



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 8OQ2 / pdb_00008oq2
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

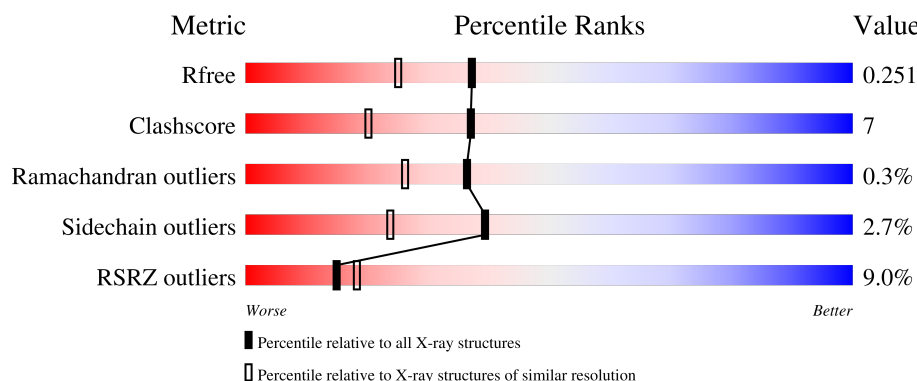
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	381	9% 86% 13%
1	B	381	8% 80% 19%
1	C	381	6% 81% 19%
1	D	381	7% 86% 13%
1	E	381	13% 81% 16%

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Mol	Chain	Length	Quality of chain
1	F	381	

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
3	AZI	B	402	-	X	-	-
3	AZI	B	403	-	X	-	-
3	AZI	B	404	-	X	-	-
3	AZI	B	405	-	X	-	-
3	AZI	B	406	-	X	-	-
3	AZI	B	407	-	X	-	-
3	AZI	B	408	-	X	-	-
3	AZI	C	402	-	X	-	-
3	AZI	C	403	-	X	-	-
3	AZI	C	404	-	X	-	-
3	AZI	C	405	-	X	-	-
3	AZI	C	406	-	X	-	-
3	AZI	C	407	-	X	-	-
3	AZI	C	408	-	X	-	-

2 Entry composition

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

There are 30 discrepancies between the modelled and reference sequences:

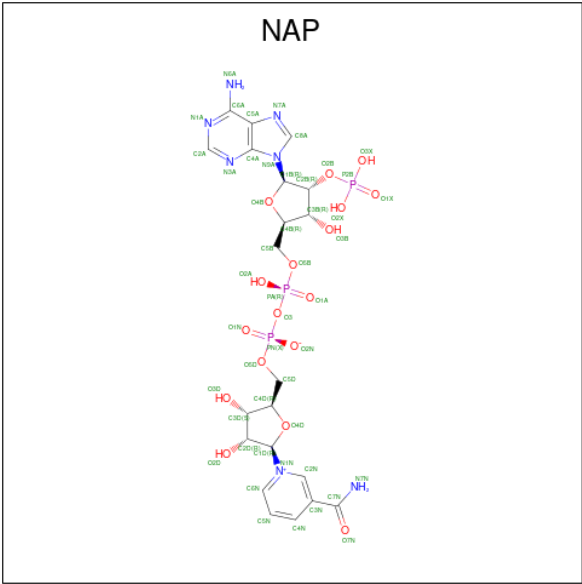
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP D7A8L2
A	200	GLY	ALA	engineered mutation	UNP D7A8L2
A	223	GLN	ASP	engineered mutation	UNP D7A8L2
A	381	LYS	HIS	engineered mutation	UNP D7A8L2
A	382	VAL	SER	engineered mutation	UNP D7A8L2
B	2	SER	-	expression tag	UNP D7A8L2
B	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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



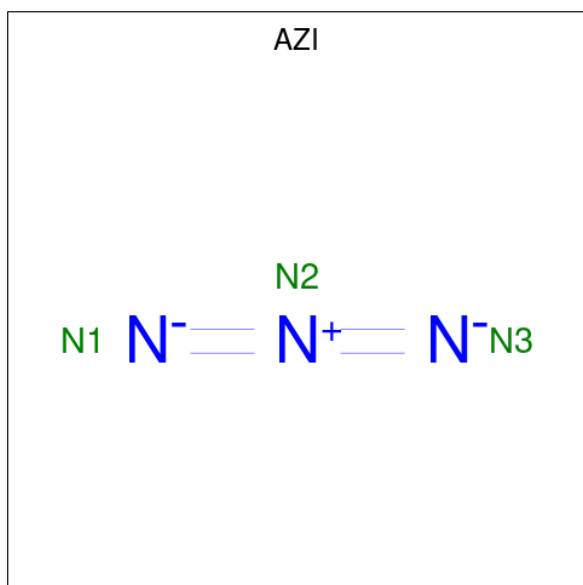
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

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

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



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 3	N 3	0	0
3	C	1	Total 3	N 3	0	0
3	C	1	Total 3	N 3	0	0
3	C	1	Total 3	N 3	0	0
3	C	1	Total 3	N 3	0	0

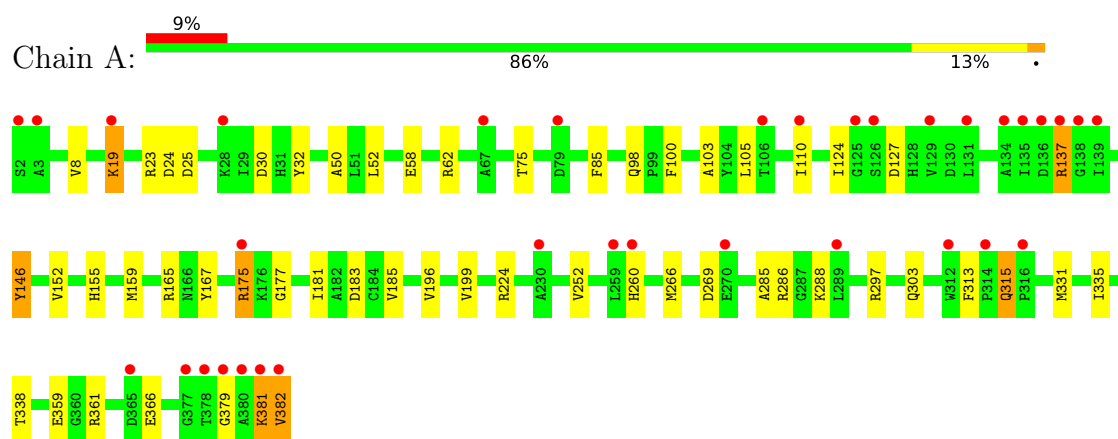
- Molecule 4 is water.

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

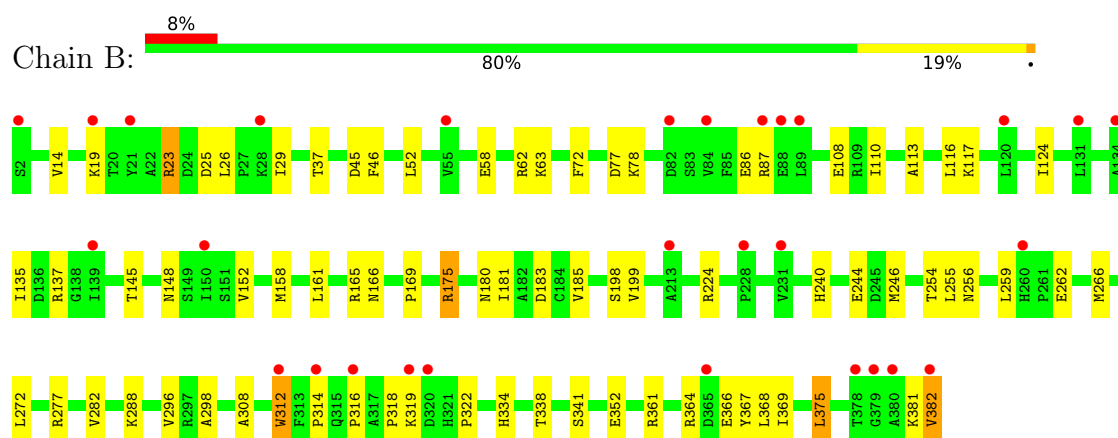
3 Residue-property plots [i](#)

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.

