



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:32 AM UTC

PDB ID : 6T9W / pdb_00006t9w
Title : Crystal structure of formate dehydrogenase FDH2 D222A/Q223R enzyme from *Granulicella mallensis* MP5ACTX8 in complex with NADP and azide.
Authors : Robescu, M.S.; Rubini, R.; Filippini, F.; Bergantino, B.; Cendron, L.
Deposited on : 2019-10-29
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

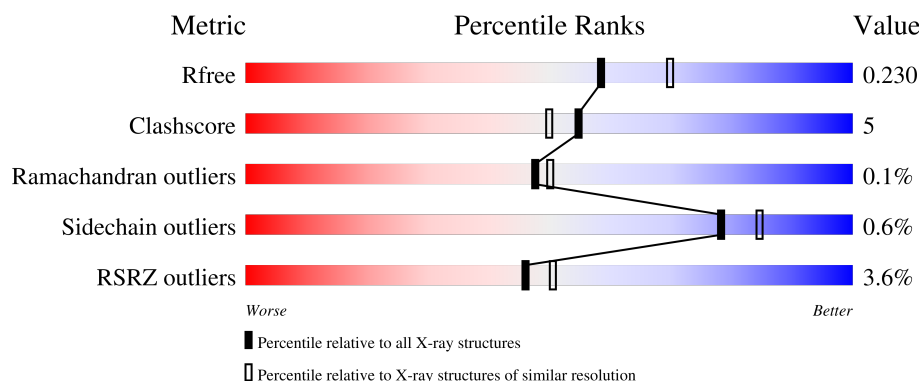
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	386	3% 87% 12% ..
1	B	386	% 89% 10% .
1	C	386	6% 88% 11% .
1	D	386	5% 85% 11% ..

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	A	802	-	X	-	-
3	AZI	B	802	-	X	-	-
3	AZI	C	802	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12872 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.

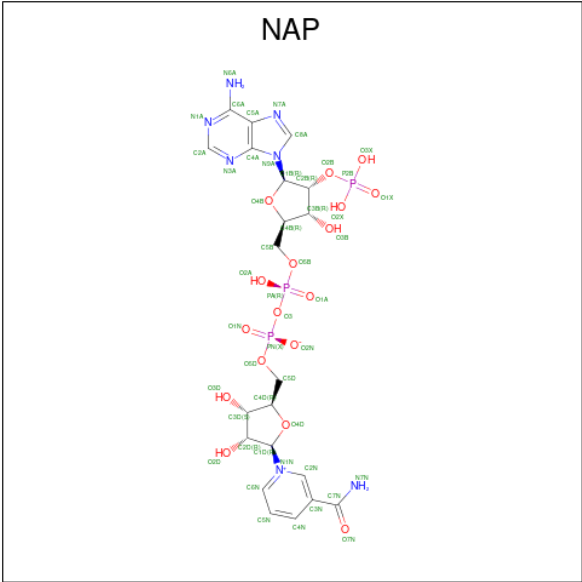
- Molecule 1 is a protein called Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	383	Total	C	N	O	S	0	4	0
			3012	1920	518	562	12			
1	A	383	Total	C	N	O	S	0	6	0
			3033	1935	521	565	12			
1	C	383	Total	C	N	O	S	0	3	0
			2999	1912	517	558	12			
1	D	374	Total	C	N	O	S	0	2	0
			2930	1869	506	543	12			

There are 8 discrepancies between the modelled and reference sequences:

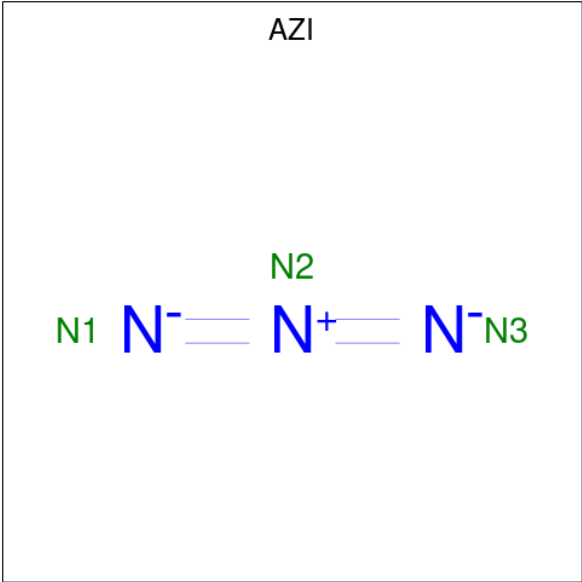
Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ALA	ASP	engineered mutation	UNP G8NTI5
B	223	ARG	GLN	engineered mutation	UNP G8NTI5
A	222	ALA	ASP	engineered mutation	UNP G8NTI5
A	223	ARG	GLN	engineered mutation	UNP G8NTI5
C	222	ALA	ASP	engineered mutation	UNP G8NTI5
C	223	ARG	GLN	engineered mutation	UNP G8NTI5
D	222	ALA	ASP	engineered mutation	UNP G8NTI5
D	223	ARG	GLN	engineered mutation	UNP G8NTI5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃) (labeled as "Ligand of Interest" by depositor).



