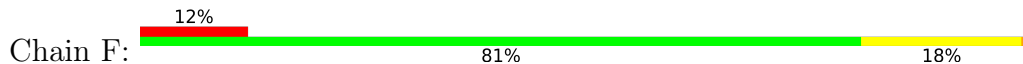
● Molecule 1: Formate dehydrogenase



● Molecule 1: Formate dehydrogenase



● Molecule 1: Formate dehydrogenase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.26Å 132.26Å 302.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.60 – 1.91 46.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (114.60-1.91) 99.5 (46.20-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.237 , 0.275 0.238 , 0.273	Depositor DCC
$R_{free}$ test set	1077 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: AZI, NAP

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	0.39	0/3043	0.67	0/4141
1	B	0.38	0/3032	0.63	0/4127
1	C	0.39	0/3032	0.66	0/4127
1	D	0.46	2/3032 (0.1%)	0.67	0/4127
1	E	0.39	0/3026	0.63	0/4119
1	F	0.38	0/3032	0.64	0/4127
All	All	0.40	2/18197 (0.0%)	0.65	0/24768

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	1
1	B	0	4
1	C	0	1
1	D	0	3
1	E	0	3
1	F	0	2
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	LEU	C-N	11.26	1.59	1.34
1	D	220	HIS	C-N	-5.09	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	87	ARG	Sidechain
1	C	109	ARG	Sidechain
1	D	109	ARG	Sidechain
1	D	175	ARG	Sidechain
1	D	361	ARG	Sidechain
1	E	165	ARG	Sidechain
1	E	175	ARG	Sidechain
1	E	364	ARG	Sidechain
1	F	109	ARG	Sidechain
1	F	23	ARG	Sidechain

## 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	2966	0	2932	38	0
1	B	2958	0	2919	56	0
1	C	2958	0	2919	44	0
1	D	2958	0	2919	28	0
1	E	2952	0	2914	35	0
1	F	2958	0	2919	49	0
2	A	48	0	25	7	0
2	B	48	0	25	4	0
2	C	48	0	25	5	0
2	D	48	0	25	1	0
2	E	48	0	25	4	0
2	F	48	0	25	4	0
3	B	21	0	0	0	0
3	C	21	0	0	0	0
4	A	36	0	0	1	0
4	B	30	0	0	0	0
4	C	21	0	0	0	0
4	D	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	15	0	0	0	0
4	F	24	0	0	0	0
All	All	18219	0	17672	231	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 7.