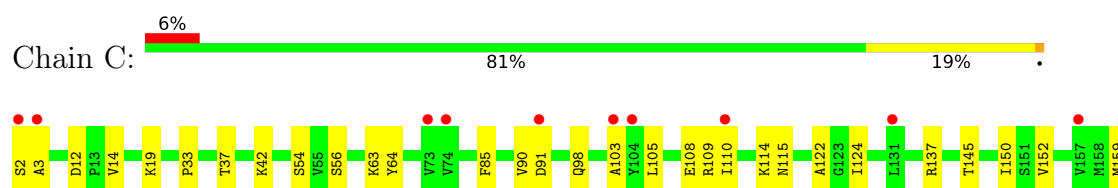
- Molecule 1: Formate dehydrogenase

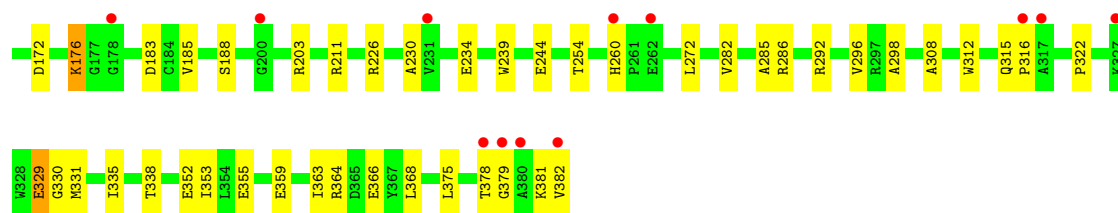


- Molecule 1: Formate dehydrogenase

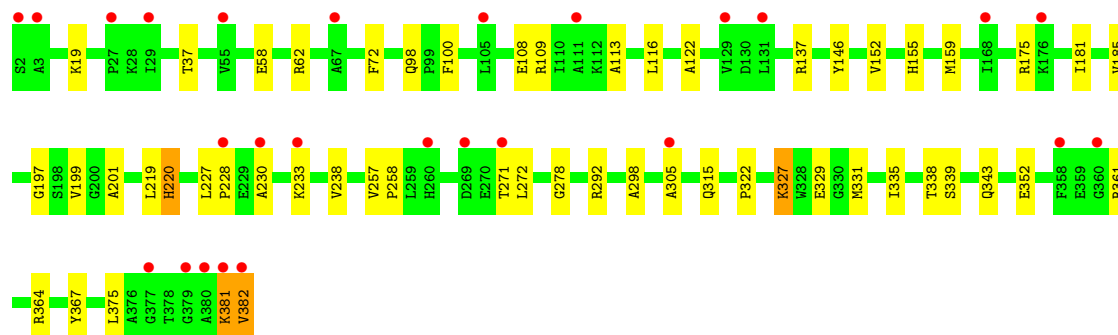
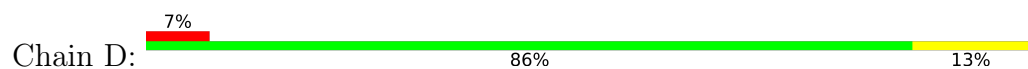


- Molecule 1: Formate dehydrogenase

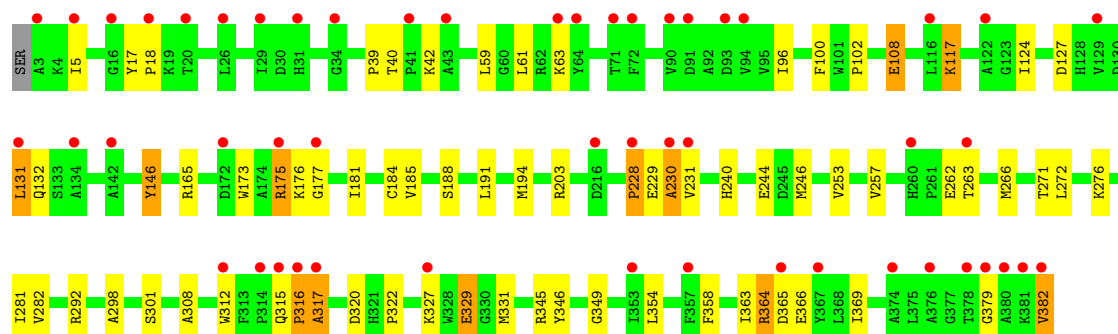
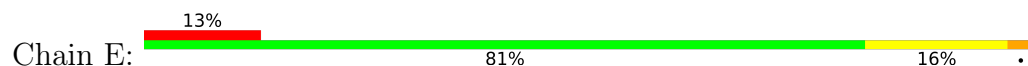




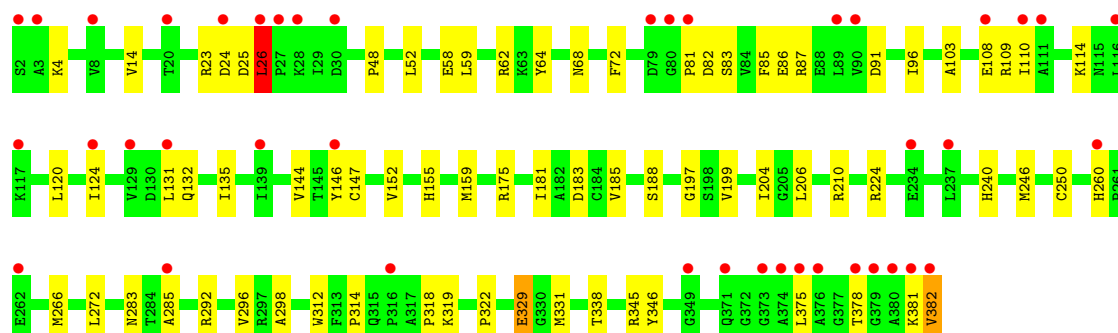
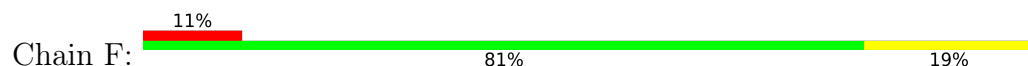
• Molecule 1: Formate dehydrogenase



• Molecule 1: Formate dehydrogenase



• Molecule 1: Formate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	132.26Å 132.26Å 302.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.60 – 1.91 114.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (114.60-1.91) 99.5 (114.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.275 (Not available) , 0.251	Depositor DCC
R_{free} test set	1077 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 8.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18219	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage'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.*

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 [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	0.48	1/3043 (0.0%)	0.75	2/4141 (0.0%)
1	B	0.45	0/3032	0.70	2/4127 (0.0%)
1	C	0.47	1/3032 (0.0%)	0.70	1/4127 (0.0%)
1	D	0.66	2/3032 (0.1%)	0.81	2/4127 (0.0%)
1	E	0.47	4/3026 (0.1%)	0.72	5/4119 (0.1%)
1	F	0.47	1/3032 (0.0%)	0.74	2/4127 (0.0%)
All	All	0.50	9/18197 (0.0%)	0.74	14/24768 (0.1%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	LEU	C-N	19.43	1.59	1.33
1	D	220	HIS	C-N	-9.09	1.22	1.33
1	A	366	GLU	C-O	-6.95	1.16	1.24
1	C	172	ASP	C-O	-6.68	1.16	1.24
1	E	345	ARG	C-O	-5.99	1.16	1.24
1	E	131	LEU	C-O	-5.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	346	TYR	C-O	-5.37	1.17	1.24
1	E	366	GLU	C-O	-5.23	1.17	1.24
1	F	345	ARG	C-O	-5.21	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	316	PRO	N-CA-C	-6.37	104.26	113.75
1	E	228	PRO	CA-C-O	-6.08	114.73	121.23
1	A	19	LYS	N-CA-C	-5.75	105.60	113.30
1	F	110	ILE	N-CA-C	-5.74	104.76	110.62
1	F	132	GLN	CA-C-O	-5.32	114.33	120.24
1	D	258	PRO	CA-C-O	-5.24	114.92	122.31
1	B	117	LYS	N-CA-C	-5.19	108.70	114.62
1	C	19	LYS	N-CA-C	-5.17	107.53	113.88
1	E	231	VAL	N-CA-C	-5.15	105.52	110.72
1	A	303	GLN	N-CA-C	-5.14	105.68	111.28
1	B	19	LYS	N-CA-C	-5.11	107.11	113.55
1	E	131	LEU	CA-C-O	-5.08	115.67	121.00
1	D	19	LYS	N-CA-C	-5.06	106.53	113.30
1	E	365	ASP	N-CA-C	-5.02	105.94	111.71