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

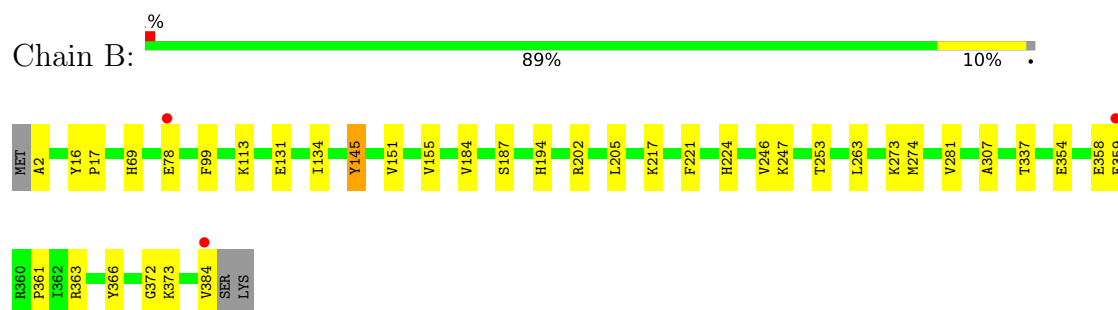
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	208	Total O 208 208	0	0
4	A	194	Total O 194 194	0	0
4	C	147	Total O 147 147	0	0
4	D	196	Total O 196 196	0	0

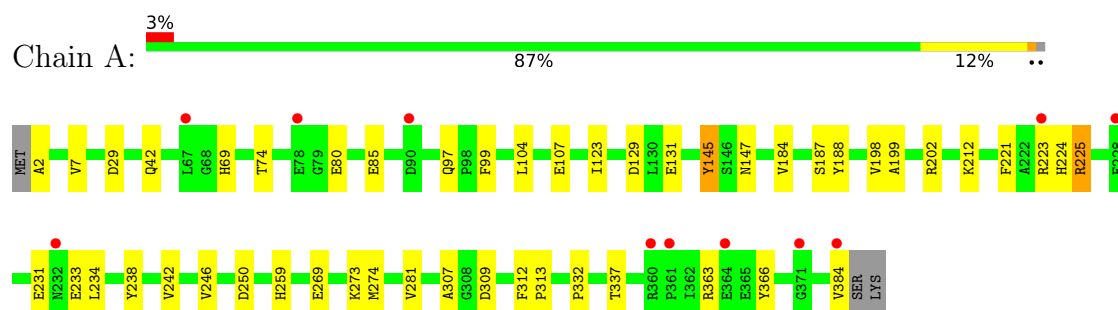
3 Residue-property plots [i](#)

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.