All (231) 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:D:220:HIS:CD2	1:D:238:VAL:HB	2.07	0.89
1:C:211:ARG:HG3	1:C:211:ARG:HH11	1.44	0.80
1:C:108:GLU:OE2	1:C:108:GLU:N	2.16	0.79
1:C:355:GLU:O	1:C:359:GLU:HG3	1.85	0.77
1:C:338:THR:HG23	1:F:185:VAL:HG11	1.70	0.73
1:F:243:ARG:HD3	1:F:266:MET:HE3	1.69	0.73
1:B:62:ARG:NH2	1:B:72:PHE:O	2.21	0.73
1:D:220:HIS:HD2	1:D:238:VAL:HB	1.53	0.73
1:B:352:GLU:OE1	1:B:364:ARG:HD2	1.90	0.72
1:A:338:THR:HG23	1:B:185:VAL:HG11	1.69	0.72
1:A:260:HIS:NE2	2:A:401:NAP:N1A	2.38	0.70
1:B:110:ILE:O	1:B:137:ARG:NH1	2.25	0.68
1:C:292:ARG:HH11	1:C:322:PRO:HG3	1.57	0.68
1:B:124:ILE:HD12	1:B:148:ASN:OD1	1.94	0.67
1:F:62:ARG:NH2	1:F:72:PHE:O	2.26	0.67
1:C:185:VAL:HG11	1:F:338:THR:HG23	1.76	0.67
1:A:185:VAL:HG11	1:B:338:THR:HG23	1.76	0.66
1:C:211:ARG:HG3	1:C:211:ARG:NH1	2.11	0.66
1:A:183:ASP:OD1	1:B:14:VAL:HG22	1.95	0.66
1:F:81:PRO:HD2	1:F:82:ASP:H	1.61	0.65
1:B:262:GLU:HG3	2:B:401:NAP:H62A	1.62	0.64
1:B:224:ARG:HH12	1:B:382:VAL:HG23	1.62	0.64
1:A:110:ILE:HG22	1:A:137[B]:ARG:HH11	1.64	0.62
1:A:285:ALA:O	1:A:286:ARG:HG2	1.99	0.61
1:D:62:ARG:NH2	1:D:72:PHE:O	2.33	0.61
1:E:5:ILE:HD11	1:E:358:PHE:CZ	2.35	0.61
1:E:5:ILE:HD11	1:E:358:PHE:HZ	1.66	0.61
1:B:58:GLU:OE2	1:B:62:ARG:NH1	2.34	0.61
1:B:272:LEU:HD13	1:B:298:ALA:HB2	1.83	0.60
1:C:375:LEU:HD13	1:C:379:GLY:O	2.01	0.60
1:A:127:ASP:OD1	1:A:286:ARG:NE	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:HE2	2:A:401:NAP:C2A	2.14	0.59
1:B:296:VAL:HG21	1:B:322:PRO:HB2	1.83	0.59
1:A:224:ARG:N	2:A:401:NAP:O3X	2.31	0.58
1:B:259:LEU:HD21	1:B:288:LYS:HE2	1.85	0.58
1:E:181:ILE:O	1:E:185:VAL:HG22	2.02	0.58
1:D:381:LYS:O	1:D:382:VAL:C	2.42	0.58
1:E:124:ILE:HB	2:E:401:NAP:H5N	1.85	0.57
1:C:368:LEU:O	1:C:378:THR:O	2.23	0.57
1:D:230:ALA:HA	1:D:233:LYS:HG3	1.86	0.57
1:B:77:ASP:CG	1:E:327:LYS:HZ3	2.08	0.56
1:C:230:ALA:O	1:C:234:GLU:HG3	2.06	0.56
1:C:203:ARG:HD2	2:C:401:NAP:O1A	2.07	0.55
1:B:198:SER:OG	1:B:256:ASN:ND2	2.40	0.55
1:B:26:LEU:HD13	1:B:341:SER:HA	1.87	0.55
1:E:185:VAL:HA	1:E:188:SER:HB2	1.88	0.54
1:F:152:VAL:HG21	2:F:401:NAP:C4N	2.37	0.54
1:B:77:ASP:OD2	1:E:327:LYS:NZ	2.39	0.54
1:B:46:PHE:CD1	1:B:52:LEU:HD11	2.43	0.54
1:D:152:VAL:HG21	2:D:401:NAP:C4N	2.38	0.54
1:F:131:LEU:HD11	1:F:375:LEU:HD11	1.90	0.54
1:B:45:ASP:OD2	1:B:63:LYS:HD3	2.08	0.54
1:B:46:PHE:CE1	1:B:52:LEU:HD11	2.42	0.54
1:E:102:PRO:HD3	1:E:315:GLN:HG2	1.90	0.54
1:B:319:LYS:NZ	1:E:320:ASP:HB2	2.23	0.53
1:F:224:ARG:N	2:F:401:NAP:O3X	2.37	0.53
1:A:152:VAL:HG21	2:A:401:NAP:C4N	2.39	0.53
1:F:199:VAL:HG11	1:F:266:MET:HE3	1.91	0.53
1:B:364:ARG:HD3	1:B:367:TYR:CE2	2.43	0.53
1:B:77:ASP:CG	1:E:327:LYS:NZ	2.63	0.53
1:C:14:VAL:HG22	1:F:183:ASP:OD1	2.08	0.53
1:F:58:GLU:OE2	1:F:62:ARG:NH1	2.42	0.53
1:A:381:LYS:O	1:A:382:VAL:C	2.47	0.52
1:C:185:VAL:HA	1:C:188:SER:HB2	1.89	0.52
1:E:369:ILE:HA	1:E:379:GLY:HA3	1.92	0.52
1:D:220:HIS:CD2	1:D:238:VAL:CB	2.90	0.52
1:A:50:ALA:O	1:A:52:LEU:HD22	2.09	0.52
1:F:135:ILE:HD11	1:F:375:LEU:HD13	1.93	0.51
1:A:181:ILE:O	1:A:185:VAL:HG22	2.11	0.51
1:A:185:VAL:HG11	1:B:338:THR:CG2	2.40	0.51
1:E:382:VAL:HG12	2:E:401:NAP:H8A	1.93	0.51
1:F:87:ARG:HH11	1:F:87:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:GLU:CG	1:F:331:MET:HG2	2.41	0.50
1:A:85:PHE:CZ	1:A:103:ALA:HB1	2.47	0.50
1:C:272:LEU:HD13	1:C:298:ALA:HB2	1.93	0.50
1:F:181:ILE:O	1:F:185:VAL:HG22	2.11	0.50
1:B:124:ILE:HG22	2:B:401:NAP:H3D	1.92	0.50
1:A:165:ARG:HD3	1:B:158:MET:CE	2.42	0.50
1:A:379:GLY:O	1:A:382:VAL:HG23	2.11	0.50
1:D:113:ALA:HB1	1:D:116:LEU:HB2	1.94	0.49
1:D:201:ALA:CB	1:D:227:LEU:HD11	2.43	0.49
1:A:359:GLU:OE1	1:A:361:ARG:NH1	2.46	0.49
1:B:181:ILE:O	1:B:185:VAL:HG22	2.12	0.49
1:B:244:GLU:CD	1:B:244:GLU:H	2.16	0.49
1:E:240:HIS:CD2	1:E:246:MET:HG3	2.47	0.49
1:F:329:GLU:HG2	1:F:331:MET:HG2	1.94	0.49
1:E:329:GLU:HG2	1:E:331:MET:HG2	1.95	0.49
1:D:181:ILE:O	1:D:185:VAL:HG22	2.12	0.49
1:C:37:THR:OG1	1:C:364:ARG:NH2	2.46	0.48
1:D:201:ALA:HB1	1:D:227:LEU:HD11	1.95	0.48
1:E:253:VAL:O	1:E:281:ILE:HA	2.13	0.48
1:C:353:ILE:HG23	1:C:363:ILE:HD13	1.95	0.48
1:A:155:HIS:O	1:A:159:MET:HG3	2.14	0.48
1:C:2:SER:OG	1:C:3:ALA:N	2.47	0.48
1:C:329:GLU:OE1	1:F:175:ARG:NH1	2.46	0.48
1:B:368:LEU:C	1:B:369:ILE:HD13	2.34	0.48
1:A:85:PHE:CE2	1:A:103:ALA:HB1	2.48	0.48
1:A:177:GLY:O	1:B:319:LYS:HG2	2.14	0.48
1:E:244:GLU:H	1:E:244:GLU:CD	2.16	0.48
1:E:272:LEU:HD13	1:E:298:ALA:HB2	1.96	0.47
1:B:152:VAL:HG21	2:B:401:NAP:C4N	2.44	0.47
1:C:282:VAL:HA	1:C:308:ALA:O	2.14	0.47
1:C:152:VAL:HG21	2:C:401:NAP:C4N	2.45	0.47
1:D:137:ARG:HE	1:D:137:ARG:HB3	1.57	0.47
1:D:339:SER:O	1:D:343:GLN:HG3	2.15	0.47
1:C:226:ARG:HG3	1:C:239:TRP:CD2	2.50	0.47
1:E:40:THR:O	1:E:40:THR:OG1	2.27	0.47
1:A:32:TYR:CE1	1:A:146:TYR:O	2.68	0.47
1:B:240:HIS:CD2	1:B:246:MET:HG3	2.50	0.47
1:C:176:LYS:HB2	1:C:176:LYS:HE2	1.69	0.47
1:F:144:VAL:HG12	1:F:147:CYS:HB3	1.97	0.47
1:A:23:ARG:HD3	1:A:25:ASP:O	2.14	0.46
1:B:338:THR:HG23	1:B:338:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:HIS:HE2	2:B:401:NAP:C7N	2.29	0.46
1:C:110:ILE:O	1:C:137:ARG:NH1	2.48	0.46
1:E:315:GLN:O	1:E:316:PRO:C	2.51	0.46
1:E:175:ARG:O	1:E:177:GLY:N	2.49	0.46
1:C:124:ILE:HB	2:C:401:NAP:H5N	1.98	0.46
1:C:335:ILE:HA	1:C:338:THR:HG22	1.98	0.46
1:D:199:VAL:O	1:D:257:VAL:HG13	2.15	0.46
1:E:191:LEU:O	1:E:194:MET:HB2	2.15	0.46
1:C:63:LYS:HD3	1:C:64:TYR:N	2.31	0.46
1:C:329:GLU:HG2	1:C:331:MET:HG2	1.97	0.46
1:F:87:ARG:HG2	1:F:87:ARG:NH1	2.31	0.46
1:C:124:ILE:HB	2:C:401:NAP:C5N	2.47	0.45
1:A:288:LYS:HE3	1:A:313:PHE:CE2	2.52	0.45
1:F:52:LEU:HB3	1:F:59:LEU:HA	1.99	0.45
1:E:175:ARG:C	1:E:177:GLY:N	2.69	0.45
1:F:283:ASN:ND2	1:F:285:ALA:H	2.14	0.45
1:F:314:PRO:HG2	1:F:318:PRO:HD3	1.99	0.45
1:E:17:TYR:CD1	1:E:18:PRO:HD2	2.51	0.45
1:F:292:ARG:HD2	1:F:322:PRO:HD2	1.99	0.45
1:B:29:ILE:N	1:B:29:ILE:HD12	2.32	0.45
1:C:338:THR:CG2	1:F:185:VAL:HG11	2.44	0.45
1:D:327:LYS:HE2	1:D:327:LYS:HB2	1.75	0.45
1:A:269:ASP:CG	1:A:297:ARG:HH21	2.19	0.44
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.90	0.44
1:A:24:ASP:OD1	1:B:277:ARG:NH2	2.33	0.44
1:D:335:ILE:HA	1:D:338:THR:HG22	1.98	0.44
1:E:146:TYR:CD2	1:E:203:ARG:HD3	2.52	0.44
1:F:83:SER:O	1:F:87:ARG:HG3	2.17	0.44
1:F:296:VAL:HG21	1:F:322:PRO:HB2	1.98	0.44
1:C:296:VAL:HG21	1:C:322:PRO:HB2	1.99	0.44
1:F:199:VAL:HG11	1:F:266:MET:CE	2.47	0.44
1:F:260:HIS:CE1	1:F:382:VAL:HG22	2.53	0.44
1:B:314:PRO:HD2	1:B:318:PRO:HD3	1.99	0.44
1:B:78:LYS:NZ	1:B:316:PRO:HD3	2.32	0.44
1:B:368:LEU:O	1:B:369:ILE:HD13	2.18	0.44
1:D:58:GLU:OE2	1:D:62:ARG:NH1	2.50	0.44
1:E:257:VAL:HG12	2:E:401:NAP:C1B	2.48	0.44
1:C:85:PHE:CZ	1:C:103:ALA:HB1	2.53	0.44
1:D:375:LEU:HD12	1:E:262:GLU:HA	1.99	0.44
1:F:260:HIS:NE2	1:F:382:VAL:HG22	2.32	0.44
1:F:81:PRO:HA	1:F:86:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HD13	4:A:520:HOH:O	2.16	0.43
1:B:137:ARG:HE	1:B:137:ARG:HB3	1.64	0.43
1:E:228:PRO:O	1:E:230:ALA:N	2.51	0.43
1:C:108:GLU:H	1:C:108:GLU:CD	2.12	0.43
1:D:352:GLU:OE2	1:D:364:ARG:HD2	2.18	0.43
1:A:196:VAL:HG22	1:A:252:VAL:HB	2.00	0.43
1:D:364:ARG:HD3	1:D:367:TYR:CE2	2.54	0.43
1:D:272:LEU:HD13	1:D:298:ALA:HB2	2.00	0.43
1:D:278:GLY:HA2	1:D:305:ALA:HB2	2.01	0.43
1:E:96:ILE:HD11	1:E:354:LEU:HD11	2.00	0.43
1:E:124:ILE:HB	2:E:401:NAP:C5N	2.48	0.43
1:F:155:HIS:CD2	1:F:159:MET:CE	3.01	0.43
1:A:8:VAL:HA	1:A:75:THR:O	2.19	0.43
1:B:312:TRP:CD1	1:B:312:TRP:N	2.86	0.43
1:F:292:ARG:HH11	1:F:322:PRO:HG3	1.84	0.43
1:C:260:HIS:CE1	2:C:401:NAP:N1A	2.87	0.43
1:D:37:THR:OG1	1:D:364:ARG:NH2	2.52	0.43
1:F:64:TYR:O	1:F:68:ASN:ND2	2.47	0.43
1:B:224:ARG:NH2	1:B:381:LYS:O	2.46	0.43
1:B:282:VAL:HA	1:B:308:ALA:O	2.18	0.43
1:E:315:GLN:HA	1:E:315:GLN:NE2	2.33	0.43
1:F:185:VAL:HA	1:F:188:SER:CB	2.49	0.43
1:A:124:ILE:HB	2:A:401:NAP:H5N	2.02	0.42
1:F:85:PHE:CZ	1:F:103:ALA:HB1	2.53	0.42
1:B:166:ASN:OD1	1:B:169:PRO:HG2	2.19	0.42
1:C:12:ASP:OD2	1:C:56:SER:OG	2.35	0.42
1:B:314:PRO:HD2	1:B:318:PRO:CD	2.49	0.42
1:C:98:GLN:HG2	1:C:122:ALA:HB3	2.00	0.42
1:F:81:PRO:CD	1:F:82:ASP:H	2.32	0.42
1:A:335:ILE:HA	1:A:338:THR:HG22	2.02	0.42
1:B:108:GLU:OE1	1:B:108:GLU:N	2.42	0.42
1:C:183:ASP:OD1	1:F:14:VAL:HG22	2.20	0.42
1:C:254:THR:HA	1:C:282:VAL:O	2.20	0.42
1:D:329:GLU:HB2	1:D:331:MET:HG2	2.02	0.42
1:F:124:ILE:HB	2:F:401:NAP:H5N	2.01	0.42
1:C:352:GLU:OE2	1:C:364:ARG:CD	2.68	0.42
1:F:147:CYS:HB2	1:F:346:TYR:HB3	2.01	0.42
1:B:25:ASP:OD1	1:B:25:ASP:O	2.37	0.41
1:B:78:LYS:HZ1	1:B:316:PRO:HD3	1.84	0.41
1:B:254:THR:HG23	1:B:256:ASN:HD21	1.85	0.41
1:C:33:PRO:HG2	1:C:150:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:LEU:HD13	1:F:298:ALA:HB2	2.01	0.41
1:B:37:THR:OG1	1:B:364:ARG:NH2	2.52	0.41
1:E:117:LYS:HE2	1:E:117:LYS:HB2	1.67	0.41
1:F:81:PRO:HD2	1:F:82:ASP:N	2.32	0.41
1:B:113:ALA:HB1	1:B:116:LEU:HB2	2.02	0.41
1:B:135:ILE:HD11	1:B:375:LEU:CD1	2.50	0.41
1:D:292:ARG:HD3	1:D:322:PRO:HD2	2.02	0.41
1:F:96:ILE:HG12	1:F:120:LEU:HB3	2.02	0.41
1:F:206:LEU:O	1:F:210:ARG:HG3	2.20	0.41
1:A:331:MET:HE3	1:A:331:MET:HB3	1.93	0.41
1:C:379:GLY:O	1:C:382:VAL:HB	2.20	0.41
1:F:26:LEU:HD22	1:F:48:PRO:C	2.41	0.41
1:A:124:ILE:HB	2:A:401:NAP:C5N	2.50	0.41
1:B:23:ARG:HD3	1:B:25:ASP:O	2.20	0.41
1:E:39:PRO:HB3	1:E:349:GLY:HA2	2.03	0.41
1:E:59:LEU:HB2	1:E:61:LEU:HD12	2.02	0.41
1:A:98:GLN:HB3	1:A:100:PHE:CD2	2.55	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.90	0.41
1:A:152:VAL:HG21	2:A:401:NAP:C3N	2.51	0.41
1:C:285:ALA:O	1:C:286:ARG:HG2	2.21	0.41
1:C:352:GLU:OE2	1:C:364:ARG:HD2	2.21	0.41
1:A:167:TYR:CD2	1:B:158:MET:SD	3.14	0.41
1:B:180:ASN:HB3	1:B:183:ASP:OD2	2.21	0.41
1:E:292:ARG:HD2	1:E:322:PRO:HD2	2.03	0.41
1:F:4:LYS:HE3	1:F:91:ASP:OD1	2.21	0.41
1:A:58:GLU:OE2	1:A:62:ARG:NH1	2.54	0.41
1:C:211:ARG:NH1	1:C:211:ARG:CG	2.81	0.41
1:B:161:LEU:O	1:B:165:ARG:HG3	2.22	0.40
1:D:292:ARG:HD2	1:D:322:PRO:CG	2.51	0.40
1:F:197:GLY:HA3	1:F:250:CYS:SG	2.60	0.40
1:F:204:ILE:HG13	2:F:401:NAP:PN	2.61	0.40
1:D:197:GLY:HA2	1:D:220:HIS:O	2.21	0.40
1:E:282:VAL:HA	1:E:308:ALA:O	2.21	0.40
1:F:155:HIS:CD2	1:F:159:MET:HE1	2.57	0.40
1:D:98:GLN:HG2	1:D:122:ALA:HB3	2.03	0.40
1:F:240:HIS:CD2	1:F:246:MET:HG3	2.56	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	380/381 (100%)	365 (96%)	14 (4%)	1 (0%)	41	31
1	B	379/381 (100%)	364 (96%)	15 (4%)	0	100	100
1	C	379/381 (100%)	367 (97%)	12 (3%)	0	100	100
1	D	379/381 (100%)	367 (97%)	12 (3%)	0	100	100
1	E	378/381 (99%)	360 (95%)	14 (4%)	4 (1%)	14	5
1	F	379/381 (100%)	362 (96%)	16 (4%)	1 (0%)	41	31
All	All	2274/2286 (100%)	2185 (96%)	83 (4%)	6 (0%)	41	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	229	GLU
1	E	230	ALA
1	F	26	LEU
1	E	176	LYS
1	E	317	ALA
1	A	315	GLN