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 ⓘ

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	41	0
1	B	2958	0	2919	59	0
1	C	2958	0	2919	52	0
1	D	2958	0	2919	31	0
1	E	2952	0	2914	42	0
1	F	2958	0	2919	46	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
4	E	15	0	0	0	0
4	F	24	0	0	0	0
All	All	18219	0	17672	252	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 (252) 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:F:199:VAL:HG11	1:F:266:MET:HE1	1.51	0.93
1:D:220:HIS:CD2	1:D:238:VAL:HB	2.07	0.89
1:D:155:HIS:CD2	1:D:159:MET:HE3	2.15	0.81
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:F:155:HIS:CD2	1:F:159:MET:HE3	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:THR:HG23	1:F:185:VAL:HG11	1.70	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:199:VAL:HG11	1:B:266:MET:HE1	1.80	0.64
1:A:199:VAL:HG11	1:A:266:MET:HE1	1.80	0.64
1:B:224:ARG:HH12	1:B:382:VAL:HG23	1.62	0.64
1:D:381:LYS:O	1:D:382:VAL:C	2.42	0.63
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:B:77:ASP:CG	1:E:327:LYS:HZ3	2.08	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
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:B:77:ASP:CG	1:E:327:LYS:NZ	2.63	0.57
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:A:381:LYS:O	1:A:382:VAL:C	2.47	0.57
1:D:230:ALA:HA	1:D:233:LYS:HG3	1.86	0.57
1:C:230:ALA:O	1:C:234:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:364:ARG:HD3	1:B:367:TYR:CE2	2.43	0.53
1:B:244:GLU:CD	1:B:244:GLU:H	2.16	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:B:368:LEU:C	1:B:369:ILE:HD13	2.34	0.52
1:C:185:VAL:HA	1:C:188:SER:HB2	1.89	0.52
1:E:244:GLU:H	1:E:244:GLU:CD	2.16	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:315:GLN:O	1:E:316:PRO:C	2.51	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
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:E:175:ARG:C	1:E:177:GLY:N	2.69	0.49
1:D:201:ALA:CB	1:D:227:LEU:HD11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLU:OE1	1:A:361:ARG:NH1	2.46	0.49
1:A:269:ASP:CG	1:A:297:ARG:HH21	2.19	0.49
1:B:181:ILE:O	1:B:185:VAL:HG22	2.12	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:C:12:ASP:OD1	1:C:54:SER:OG	2.28	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:159:MET:HE2	1:C:330:GLY:O	2.14	0.48
1:C:108:GLU:H	1:C:108:GLU:CD	2.12	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:E:173:TRP:CD1	1:E:184:CYS:HG	2.32	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:145:THR:OG1	1:C:366:GLU:O	2.25	0.45
1:E:263:THR:HB	1:E:266:MET:HE3	1.98	0.45
1:F:52:LEU:HB3	1:F:59:LEU:HA	1.99	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:D:155:HIS:NE2	1:D:159:MET:HE3	2.31	0.45
1:E:17:TYR:CD1	1:E:18:PRO:HD2	2.51	0.45
1:C:12:ASP:OD2	1:C:56:SER:OG	2.35	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:F:26:LEU:HD22	1:F:48:PRO:C	2.41	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: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:246:MET:HE2	1:E:246:MET:HB3	1.91	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: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:E:363:ILE:O	1:E:364:ARG:C	2.61	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
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:C:114:LYS:C	1:C:115:ASN:HD22	2.26	0.43
1:E:228:PRO:O	1:E:230:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:244:GLU:H	1:C:244:GLU:CD	2.26	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: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:C:226:ARG:HE	1:C:239:TRP:CD1	2.36	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:78:LYS:HZ1	1:B:316:PRO:HD3	1.83	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:E:108:GLU:CD	1:E:108:GLU:H	2.26	0.42
1:A:30:ASP:OD1	1:A:30:ASP:C	2.63	0.42
1:B:255:LEU:HD22	1:B:266:MET:HE2	2.01	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:B:145:THR:OG1	1:B:366:GLU:O	2.35	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:A:127:ASP:CG	1:A:286:ARG:HE	2.27	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:254:THR:HG23	1:B:256:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PRO:HG2	1:C:150:ILE:HD11	2.01	0.41
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:E:315:GLN:C	1:E:317:ALA:N	2.77	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:C:381:LYS:O	1:C:382:VAL:C	2.63	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:C:379:GLY:O	1:C:382:VAL:HB	2.20	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:D:227:LEU:O	1:D:228:PRO:C	2.64	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:C:315:GLN:HA	1:C:316:PRO:C	2.45	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:A:331:MET:HE3	1:A:331:MET:HB3	1.77	0.40
1:D:98:GLN:HG2	1:D:122:ALA:HB3	2.03	0.40
1:E:131:LEU:O	1:E:132:GLN:C	2.64	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

5.3.1 Protein backbone

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%)	36	26
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%)	11	3
1	F	379/381 (100%)	362 (96%)	16 (4%)	1 (0%)	36	26
All	All	2274/2286 (100%)	2185 (96%)	83 (4%)	6 (0%)	36	26

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

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%)	305 (97%)	8 (3%)	40	24
1	B	312/312 (100%)	307 (98%)	5 (2%)	55	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	312/312 (100%)	306 (98%)	6 (2%)	50	37
1	D	312/312 (100%)	304 (97%)	8 (3%)	40	24
1	E	311/312 (100%)	298 (96%)	13 (4%)	26	11
1	F	312/312 (100%)	300 (96%)	12 (4%)	29	14
All	All	1872/1872 (100%)	1820 (97%)	52 (3%)	39	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	137[A]	ARG
1	A	137[B]	ARG
1	A	146	TYR
1	A	175	ARG
1	A	315	GLN
1	A	381	LYS
1	A	382	VAL
1	B	86	GLU
1	B	175	ARG
1	B	312	TRP
1	B	375	LEU
1	B	382	VAL
1	C	42	LYS
1	C	90	VAL
1	C	91	ASP
1	C	176	LYS
1	C	312	TRP
1	C	329	GLU
1	D	100	PHE
1	D	108	GLU
1	D	146	TYR
1	D	271	THR
1	D	315	GLN
1	D	327	LYS
1	D	381	LYS
1	D	382	VAL
1	E	42	LYS
1	E	63	LYS
1	E	100	PHE
1	E	108	GLU
1	E	117	LYS

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Mol	Chain	Res	Type
1	E	127	ASP
1	E	146	TYR
1	E	271	THR
1	E	276	LYS
1	E	301	SER
1	E	312	TRP
1	E	329	GLU
1	E	382	VAL
1	F	24	ASP
1	F	25	ASP
1	F	26	LEU
1	F	108	GLU
1	F	114	LYS
1	F	146	TYR
1	F	312	TRP
1	F	319	LYS
1	F	329	GLU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	132	GLN
1	A	303	GLN
1	B	70	HIS
1	B	256	ASN
1	C	115	ASN
1	C	180	ASN
1	C	315	GLN
1	C	371	GLN
1	D	70	HIS
1	D	155	HIS
1	D	220	HIS
1	D	225	HIS
1	D	256	ASN
1	E	115	ASN
1	E	260	HIS
1	E	315	GLN
1	E	371	GLN

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Mol	Chain	Res	Type
1	F	70	HIS
1	F	283	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	NAP	A	401	-	50,52,52	0.69	1 (2%)	71,80,80	0.96	4 (5%)
3	AZI	B	403	-	2,2,2	3.24	2 (100%)	0,1,1	-	-
2	NAP	B	401	-	50,52,52	0.67	1 (2%)	71,80,80	0.97	2 (2%)
2	NAP	F	401	-	50,52,52	0.67	1 (2%)	71,80,80	1.05	7 (9%)
3	AZI	C	407	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
3	AZI	C	403	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
3	AZI	B	405	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
3	AZI	C	404	-	2,2,2	3.23	2 (100%)	0,1,1	-	-
3	AZI	C	406	-	2,2,2	3.26	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AZI	B	406	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
3	AZI	C	408	-	2,2,2	3.23	2 (100%)	0,1,1	-	-
3	AZI	B	404	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
2	NAP	D	401	-	50,52,52	0.69	1 (2%)	71,80,80	0.93	3 (4%)
2	NAP	E	401	-	50,52,52	0.65	1 (2%)	71,80,80	0.84	2 (2%)
3	AZI	C	405	-	2,2,2	3.24	2 (100%)	0,1,1	-	-
3	AZI	B	408	-	2,2,2	3.23	2 (100%)	0,1,1	-	-
2	NAP	C	401	-	50,52,52	0.69	1 (2%)	71,80,80	0.89	4 (5%)
3	AZI	C	402	-	2,2,2	3.61	2 (100%)	0,1,1	-	-
3	AZI	B	402	-	2,2,2	3.36	2 (100%)	0,1,1	-	-
3	AZI	B	407	-	2,2,2	3.25	2 (100%)	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	A	401	-	-	3/35/67/67	0/5/5/5
2	NAP	B	401	-	-	3/35/67/67	0/5/5/5
2	NAP	C	401	-	-	3/35/67/67	0/5/5/5
2	NAP	F	401	-	-	4/35/67/67	0/5/5/5
2	NAP	D	401	-	-	3/35/67/67	0/5/5/5
2	NAP	E	401	-	-	3/35/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	AZI	N1-N2	-3.63	1.15	1.23
3	C	402	AZI	N3-N2	-3.60	1.15	1.23
3	B	402	AZI	N3-N2	-3.37	1.16	1.23
3	B	402	AZI	N1-N2	-3.35	1.16	1.23
3	B	404	AZI	N1-N2	-3.30	1.16	1.23
3	C	406	AZI	N3-N2	-3.29	1.16	1.23
3	C	407	AZI	N3-N2	-3.27	1.16	1.23
3	B	406	AZI	N1-N2	-3.27	1.16	1.23
3	C	403	AZI	N1-N2	-3.27	1.16	1.23
3	C	404	AZI	N1-N2	-3.27	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	AZI	N3-N2	-3.26	1.16	1.23
3	B	405	AZI	N3-N2	-3.26	1.16	1.23
3	B	405	AZI	N1-N2	-3.26	1.16	1.23
3	B	403	AZI	N3-N2	-3.26	1.16	1.23
3	C	408	AZI	N1-N2	-3.25	1.16	1.23
3	B	407	AZI	N3-N2	-3.25	1.16	1.23
3	C	403	AZI	N3-N2	-3.25	1.16	1.23
3	C	407	AZI	N1-N2	-3.25	1.16	1.23
3	C	405	AZI	N3-N2	-3.25	1.16	1.23
3	B	407	AZI	N1-N2	-3.24	1.16	1.23
3	C	405	AZI	N1-N2	-3.24	1.16	1.23
3	B	408	AZI	N1-N2	-3.23	1.16	1.23
3	B	408	AZI	N3-N2	-3.23	1.16	1.23
3	C	406	AZI	N1-N2	-3.23	1.16	1.23
3	B	404	AZI	N3-N2	-3.23	1.16	1.23
3	B	403	AZI	N1-N2	-3.22	1.16	1.23
3	C	408	AZI	N3-N2	-3.20	1.16	1.23
3	C	404	AZI	N3-N2	-3.20	1.16	1.23
2	C	401	NAP	C2N-N1N	2.96	1.38	1.35
2	A	401	NAP	C2N-N1N	2.95	1.38	1.35
2	D	401	NAP	C2N-N1N	2.92	1.38	1.35
2	B	401	NAP	C2N-N1N	2.86	1.38	1.35
2	E	401	NAP	C2N-N1N	2.85	1.38	1.35
2	F	401	NAP	C2N-N1N	2.78	1.38	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	P2B-O2B-C2B	-4.25	112.09	123.43
2	D	401	NAP	P2B-O2B-C2B	-3.88	113.06	123.43
2	B	401	NAP	P2B-O2B-C2B	-3.49	114.11	123.43
2	F	401	NAP	P2B-O2B-C2B	-3.21	114.85	123.43
2	C	401	NAP	P2B-O2B-C2B	-2.92	115.63	123.43
2	F	401	NAP	C1B-N9A-C8A	-2.81	120.85	127.09
2	E	401	NAP	P2B-O2B-C2B	-2.66	116.32	123.43
2	B	401	NAP	C6N-N1N-C2N	-2.62	119.65	121.88
2	D	401	NAP	C6N-N1N-C2N	-2.57	119.69	121.88
2	F	401	NAP	C3B-C2B-C1B	-2.57	97.89	102.81
2	E	401	NAP	C6N-N1N-C2N	-2.56	119.70	121.88
2	C	401	NAP	C6N-N1N-C2N	-2.50	119.75	121.88
2	F	401	NAP	C4A-N9A-C1B	2.44	132.33	126.63
2	F	401	NAP	C2B-C1B-N9A	2.35	117.61	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAP	C6N-N1N-C2N	-2.34	119.89	121.88
2	A	401	NAP	C6N-N1N-C2N	-2.33	119.89	121.88
2	F	401	NAP	O4B-C1B-C2B	-2.29	102.64	106.59
2	A	401	NAP	O4B-C1B-C2B	-2.28	102.66	106.59
2	C	401	NAP	O4B-C1B-C2B	-2.24	102.74	106.59
2	D	401	NAP	O4B-C1B-C2B	-2.20	102.80	106.59
2	A	401	NAP	C3B-C2B-C1B	-2.20	98.60	102.81
2	C	401	NAP	C3B-C2B-C1B	-2.08	98.83	102.81