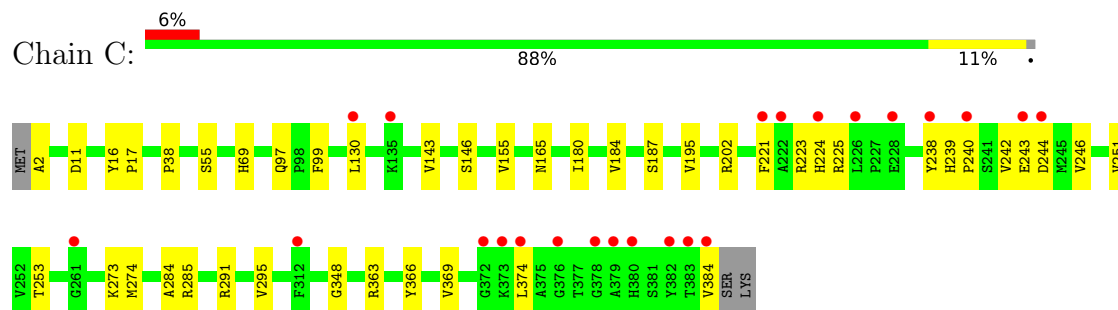
- Molecule 1: Formate dehydrogenase



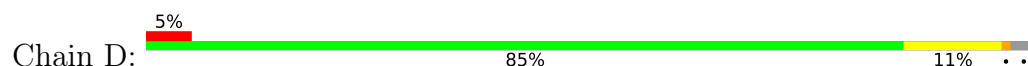
- Molecule 1: Formate dehydrogenase

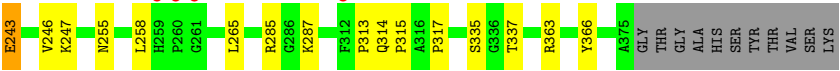
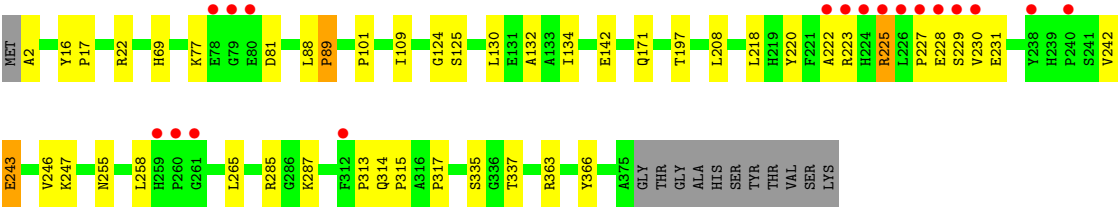


- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.53Å 62.08Å 211.75Å 90.00° 91.25° 90.00°	Depositor
Resolution (Å)	54.10 – 2.15 54.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	87.7 (54.10-2.15) 83.0 (54.10-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.191 , 0.231 0.191 , 0.230	Depositor DCC
R_{free} test set	4424 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12872	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: NAP, AZI

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	0.30	2/3109 (0.1%)	0.54	3/4229 (0.1%)
1	B	0.27	1/3087 (0.0%)	0.50	0/4200
1	C	0.32	0/3073	0.54	1/4181 (0.0%)
1	D	0.56	3/3002 (0.1%)	0.70	1/4083 (0.0%)
All	All	0.38	6/12271 (0.0%)	0.57	5/16693 (0.0%)

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	D	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	335	SER	C-O	-6.45	1.16	1.24
1	B	361	PRO	C-O	-6.31	1.16	1.23
1	D	125	SER	C-O	-5.91	1.18	1.24
1	D	89	PRO	C-O	-5.78	1.17	1.24
1	A	225	ARG	C-O	-5.21	1.17	1.23
1	A	224	HIS	C-O	-5.02	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	GLU	N-CA-C	-6.62	104.14	111.36
1	A	225	ARG	CG-CD-NE	-6.03	98.74	112.00
1	A	198	VAL	CA-C-N	5.48	132.00	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	VAL	C-N-CA	5.48	132.00	121.54
1	C	224	HIS	CB-CA-C	-5.12	100.16	109.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	222	ALA	Mainchain
1	D	223[A]	ARG	Mainchain
1	D	223[B]	ARG	Mainchain

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	3033	0	3006	39	0
1	B	3012	0	2989	22	0
1	C	2999	0	2986	25	0
1	D	2930	0	2925	33	0
2	A	48	0	24	5	0
2	B	48	0	24	2	0
2	C	48	0	24	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	194	0	0	1	0
4	B	208	0	0	2	0
4	C	147	0	0	1	0
4	D	196	0	0	2	0
All	All	12872	0	11978	116	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 5.