### 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	313/312 (100%)	301 (96%)	12 (4%)	33	22
1	B	312/312 (100%)	303 (97%)	9 (3%)	42	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	312/312 (100%)	302 (97%)	10 (3%)	39	29
1	D	312/312 (100%)	300 (96%)	12 (4%)	33	22
1	E	311/312 (100%)	297 (96%)	14 (4%)	27	17
1	F	312/312 (100%)	302 (97%)	10 (3%)	39	29
All	All	1872/1872 (100%)	1805 (96%)	67 (4%)	36	24

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	100	PHE
1	A	108	GLU
1	A	137[A]	ARG
1	A	137[B]	ARG
1	A	146	TYR
1	A	175	ARG
1	A	186	GLU
1	A	320	ASP
1	A	346	TYR
1	A	381	LYS
1	A	382	VAL
1	B	23	ARG
1	B	100	PHE
1	B	127	ASP
1	B	146	TYR
1	B	241	ASP
1	B	312	TRP
1	B	329	GLU
1	B	346	TYR
1	B	365	ASP
1	C	54	SER
1	C	91	ASP
1	C	100	PHE
1	C	146	TYR
1	C	218	LYS
1	C	226	ARG
1	C	312	TRP
1	C	329	GLU
1	C	346	TYR
1	C	381	LYS
1	D	100	PHE

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Mol	Chain	Res	Type
1	D	108	GLU
1	D	127	ASP
1	D	146	TYR
1	D	229	GLU
1	D	271	THR
1	D	315	GLN
1	D	327	LYS
1	D	346	TYR
1	D	365	ASP
1	D	381	LYS
1	D	382	VAL
1	E	24	ASP
1	E	42	LYS
1	E	63	LYS
1	E	64	TYR
1	E	78	LYS
1	E	100	PHE
1	E	108	GLU
1	E	117	LYS
1	E	127	ASP
1	E	146	TYR
1	E	276	LYS
1	E	312	TRP
1	E	329	GLU
1	E	382	VAL
1	F	24	ASP
1	F	100	PHE
1	F	146	TYR
1	F	241	ASP
1	F	312	TRP
1	F	329	GLU
1	F	365	ASP
1	F	378	THR
1	F	381	LYS
1	F	382	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	C	115	ASN
1	D	155	HIS

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Mol	Chain	Res	Type
1	D	220	HIS
1	E	115	ASN
1	E	315	GLN
1	F	283	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AZI	B	402	-	0,2,2	-	-	0,1,1	-	-
2	NAP	C	401	-	45,52,52	0.74	2 (4%)	56,80,80	0.95	4 (7%)
3	AZI	C	408	-	0,2,2	-	-	0,1,1	-	-
3	AZI	B	407	-	0,2,2	-	-	0,1,1	-	-
2	NAP	E	401	-	45,52,52	0.70	1 (2%)	56,80,80	0.88	2 (3%)
3	AZI	C	402	-	0,2,2	-	-	0,1,1	-	-
3	AZI	C	407	-	0,2,2	-	-	0,1,1	-	-
3	AZI	C	405	-	0,2,2	-	-	0,1,1	-	-
3	AZI	B	406	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AZI	C	406	-	0,2,2	-	-	0,1,1	-	-
2	NAP	F	401	-	45,52,52	0.74	2 (4%)	56,80,80	1.03	4 (7%)
3	AZI	B	408	-	0,2,2	-	-	0,1,1	-	-
3	AZI	C	404	-	0,2,2	-	-	0,1,1	-	-
3	AZI	B	403	-	0,2,2	-	-	0,1,1	-	-
2	NAP	B	401	-	45,52,52	0.73	2 (4%)	56,80,80	0.96	2 (3%)
3	AZI	B	404	-	0,2,2	-	-	0,1,1	-	-
2	NAP	D	401	-	45,52,52	0.72	2 (4%)	56,80,80	0.94	3 (5%)
2	NAP	A	401	-	45,52,52	0.74	2 (4%)	56,80,80	0.93	4 (7%)
3	AZI	B	405	-	0,2,2	-	-	0,1,1	-	-
3	AZI	C	403	-	0,2,2	-	-	0,1,1	-	-