There are no chirality outliers.

All (19) 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	A	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C2N
2	E	401	NAP	O4D-C1D-N1N-C2N
2	F	401	NAP	O4D-C1D-N1N-C2N
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	F	401	NAP	C2B-O2B-P2B-O3X
2	D	401	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 25 short contacts:

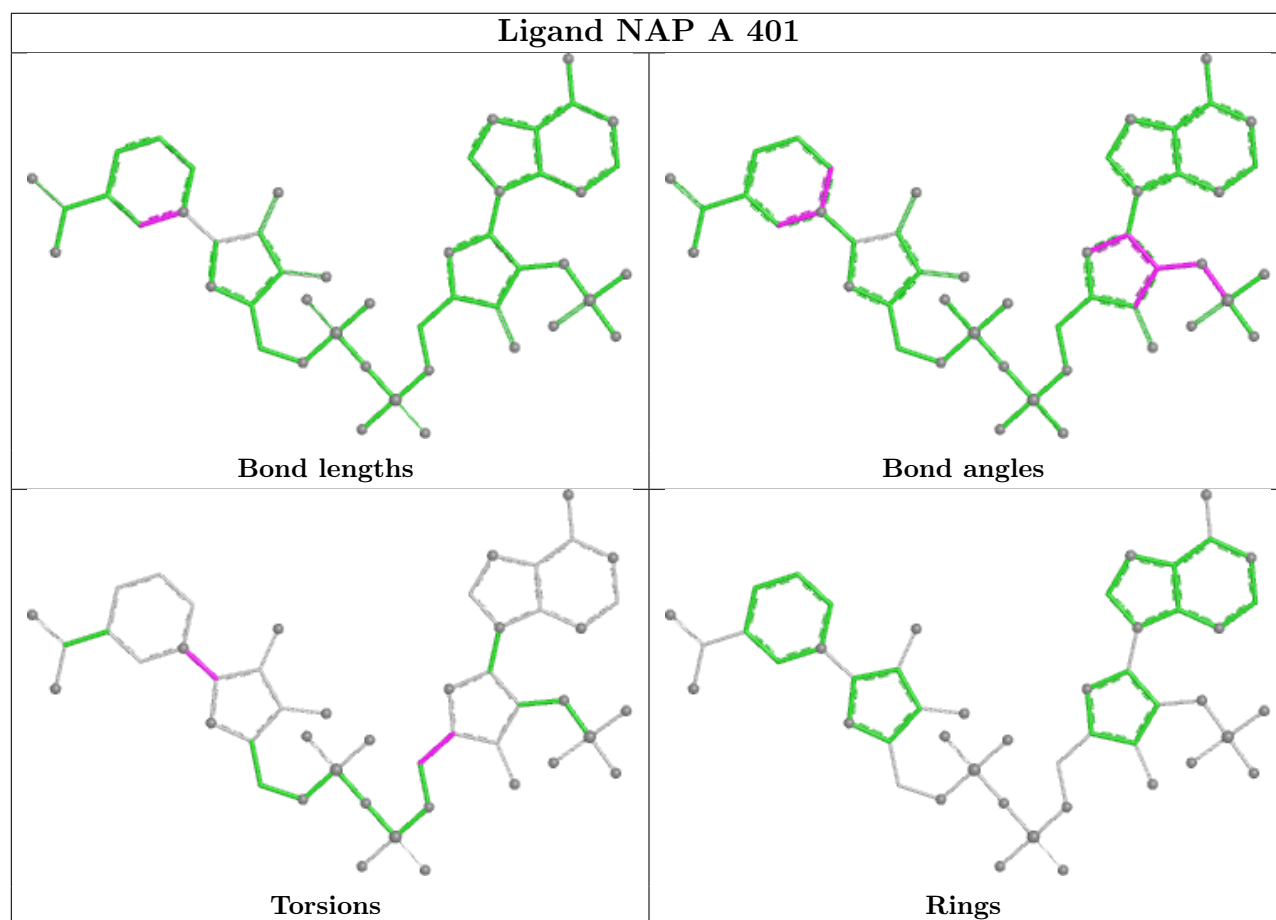
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	7	0
2	B	401	NAP	4	0
2	F	401	NAP	4	0
2	D	401	NAP	1	0

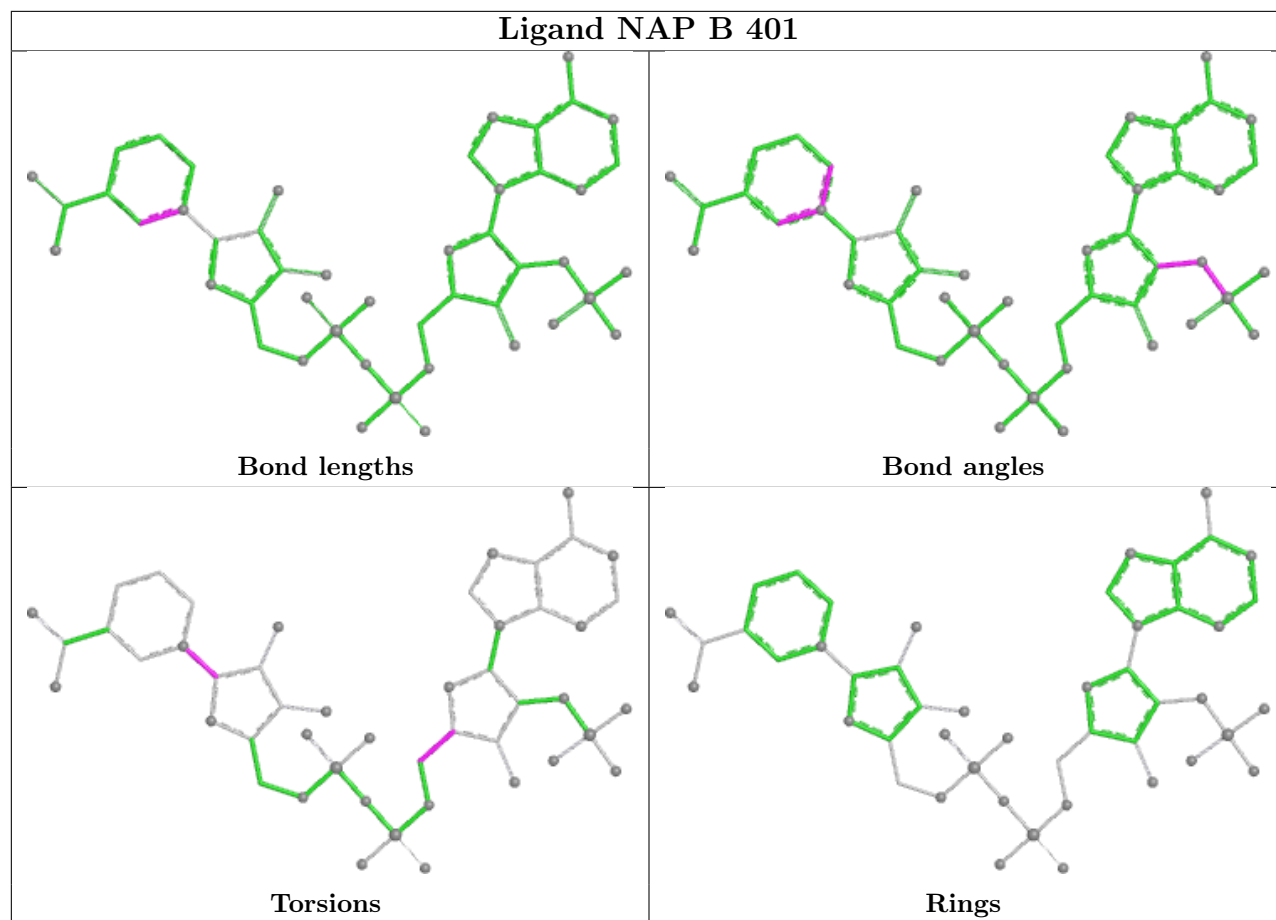
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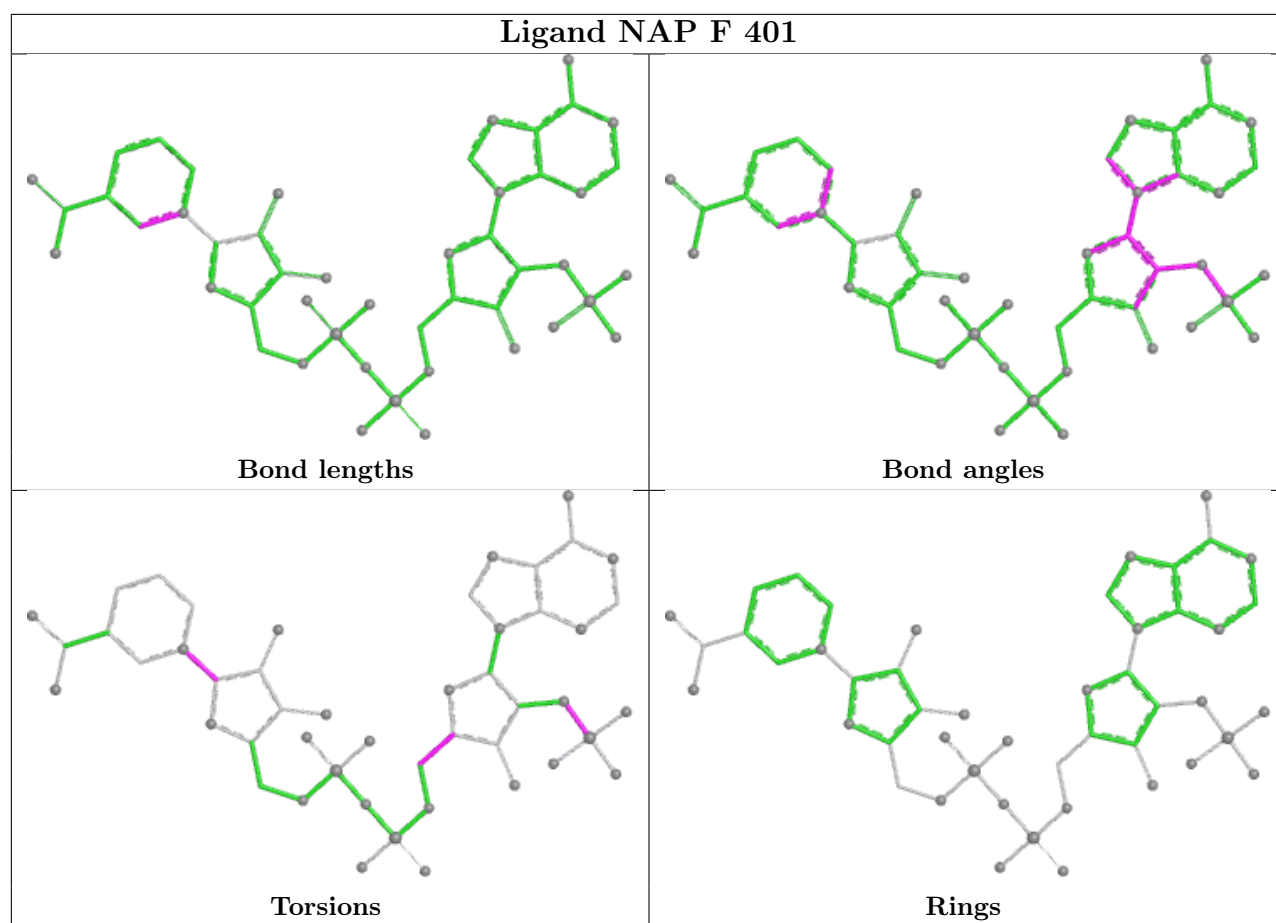
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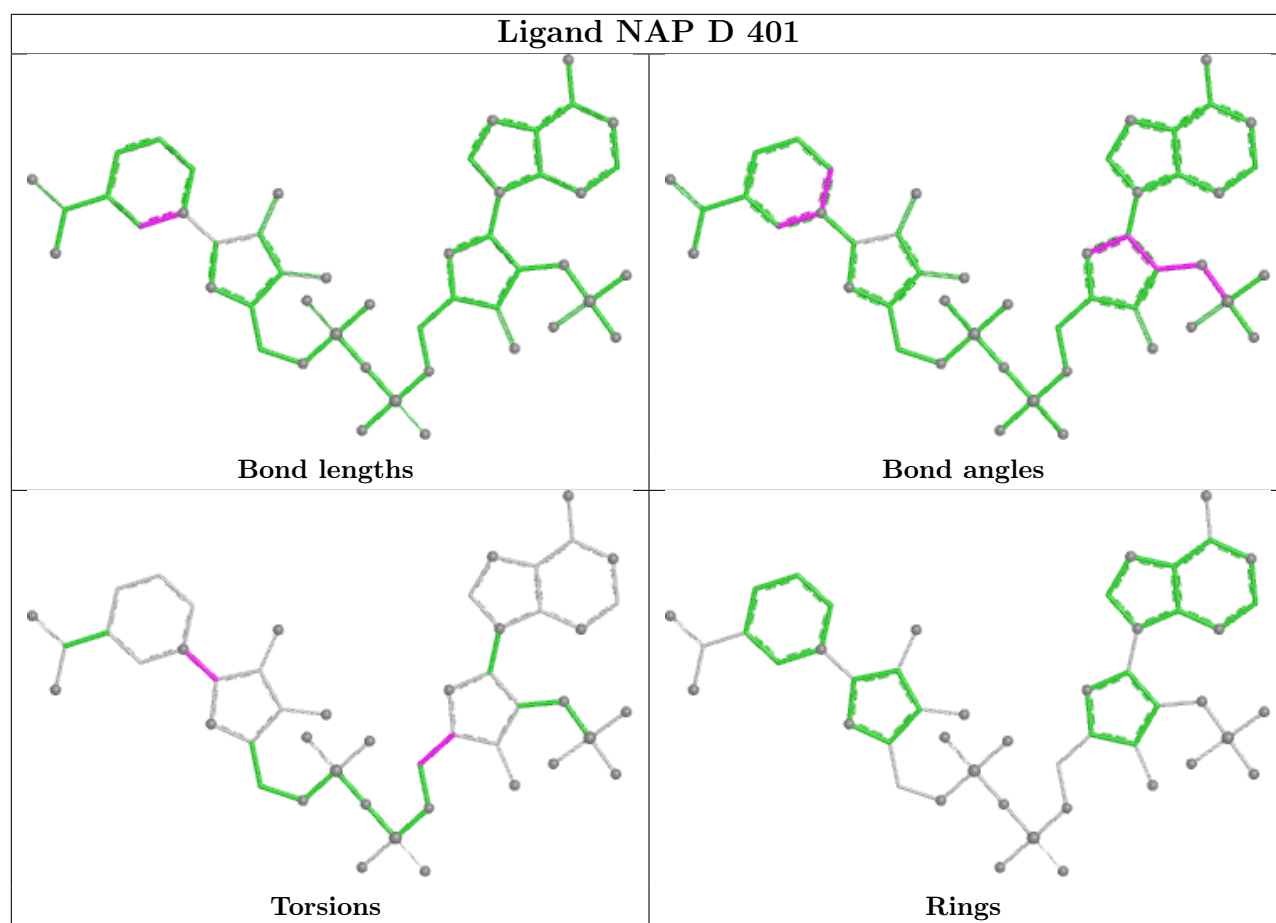
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	NAP	4	0
2	C	401	NAP	5	0