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	NAP	C	401	-	-	2/31/67/67	0/5/5/5
2	NAP	B	401	-	-	2/31/67/67	0/5/5/5
2	NAP	E	401	-	-	2/31/67/67	0/5/5/5
2	NAP	D	401	-	-	2/31/67/67	0/5/5/5
2	NAP	A	401	-	-	2/31/67/67	0/5/5/5
2	NAP	F	401	-	-	3/31/67/67	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	C2N-N1N	2.69	1.38	1.35
2	A	401	NAP	C2N-N1N	2.68	1.38	1.35
2	D	401	NAP	C2N-N1N	2.65	1.38	1.35
2	B	401	NAP	C2N-N1N	2.60	1.38	1.35
2	E	401	NAP	C2N-N1N	2.59	1.38	1.35
2	F	401	NAP	C2N-N1N	2.53	1.38	1.35
2	F	401	NAP	C8A-N7A	-2.27	1.30	1.34
2	B	401	NAP	C8A-N7A	-2.15	1.30	1.34
2	D	401	NAP	C8A-N7A	-2.10	1.31	1.34
2	C	401	NAP	C8A-N7A	-2.07	1.31	1.34
2	A	401	NAP	C8A-N7A	-2.03	1.31	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAP	C1B-N9A-C4A	3.24	132.33	126.64
2	F	401	NAP	C3B-C2B-C1B	-2.66	97.89	102.89
2	B	401	NAP	C6N-N1N-C2N	-2.55	119.65	121.97
2	D	401	NAP	C6N-N1N-C2N	-2.51	119.69	121.97
2	E	401	NAP	C6N-N1N-C2N	-2.50	119.70	121.97
2	C	401	NAP	C6N-N1N-C2N	-2.44	119.75	121.97
2	F	401	NAP	C6N-N1N-C2N	-2.29	119.89	121.97
2	A	401	NAP	C6N-N1N-C2N	-2.29	119.89	121.97
2	A	401	NAP	C3B-C2B-C1B	-2.28	98.60	102.89
2	F	401	NAP	O4B-C1B-C2B	-2.28	102.64	106.59
2	A	401	NAP	O4B-C1B-C2B	-2.26	102.66	106.59
2	C	401	NAP	O4B-C1B-C2B	-2.22	102.74	106.59
2	D	401	NAP	O4B-C1B-C2B	-2.19	102.80	106.59
2	C	401	NAP	C3B-C2B-C1B	-2.16	98.83	102.89
2	A	401	NAP	C5A-C6A-N6A	2.16	123.63	120.35
2	C	401	NAP	C5A-C6A-N6A	2.13	123.59	120.35
2	D	401	NAP	C5A-C6A-N6A	2.10	123.55	120.35
2	E	401	NAP	C5A-C6A-N6A	2.05	123.47	120.35
2	B	401	NAP	C3B-C2B-C1B	-2.00	99.13	102.89

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	E	401	NAP	O4D-C1D-N1N-C6N
2	F	401	NAP	O4D-C1D-N1N-C6N
2	E	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	O4B-C4B-C5B-O5B
2	F	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B
2	F	401	NAP	C2B-O2B-P2B-O3X

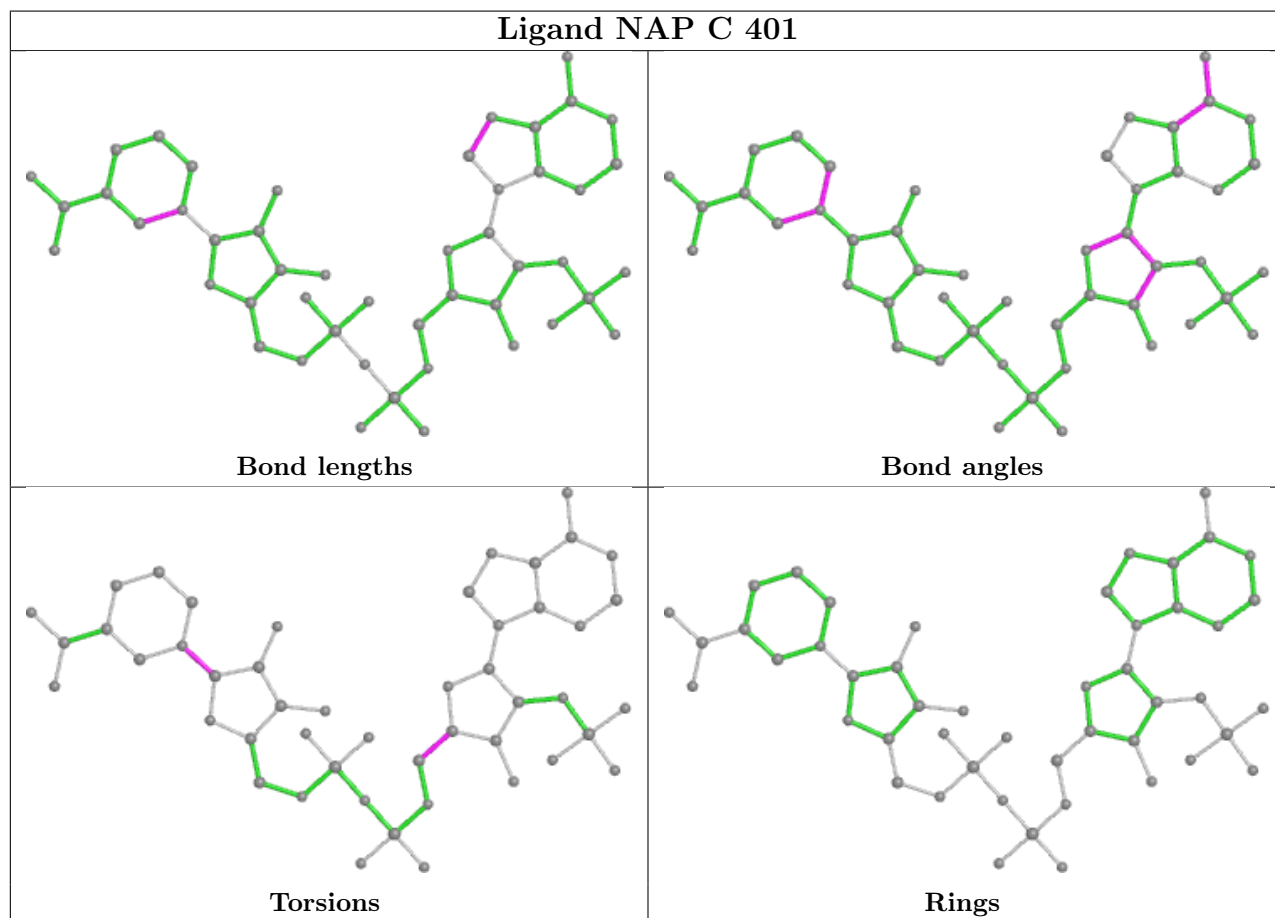
There are no ring outliers.

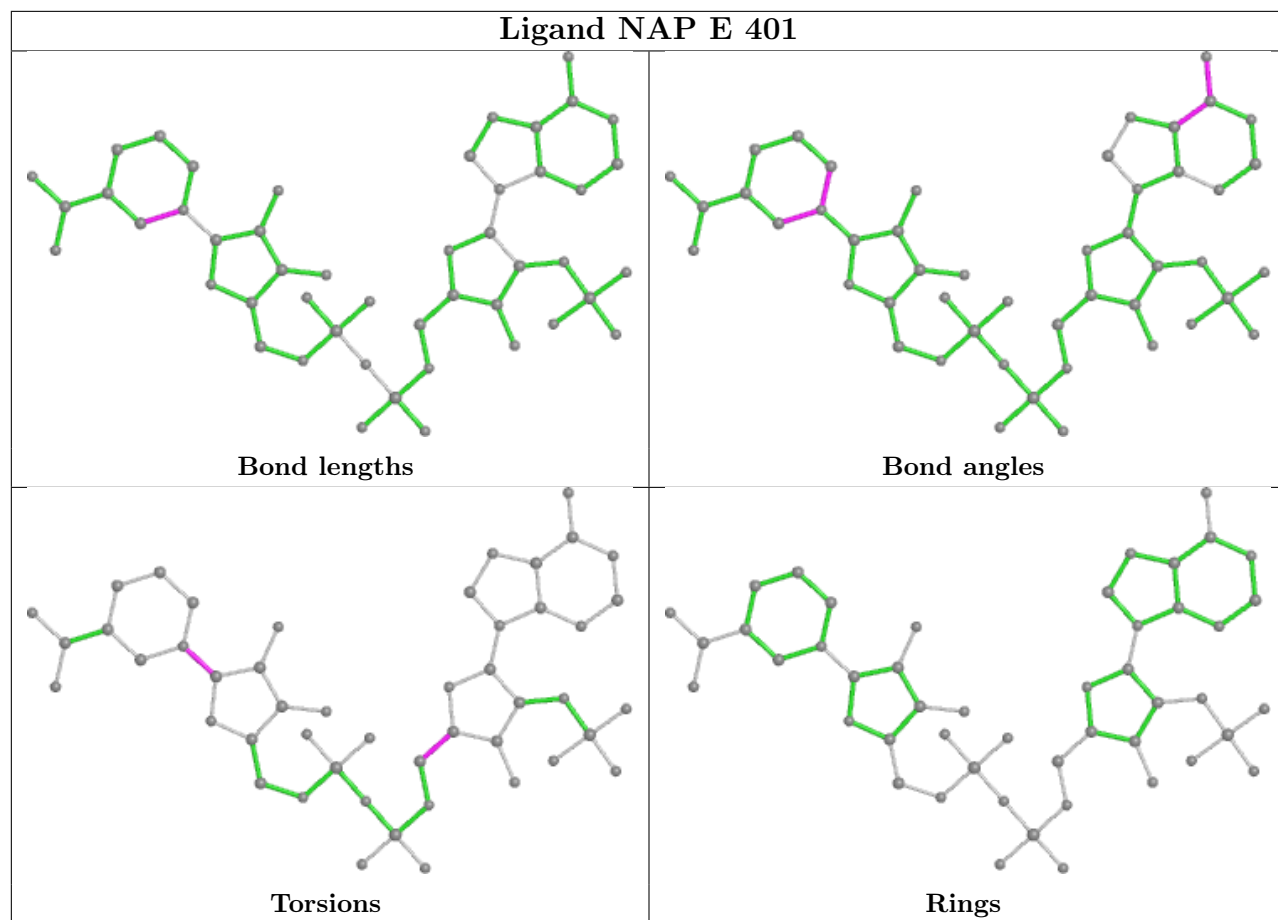
6 monomers are involved in 25 short contacts:

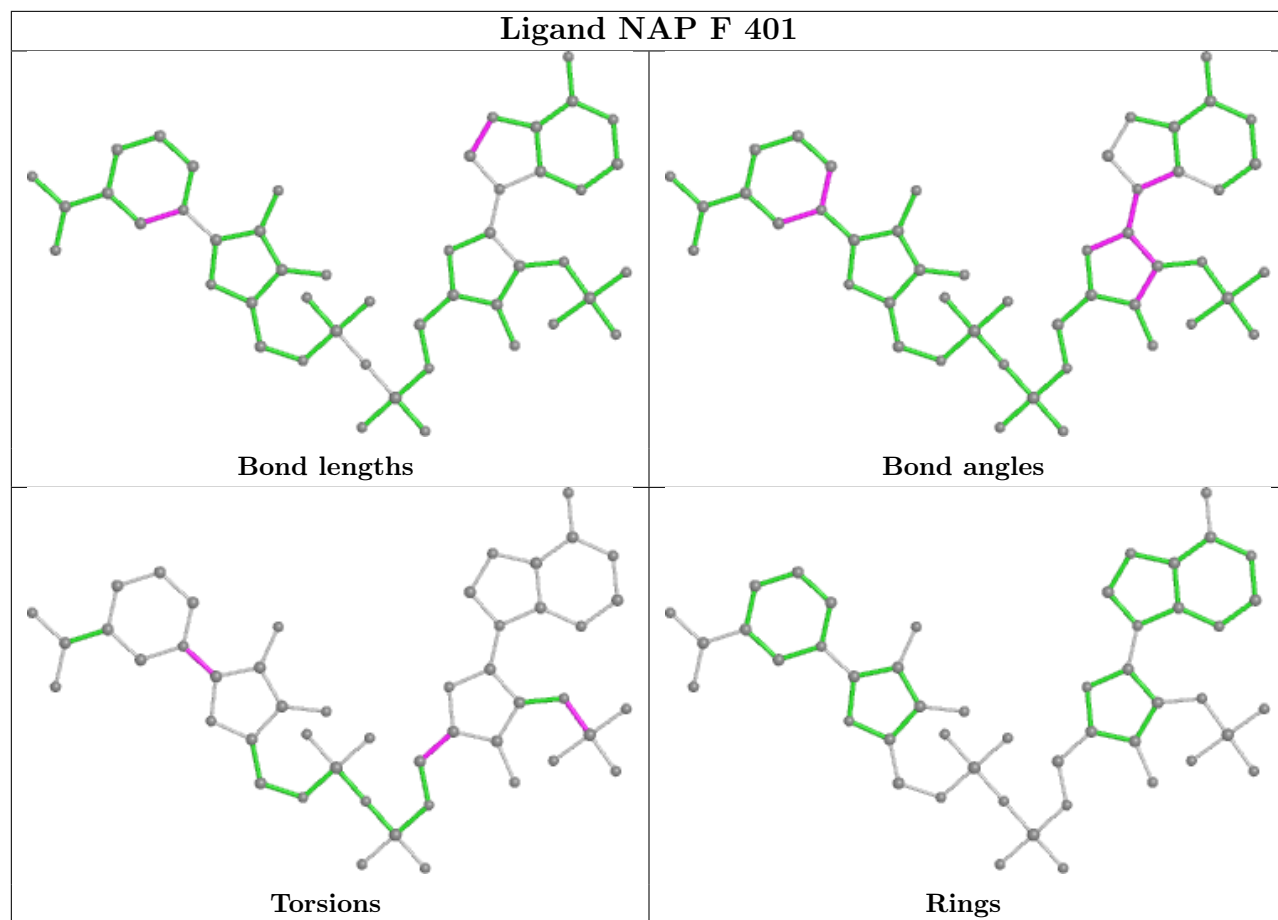


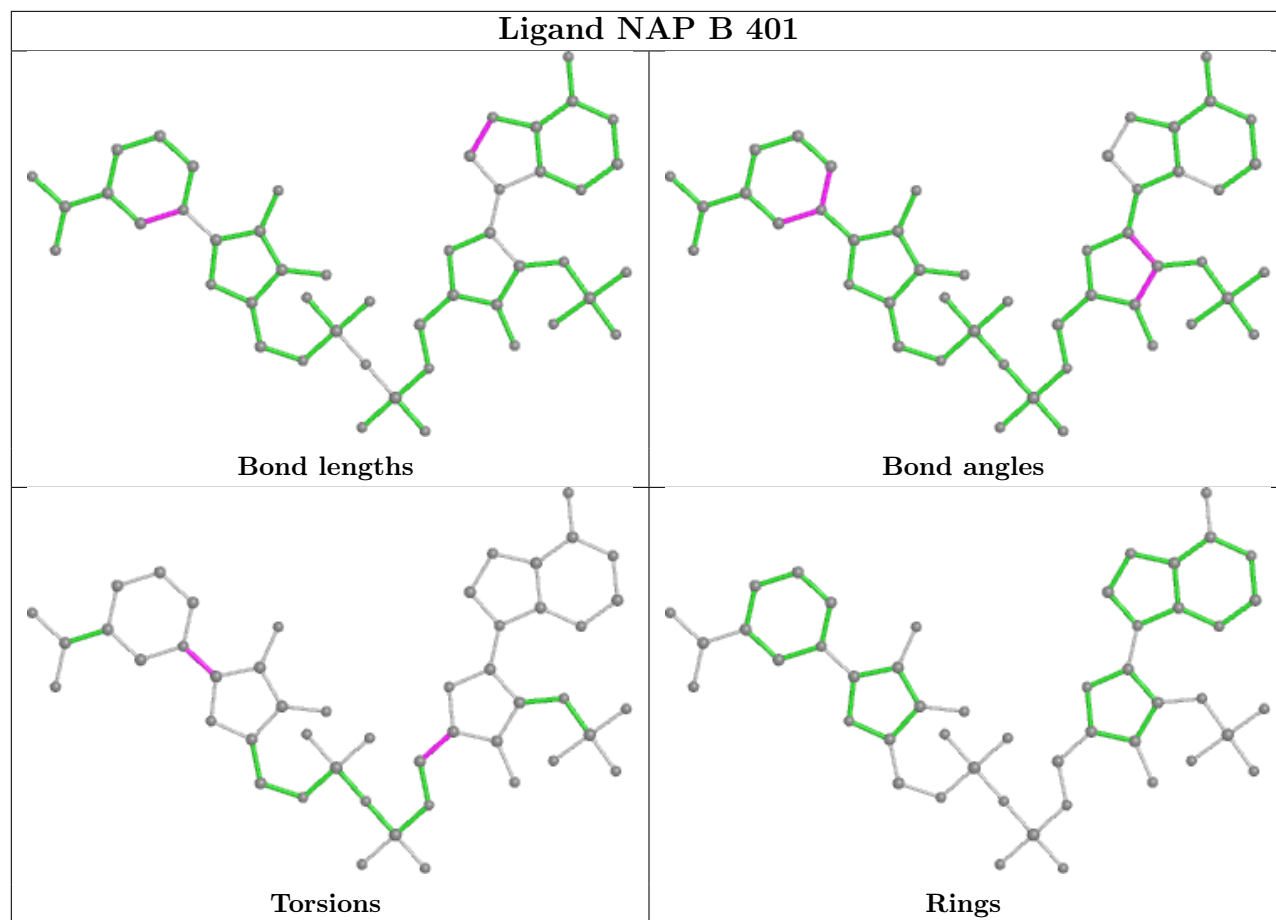
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAP	5	0
2	E	401	NAP	4	0
2	F	401	NAP	4	0
2	B	401	NAP	4	0
2	D	401	NAP	1	0
2	A	401	NAP	7	0