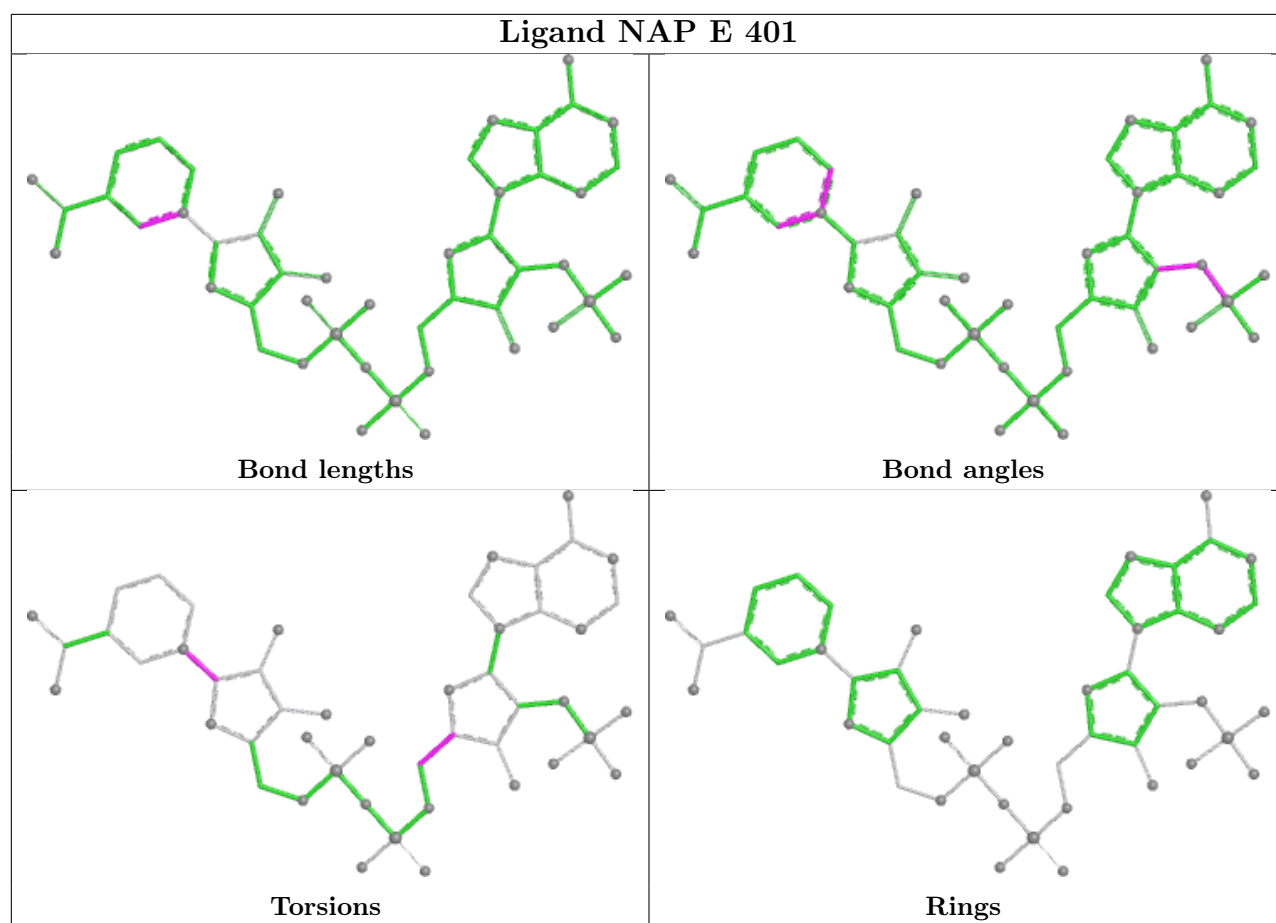
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