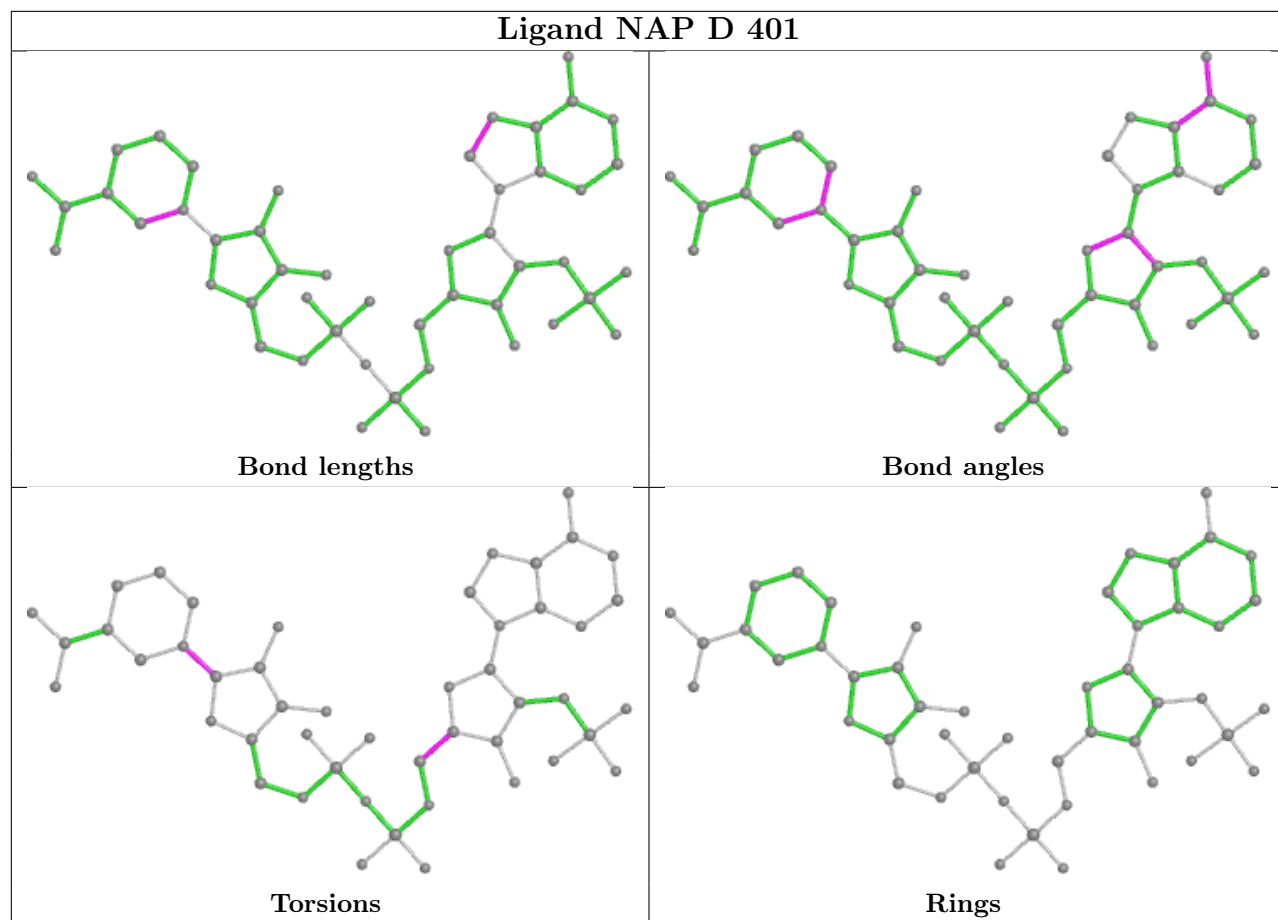
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

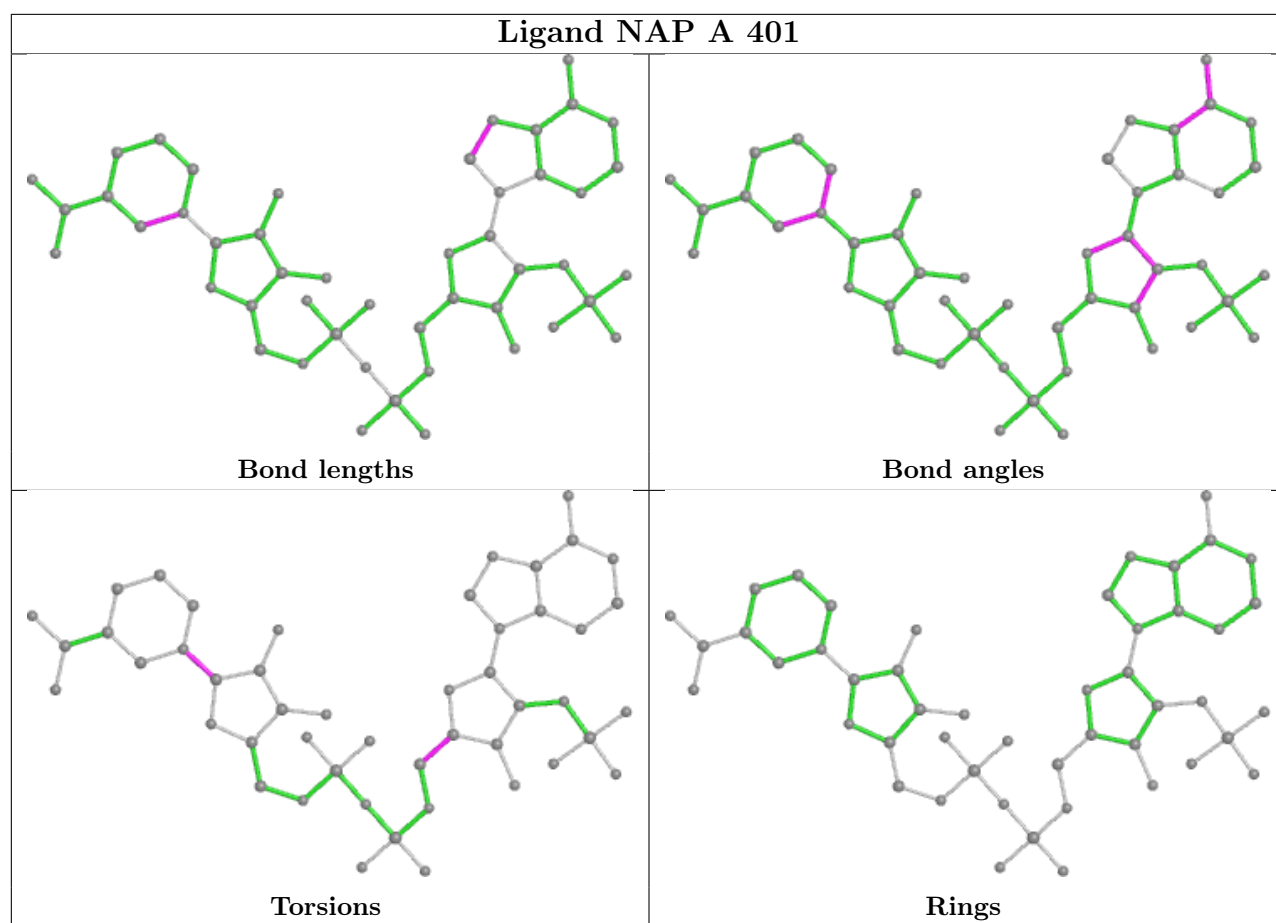












## 5.7 Other polymers [\(i\)](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	380/381 (99%)	0.89	36 (9%) 8 9	35, 40, 49, 83	0
1	B	378/381 (99%)	0.79	30 (7%) 12 14	30, 40, 45, 62	0
1	C	381/381 (100%)	0.84	28 (7%) 15 17	36, 41, 47, 55	0
1	D	379/381 (99%)	0.88	34 (8%) 9 11	39, 44, 53, 71	0
1	E	371/381 (97%)	0.97	45 (12%) 4 5	30, 45, 54, 65	0
1	F	378/381 (99%)	0.99	44 (11%) 4 5	36, 42, 52, 63	0
All	All	2267/2286 (99%)	0.89	217 (9%) 8 9	30, 42, 51, 83	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	7.8
1	D	2	SER	6.2
1	B	2	SER	5.1
1	F	2	SER	4.4
1	C	157	VAL	4.2
1	B	382	VAL	4.2
1	F	382	VAL	4.1
1	C	3	ALA	4.1
1	F	3	ALA	4.0
1	F	157	VAL	3.9
1	D	382	VAL	3.8
1	F	285	ALA	3.6
1	A	2	SER	3.5
1	D	157	VAL	3.5
1	A	204	ILE	3.5
1	C	230	ALA	3.5
1	F	89	LEU	3.4
1	E	316	PRO	3.4
1	E	90	VAL	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	161	LEU	3.3
1	F	191	LEU	3.3
1	C	382	VAL	3.2
1	A	153	ALA	3.2
1	D	379	GLY	3.2
1	A	157	VAL	3.2
1	E	382	VAL	3.2
1	C	327	LYS	3.2
1	A	139	ILE	3.2
1	C	152	VAL	3.2
1	C	124	ILE	3.2
1	C	233	LYS	3.2
1	A	152	VAL	3.2
1	D	233	LYS	3.1
1	C	153	ALA	3.1
1	E	82	ASP	3.1
1	E	241	ASP	3.0
1	D	89	LEU	3.0
1	A	150	ILE	3.0
1	E	155	HIS	3.0
1	E	72	PHE	3.0
1	D	380	ALA	3.0
1	E	157	VAL	3.0
1	D	82	ASP	3.0
1	C	208	VAL	3.0
1	E	81	PRO	2.9
1	F	67	ALA	2.9
1	D	358	PHE	2.9
1	D	161	LEU	2.9
1	F	161	LEU	2.9
1	A	3	ALA	2.9
1	B	215	PHE	2.8
1	A	146	TYR	2.8
1	B	319	LYS	2.8
1	C	91	ASP	2.8
1	F	215	PHE	2.8
1	B	191	LEU	2.8
1	E	20	THR	2.8
1	A	137[A]	ARG	2.7
1	E	379	GLY	2.7
1	A	156	VAL	2.7
1	F	124	ILE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	155	HIS	2.7
1	F	152	VAL	2.7
1	F	160	ILE	2.7
1	F	99	PRO	2.7
1	E	44	ILE	2.6
1	E	55	VAL	2.6
1	D	164	VAL	2.6
1	F	164	VAL	2.6
1	F	358	PHE	2.6
1	F	65	LEU	2.6
1	F	88	GLU	2.6
1	F	204	ILE	2.6
1	A	134	ALA	2.6
1	F	44	ILE	2.6
1	C	161	LEU	2.5
1	F	131	LEU	2.5
1	A	314	PRO	2.5
1	F	316	PRO	2.5
1	B	164	VAL	2.5
1	D	129	VAL	2.5
1	D	156	VAL	2.5
1	B	357	PHE	2.5
1	E	204	ILE	2.5
1	D	114	LYS	2.5
1	E	378	THR	2.5
1	A	257	VAL	2.5
1	B	157	VAL	2.5
1	C	73	VAL	2.5
1	E	156	VAL	2.5
1	E	161	LEU	2.5
1	F	378	THR	2.5
1	C	204	ILE	2.5
1	E	248	PRO	2.5
1	F	282	VAL	2.5
1	A	229	GLU	2.5
1	D	372	GLY	2.4
1	F	91	ASP	2.4
1	E	208	VAL	2.4
1	B	255	LEU	2.4
1	D	229	GLU	2.4
1	B	282	VAL	2.4
1	D	231	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	239	TRP	2.4
1	E	158	MET	2.4
1	D	47	THR	2.4
1	D	208	VAL	2.4
1	A	235	LEU	2.4
1	A	346	TYR	2.4
1	E	46	PHE	2.4
1	D	3	ALA	2.4
1	B	378	THR	2.4
1	A	124	ILE	2.4
1	A	335	ILE	2.4
1	D	90	VAL	2.4
1	D	204	ILE	2.4
1	D	238	VAL	2.4
1	A	259	LEU	2.3
1	B	289	LEU	2.3
1	F	114	LYS	2.3
1	E	168	ILE	2.3
1	E	311	VAL	2.3
1	F	129	VAL	2.3
1	A	161	LEU	2.3
1	E	274	LEU	2.3
1	E	308	ALA	2.3
1	A	270	GLU	2.3
1	B	204	ILE	2.3
1	D	55	VAL	2.3
1	F	155	HIS	2.3
1	A	206	LEU	2.3
1	D	191	LEU	2.3
1	A	309	GLY	2.3
1	B	160	ILE	2.3
1	E	159	MET	2.3
1	A	370	VAL	2.3
1	B	233	LYS	2.3
1	C	316	PRO	2.2
1	B	28	LYS	2.2
1	B	208	VAL	2.2
1	B	253	VAL	2.2
1	B	308	ALA	2.2
1	A	336	SER	2.2
1	B	139	ILE	2.2
1	F	110	ILE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	60	GLY	2.2
1	C	114	LYS	2.2
1	F	100	PHE	2.2
1	A	208	VAL	2.2
1	B	152	VAL	2.2
1	E	84	VAL	2.2
1	F	274	LEU	2.2
1	B	365	ASP	2.2
1	D	215	PHE	2.2
1	C	150	ILE	2.2
1	A	131	LEU	2.2
1	B	239	TRP	2.2
1	B	158	MET	2.2
1	B	153	ALA	2.2
1	E	153	ALA	2.2
1	D	353	ILE	2.2
1	C	19	LYS	2.2
1	F	289	LEU	2.2
1	D	155	HIS	2.2
1	D	239	TRP	2.2
1	E	327	LYS	2.2
1	D	228	PRO	2.1
1	E	124	ILE	2.1
1	D	354	LEU	2.1
1	E	134	ALA	2.1
1	E	245	ASP	2.1
1	E	21	TYR	2.1
1	C	336	SER	2.1
1	B	252	VAL	2.1
1	D	152	VAL	2.1
1	E	381	LYS	2.1
1	F	275	PHE	2.1
1	E	353	ILE	2.1
1	E	359	GLU	2.1
1	C	155	HIS	2.1
1	A	365	ASP	2.1
1	F	309	GLY	2.1
1	A	129	VAL	2.1
1	E	152	VAL	2.1
1	F	90	VAL	2.1
1	F	146	TYR	2.1
1	A	319	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	158	MET	2.1
1	D	91	ASP	2.1
1	E	83	SER	2.1
1	F	245	ASP	2.1
1	A	43	ALA	2.1
1	C	229	GLU	2.1
1	C	380	ALA	2.1
1	E	174	ALA	2.1
1	F	230	ALA	2.1
1	A	289	LEU	2.1
1	B	379	GLY	2.1
1	A	254	THR	2.0
1	A	284	THR	2.0
1	C	346	TYR	2.0
1	C	212	LEU	2.0
1	E	5	ILE	2.0
1	E	160	ILE	2.0
1	F	212	LEU	2.0
1	F	375	LEU	2.0
1	F	229	GLU	2.0
1	F	241	ASP	2.0
1	C	167	TYR	2.0
1	C	234	GLU	2.0
1	F	72	PHE	2.0
1	F	201	ALA	2.0
1	B	150	ILE	2.0
1	B	259	LEU	2.0
1	D	289	LEU	2.0
1	E	150	ILE	2.0
1	E	151	SER	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

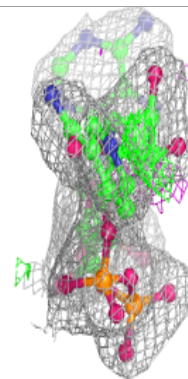
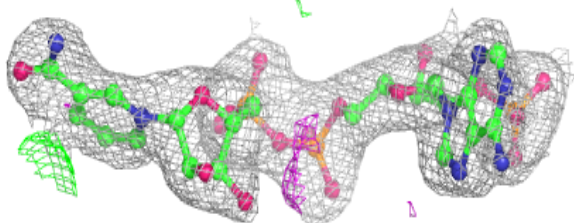
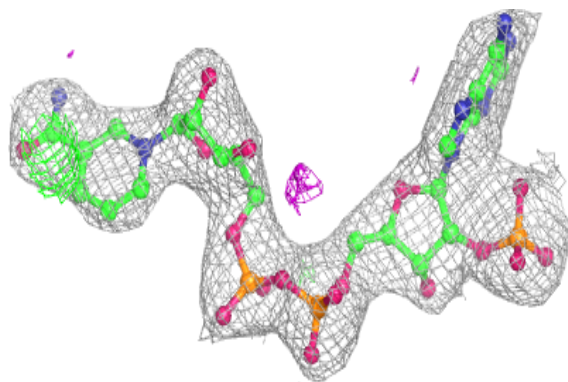
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	AZI	C	405	3/3	0.78	0.27	43,43,45,46	0
3	AZI	C	408	3/3	0.87	0.22	44,44,44,45	0
3	AZI	B	408	3/3	0.89	0.26	40,40,40,41	0
3	AZI	B	404	3/3	0.89	0.23	36,36,37,38	0
3	AZI	B	407	3/3	0.89	0.34	37,37,38,39	0
3	AZI	C	407	3/3	0.90	0.30	47,47,48,50	0
3	AZI	B	405	3/3	0.90	0.32	46,46,46,48	0
3	AZI	C	406	3/3	0.92	0.20	40,40,41,42	0
3	AZI	C	404	3/3	0.92	0.26	38,38,38,40	0
3	AZI	B	406	3/3	0.92	0.23	42,42,43,43	0
3	AZI	C	403	3/3	0.93	0.25	44,44,44,46	0
2	NAP	E	401	48/48	0.94	0.15	40,46,50,50	0
2	NAP	C	401	48/48	0.95	0.14	36,40,43,44	0
2	NAP	A	401	48/48	0.95	0.16	34,39,42,43	0
2	NAP	F	401	48/48	0.95	0.14	38,42,45,46	0
3	AZI	B	403	3/3	0.95	0.13	39,39,40,42	0
2	NAP	B	401	48/48	0.95	0.13	35,40,42,43	0
2	NAP	D	401	48/48	0.97	0.13	39,43,50,59	0
3	AZI	B	402	3/3	0.97	0.11	35,35,36,36	0
3	AZI	C	402	3/3	0.97	0.12	37,37,37,37	0