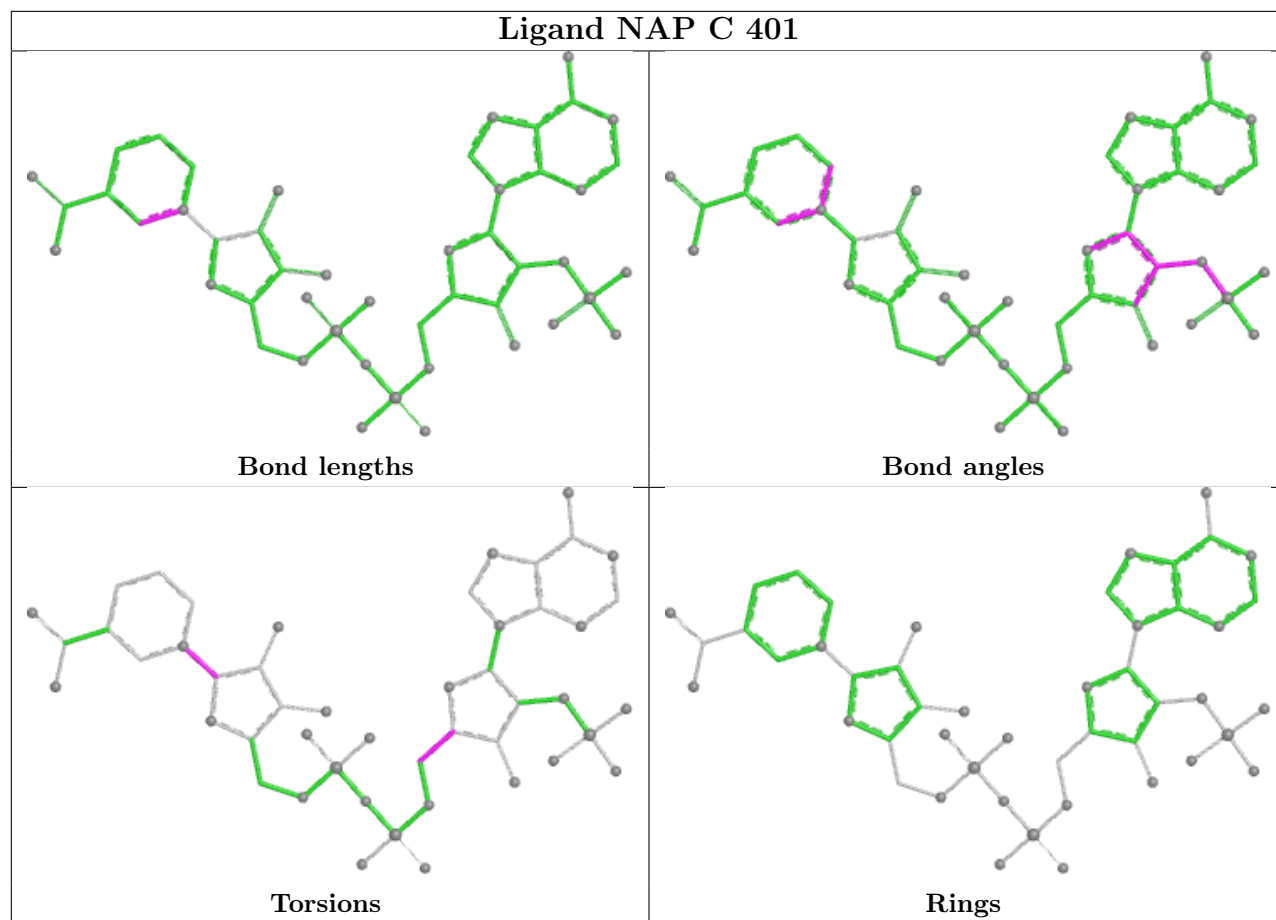












5.7 Other polymers [i](#)

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, 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	380/381 (99%)	0.92	34 (8%) 15 19	35, 40, 48, 65	1 (0%)
1	B	378/381 (99%)	0.86	29 (7%) 19 23	30, 40, 45, 62	0
1	C	381/381 (100%)	0.89	22 (5%) 29 33	36, 41, 47, 55	0
1	D	379/381 (99%)	0.99	26 (6%) 23 27	39, 44, 53, 71	0
1	E	371/381 (97%)	1.12	51 (13%) 6 9	30, 45, 54, 65	0
1	F	378/381 (99%)	0.94	41 (10%) 11 14	36, 42, 52, 63	0
All	All	2267/2286 (99%)	0.95	203 (8%) 15 18	30, 42, 51, 71	1 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	VAL	8.9
1	B	382	VAL	6.6
1	F	382	VAL	6.2
1	E	316	PRO	6.1
1	C	2	SER	5.8
1	E	230	ALA	5.6
1	C	382	VAL	5.5
1	E	379	GLY	5.3
1	C	380	ALA	4.9
1	D	380	ALA	4.9
1	E	382	VAL	4.8
1	B	2	SER	4.7
1	A	137[A]	ARG	4.6
1	F	131	LEU	4.6
1	E	177	GLY	4.5
1	A	125	GLY	4.5
1	E	378	THR	4.5
1	B	319	LYS	4.4
1	B	379	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	380	ALA	4.2
1	A	382	VAL	4.1
1	D	381	LYS	4.0
1	D	2	SER	4.0
1	D	379	GLY	3.9
1	C	3	ALA	3.9
1	F	373	GLY	3.8
1	D	176	LYS	3.8
1	C	316	PRO	3.7
1	B	378	THR	3.7
1	D	260	HIS	3.7
1	E	260	HIS	3.7
1	E	380	ALA	3.7
1	C	91	ASP	3.7
1	A	378	THR	3.7
1	E	381	LYS	3.7
1	E	16	GLY	3.6
1	B	380	ALA	3.5
1	F	375	LEU	3.5
1	D	29	ILE	3.5
1	D	131	LEU	3.5
1	F	26	LEU	3.5
1	A	316	PRO	3.4
1	A	379	GLY	3.4
1	E	3	ALA	3.4
1	F	81	PRO	3.4
1	A	380	ALA	3.3
1	E	20	THR	3.3
1	E	90	VAL	3.3
1	B	131	LEU	3.3
1	E	134	ALA	3.3
1	C	378	THR	3.2
1	E	131	LEU	3.2
1	E	374	ALA	3.2
1	A	3	ALA	3.1
1	A	314	PRO	3.1
1	D	129	VAL	3.1
1	E	315	GLN	3.1
1	E	317	ALA	3.1
1	E	327	LYS	3.1
1	B	87	ARG	3.1
1	A	365	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	93	ASP	3.0
1	F	3	ALA	3.0
1	E	175	ARG	3.0
1	A	129	VAL	3.0
1	A	134	ALA	3.0
1	B	260	HIS	2.9
1	F	381	LYS	2.9
1	F	378	THR	2.9
1	E	26	LEU	2.9
1	A	377	GLY	2.9
1	F	110	ILE	2.9
1	D	105	LEU	2.9
1	F	316	PRO	2.9
1	A	139	ILE	2.9
1	D	233	LYS	2.8
1	A	230	ALA	2.8
1	F	24	ASP	2.8
1	E	376	ALA	2.8
1	B	365	ASP	2.8
1	B	228	PRO	2.8
1	C	73	VAL	2.8
1	C	262	GLU	2.7
1	B	231	VAL	2.7
1	F	260	HIS	2.7
1	C	131	LEU	2.7
1	D	27	PRO	2.7
1	B	312	TRP	2.7
1	D	360	GLY	2.7
1	A	2	SER	2.7
1	A	110	ILE	2.7
1	F	262	GLU	2.7
1	B	88	GLU	2.6
1	F	89	LEU	2.6
1	B	28	LYS	2.6
1	B	316	PRO	2.6
1	A	138	GLY	2.6
1	D	377	GLY	2.6
1	C	103	ALA	2.6
1	A	19	LYS	2.6
1	A	381	LYS	2.6
1	E	71	THR	2.6
1	A	175	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	327	LYS	2.6
1	F	27	PRO	2.5
1	B	21	TYR	2.5
1	C	178	GLY	2.5
1	E	43	ALA	2.5
1	E	142	ALA	2.5
1	F	376	ALA	2.5
1	D	228	PRO	2.5
1	B	320	ASP	2.5
1	D	55	VAL	2.5
1	E	216	ASP	2.5
1	D	67	ALA	2.4
1	D	305	ALA	2.4
1	E	18	PRO	2.4
1	C	200	GLY	2.4
1	F	371	GLN	2.4
1	E	357	PHE	2.4
1	E	365	ASP	2.4
1	E	122	ALA	2.4
1	E	41	PRO	2.4
1	C	157	VAL	2.4
1	E	231	VAL	2.4
1	A	131	LEU	2.4
1	A	79	ASP	2.4
1	A	136	ASP	2.4
1	E	72	PHE	2.4
1	C	317	ALA	2.4
1	F	374	ALA	2.4
1	E	31	HIS	2.4
1	E	367	TYR	2.3
1	D	271	THR	2.3
1	A	67	ALA	2.3
1	D	3	ALA	2.3
1	E	353	ILE	2.3
1	E	314	PRO	2.3
1	E	129	VAL	2.3
1	B	120	LEU	2.3
1	F	111	ALA	2.3
1	B	19	LYS	2.3
1	A	289	LEU	2.3
1	F	116	LEU	2.3
1	A	135	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	349	GLY	2.3
1	F	379	GLY	2.3
1	C	260	HIS	2.3
1	E	63	LYS	2.3
1	F	20	THR	2.3
1	E	29	ILE	2.2
1	C	74	VAL	2.2
1	E	94	VAL	2.2
1	F	8	VAL	2.2
1	F	234	GLU	2.2
1	C	379	GLY	2.2
1	B	150	ILE	2.2
1	D	168	ILE	2.2
1	C	231	VAL	2.2
1	F	108	GLU	2.2
1	B	89	LEU	2.2
1	F	237	LEU	2.2
1	D	269	ASP	2.2
1	E	172	ASP	2.2
1	E	228	PRO	2.2
1	A	28	LYS	2.2
1	E	312	TRP	2.2
1	F	129	VAL	2.2
1	F	285	ALA	2.2
1	A	260	HIS	2.1
1	E	64	TYR	2.1
1	F	124	ILE	2.1
1	F	79	ASP	2.1
1	A	259	LEU	2.1
1	D	111	ALA	2.1
1	D	358	PHE	2.1
1	B	139	ILE	2.1
1	C	110	ILE	2.1
1	F	30	ASP	2.1
1	A	126	SER	2.1
1	E	263	THR	2.1
1	F	80	GLY	2.1
1	F	28	LYS	2.1
1	F	117	LYS	2.1
1	B	314	PRO	2.1
1	B	134	ALA	2.1
1	B	213	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	312	TRP	2.1
1	D	230	ALA	2.1
1	E	5	ILE	2.0
1	C	104	TYR	2.0
1	E	34	GLY	2.0
1	B	84	VAL	2.0
1	F	90	VAL	2.0
1	E	116	LEU	2.0
1	B	82	ASP	2.0
1	E	91	ASP	2.0
1	A	270	GLU	2.0
1	F	2	SER	2.0
1	F	139	ILE	2.0
1	A	106	THR	2.0
1	F	146	TYR	2.0
1	B	55	VAL	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 [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.

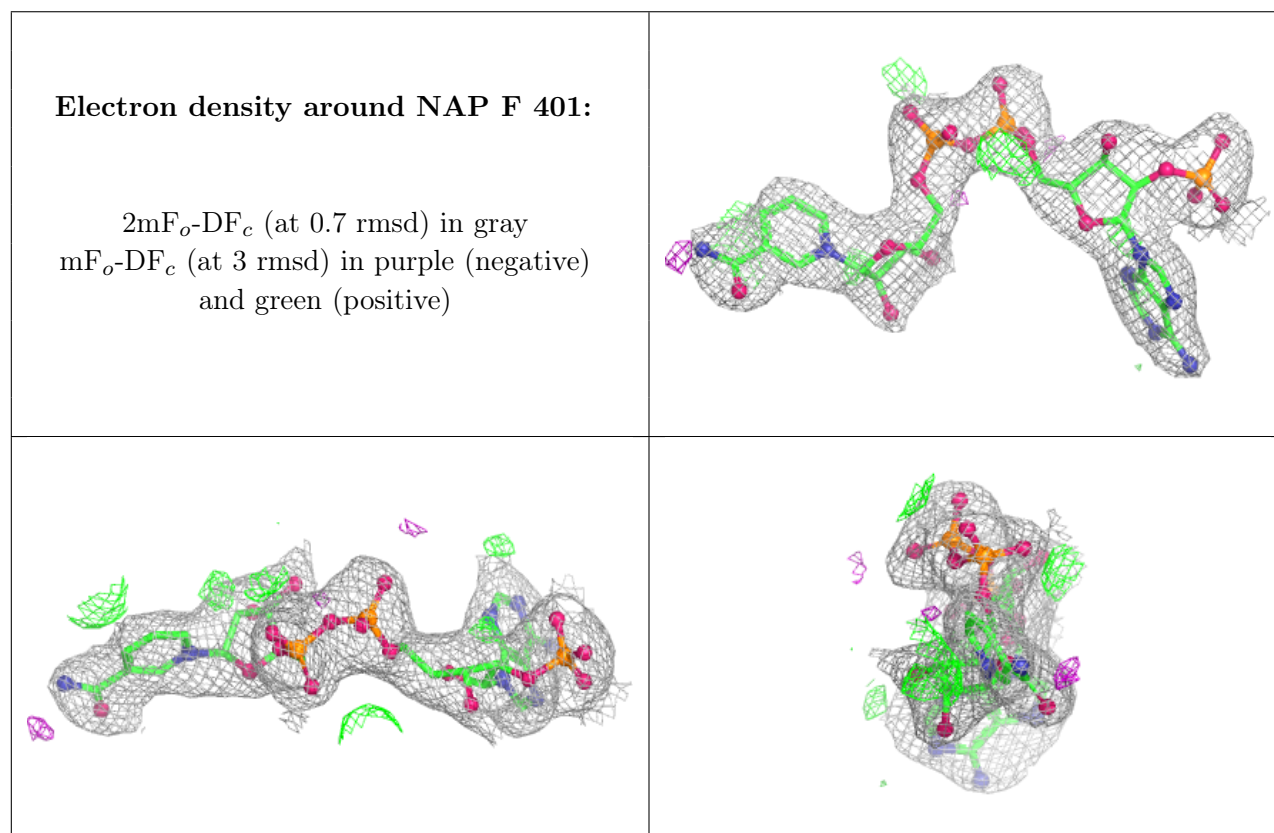
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AZI	C	407	3/3	0.76	0.12	47,47,48,50	0
3	AZI	B	405	3/3	0.78	0.14	46,46,46,48	0
3	AZI	B	404	3/3	0.78	0.16	36,36,37,38	0
3	AZI	C	408	3/3	0.78	0.14	44,44,44,45	0
3	AZI	C	405	3/3	0.81	0.12	43,43,45,46	0
3	AZI	B	408	3/3	0.82	0.18	40,40,40,41	0
3	AZI	B	403	3/3	0.84	0.10	39,39,40,42	0