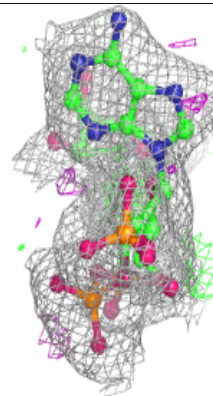
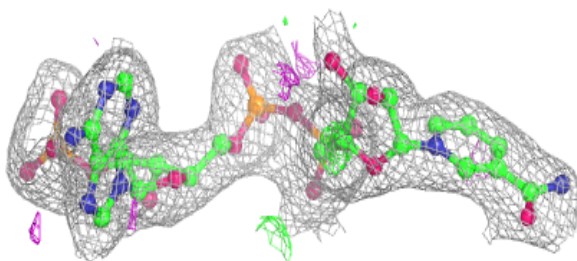
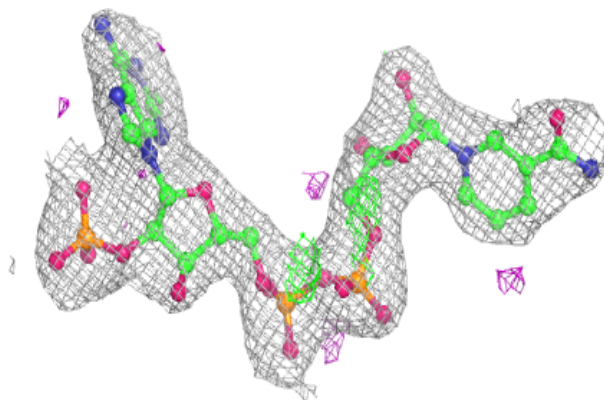
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP E 401:**

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

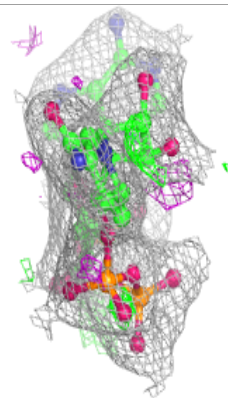
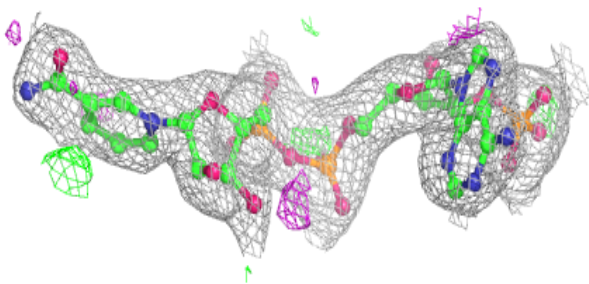
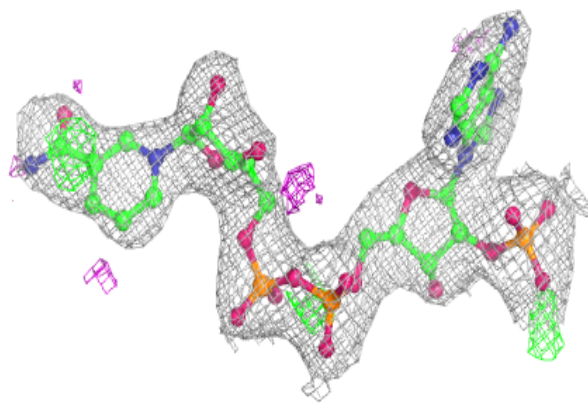
**Electron density around NAP C 401:**

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

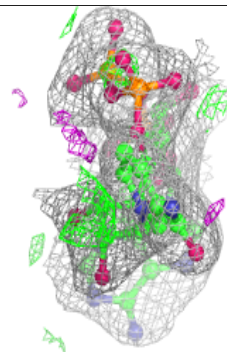
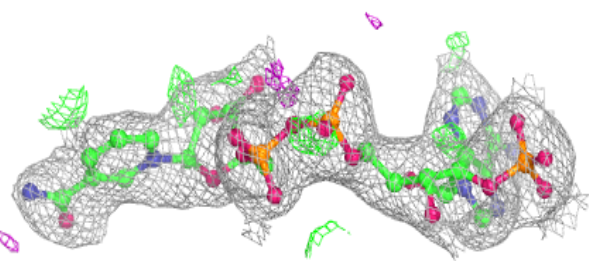
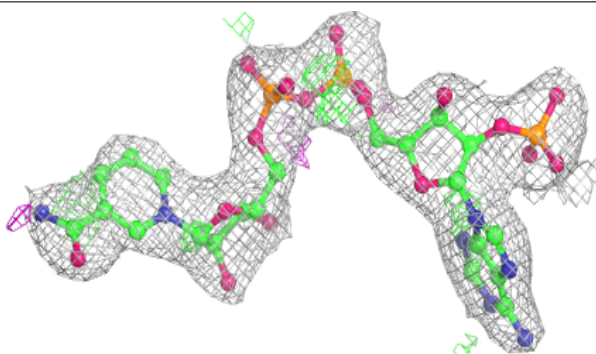


**Electron density around NAP A 401:**

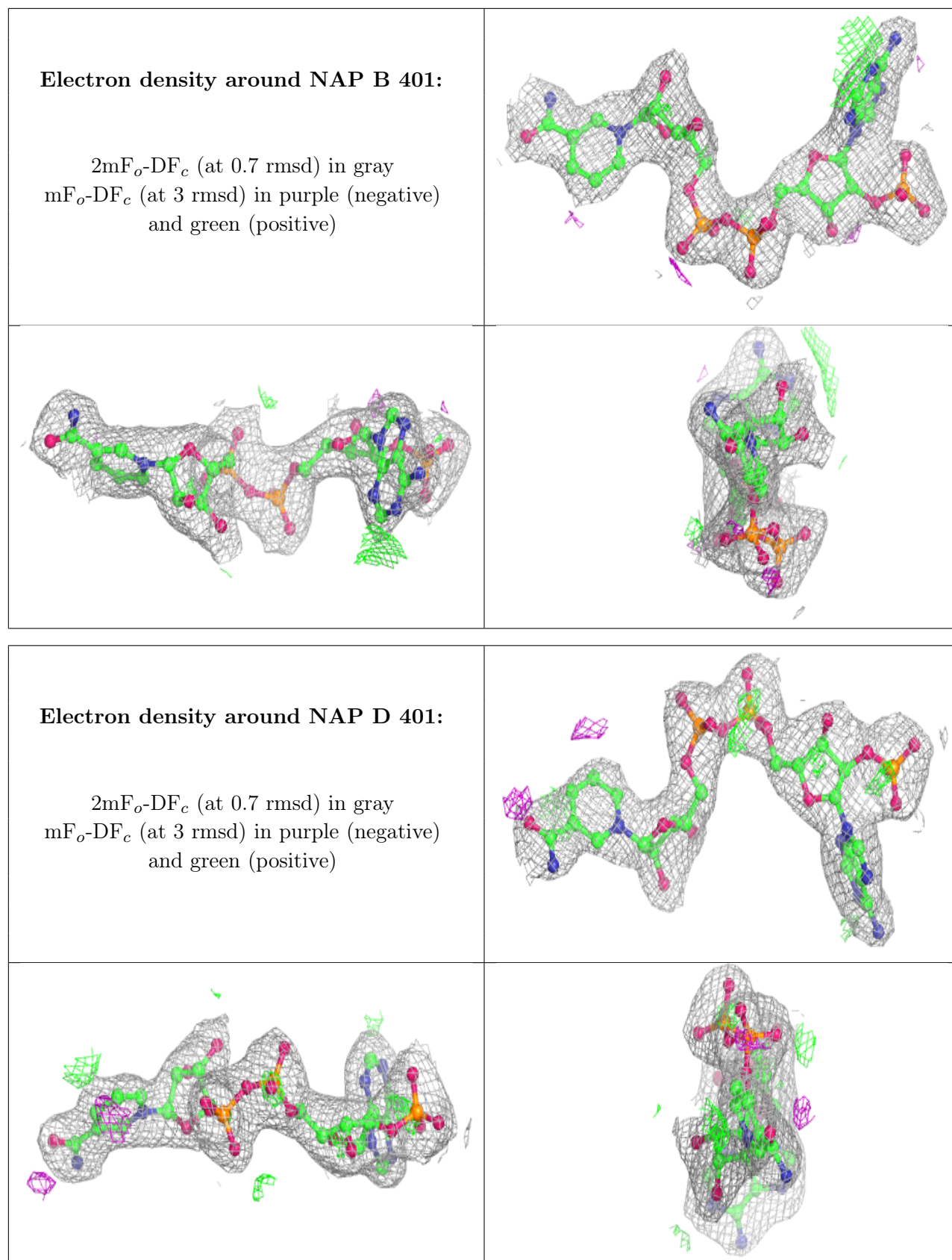
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP F 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 [i](#)

There are no such residues in this entry.