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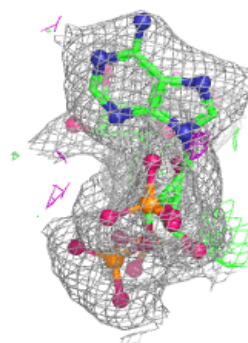
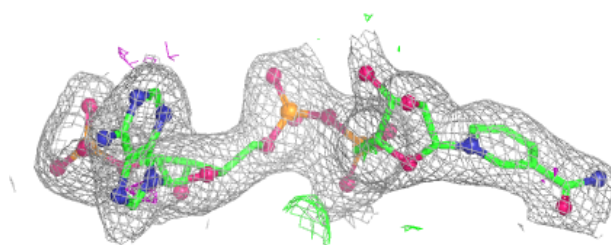
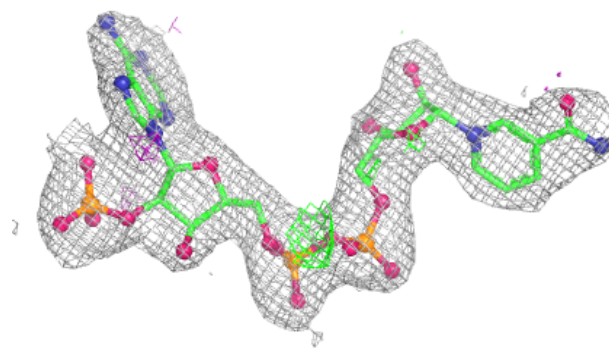
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AZI	B	406	3/3	0.87	0.14	42,42,43,43	0
3	AZI	B	407	3/3	0.88	0.20	37,37,38,39	0
3	AZI	C	406	3/3	0.88	0.12	40,40,41,42	0
3	AZI	C	404	3/3	0.90	0.15	38,38,38,40	0
3	AZI	C	403	3/3	0.91	0.10	44,44,44,46	0
2	NAP	F	401	48/48	0.94	0.09	38,42,45,46	0
3	AZI	C	402	3/3	0.94	0.13	37,37,37,37	0
2	NAP	C	401	48/48	0.95	0.09	36,40,43,44	0
2	NAP	E	401	48/48	0.95	0.09	40,46,50,50	0
2	NAP	A	401	48/48	0.95	0.09	34,39,42,43	0
2	NAP	B	401	48/48	0.95	0.08	35,40,42,43	0
3	AZI	B	402	3/3	0.96	0.07	35,35,36,36	0
2	NAP	D	401	48/48	0.96	0.08	39,43,50,59	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.

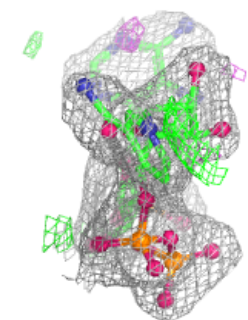
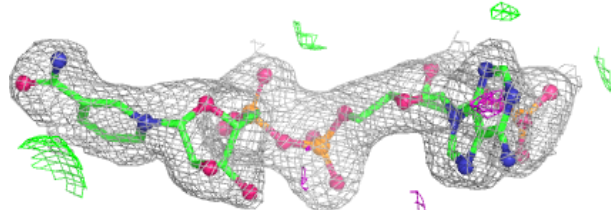
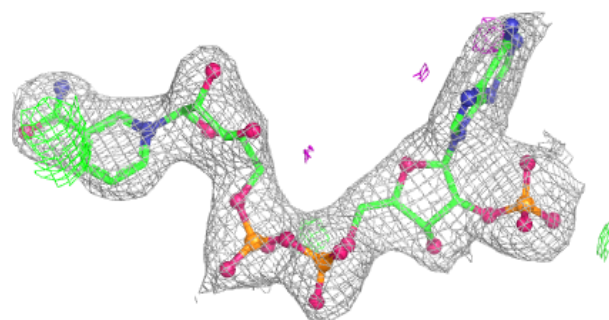


Electron density around NAP C 401:

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

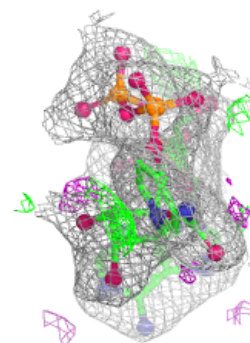
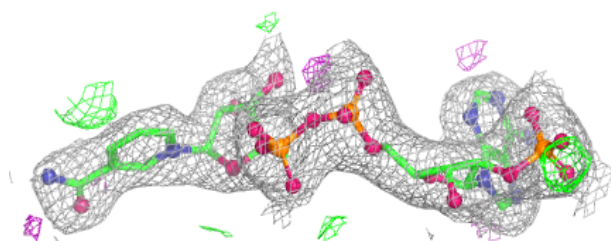
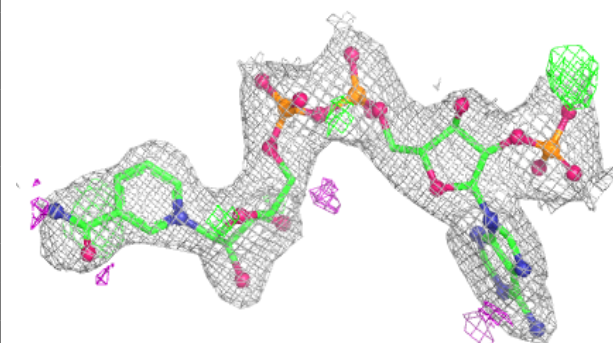
**Electron density around NAP E 401:**

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

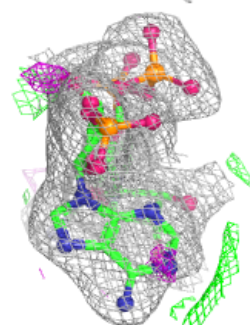
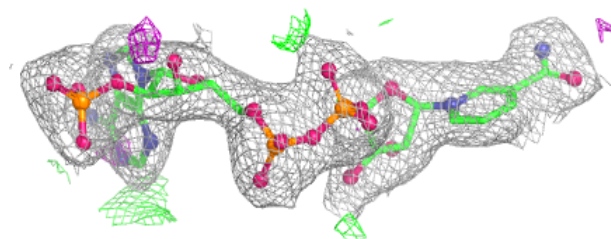
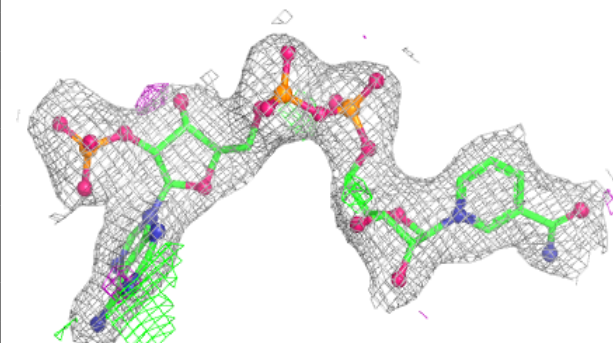


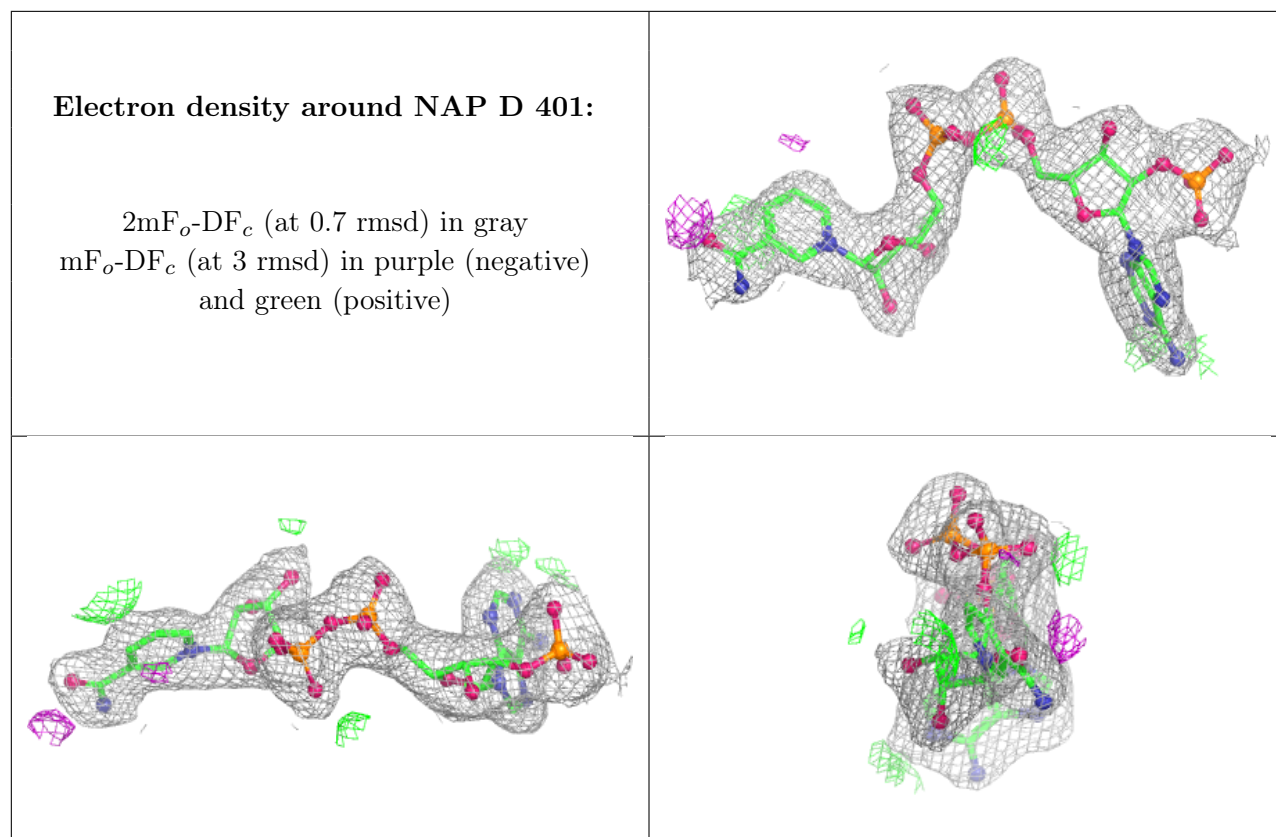
Electron density around NAP A 401:

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

**Electron density around NAP B 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.