All (116) 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:227:PRO:HB2	1:D:230:VAL:HG23	1.53	0.87
1:D:225:ARG:HH11	1:D:225:ARG:HG3	1.48	0.77
1:D:243:GLU:O	1:D:247:LYS:HG3	1.86	0.75
1:D:287:LYS:HB2	4:D:505:HOH:O	1.94	0.67
1:B:2:ALA:HB1	1:B:69:HIS:ND1	2.10	0.67
1:D:220:TYR:OH	1:D:231:GLU:OE2	2.12	0.66
1:C:374:LEU:HD11	1:C:384:VAL:HG23	1.78	0.65
1:C:239:HIS:ND1	1:C:244:ASP:OD2	2.25	0.65
1:C:165:ASN:HA	4:C:911:HOH:O	1.97	0.63
1:D:225:ARG:HH11	1:D:225:ARG:CG	2.11	0.63
1:D:227:PRO:HD2	1:D:230:VAL:HG21	1.81	0.61
1:C:2:ALA:N	1:C:69:HIS:HD1	1.98	0.61
1:A:184:VAL:HG11	1:D:337:THR:HG23	1.83	0.60
1:C:243:GLU:HG2	1:C:273:LYS:HE2	1.86	0.57
1:D:255:ASN:ND2	4:D:403:HOH:O	2.32	0.57
1:D:130:LEU:O	1:D:134:ILE:HG12	2.05	0.57
1:A:145[B]:TYR:CD2	1:A:202:ARG:HD3	2.40	0.56
1:D:208:LEU:HD23	1:D:218:LEU:HD22	1.87	0.56
1:D:313:PRO:HG2	1:D:317:PRO:HD3	1.88	0.56
1:C:284:ALA:O	1:C:285:ARG:HG2	2.07	0.55
1:A:129:ASP:OD1	1:A:131:GLU:HG3	2.07	0.54
1:D:124:GLY:N	1:D:142:GLU:OE1	2.32	0.54
1:D:2:ALA:N	1:D:69:HIS:HD1	2.06	0.54
1:A:99[A]:PHE:CE2	1:A:337:THR:HB	2.44	0.53
1:C:195:VAL:HG22	1:C:251:VAL:HB	1.89	0.53
1:B:359:GLU:HA	1:B:359:GLU:OE1	2.08	0.53
1:A:223[A]:ARG:HH21	2:A:801:NAP:H61A	1.56	0.53
1:A:223[A]:ARG:HE	2:A:801:NAP:C6A	2.22	0.53
1:B:263:LEU:HD23	1:C:240:PRO:HB2	1.89	0.52
1:D:197:THR:HG21	1:D:208:LEU:HD11	1.92	0.52
1:A:131:GLU:HB3	1:A:384:VAL:HG21	1.92	0.52
1:A:2:ALA:N	1:A:69:HIS:HD1	2.08	0.51
1:D:242:VAL:HG21	1:D:265:LEU:HD11	1.92	0.51
1:A:363:ARG:HB2	1:A:366:TYR:CD2	2.46	0.51
1:D:363:ARG:HB2	1:D:366:TYR:CD2	2.46	0.51
1:A:223[A]:ARG:NH2	1:A:259:HIS:HE1	2.08	0.50
1:A:145[B]:TYR:CD2	1:A:202:ARG:NE	2.79	0.50
1:D:225:ARG:CG	1:D:225:ARG:NH1	2.73	0.50
1:B:145[B]:TYR:CZ	1:B:202:ARG:HG2	2.47	0.50
1:A:29:ASP:OD1	1:A:29:ASP:N	2.37	0.50
1:A:221:PHE:CD2	1:A:242:VAL:HG13	2.47	0.49
1:C:97:GLN:HB3	1:C:99:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:HB2	1:D:285:ARG:HG3	1.94	0.49
1:A:145[B]:TYR:CD2	1:A:202:ARG:CD	2.95	0.48
1:A:145[B]:TYR:CG	1:A:202:ARG:HD3	2.49	0.48
1:C:246:VAL:HB	1:C:274:MET:HG2	1.95	0.48
1:D:77:LYS:HE3	1:D:101:PRO:O	2.14	0.47
1:C:223:ARG:NH2	2:C:801:NAP:O3X	2.38	0.47
1:A:250:ASP:CG	1:D:22:ARG:HH12	2.23	0.47
1:C:143:VAL:HG12	1:C:146:SER:HB3	1.97	0.46
1:A:225:ARG:HG3	1:A:238:TYR:CD1	2.50	0.46
1:A:233:GLU:OE1	1:A:234:LEU:HG	2.15	0.46
1:B:224:HIS:HD2	4:B:1095:HOH:O	1.97	0.46
1:C:225:ARG:HD3	1:C:238:TYR:CD2	2.51	0.46
1:A:97:GLN:HB3	1:A:99[B]:PHE:CD2	2.51	0.45
1:C:363:ARG:HB2	1:C:366:TYR:CD2	2.52	0.45
1:A:184:VAL:HA	1:A:187:SER:HB3	1.96	0.45
1:A:188:TYR:CE2	1:D:22:ARG:HD3	2.51	0.45
1:A:123:ILE:HB	2:A:801:NAP:H5N	1.97	0.45
1:C:38:PRO:HB3	1:C:348:GLY:HA2	1.98	0.45
1:C:180:ILE:O	1:C:184:VAL:HG22	2.17	0.45
1:D:314:GLN:HA	1:D:315:PRO:C	2.42	0.45
1:A:281:VAL:HA	1:A:307:ALA:O	2.16	0.45
1:D:81:ASP:OD1	1:D:81:ASP:N	2.50	0.45
1:B:184:VAL:HA	1:B:187:SER:HB3	1.99	0.45
1:A:42:GLN:NE2	4:A:919:HOH:O	2.50	0.45
1:B:131:GLU:HB2	1:B:384:VAL:HG21	1.98	0.45
1:B:246:VAL:HB	1:B:274:MET:HG2	1.98	0.44
1:D:227:PRO:O	1:D:230:VAL:N	2.50	0.44
1:C:16:TYR:CD1	1:C:17:PRO:HD2	2.52	0.44
1:D:88:LEU:HB3	1:D:89:PRO:HD3	1.99	0.44
1:C:130[A]:LEU:HD12	1:C:369:VAL:HG23	1.99	0.44
1:A:269:GLU:HG3	1:A:273:LYS:HE3	1.98	0.44
1:C:202:ARG:NH1	2:C:801:NAP:O2A	2.48	0.44
1:B:247:LYS:HG3	1:B:273:LYS:O	2.18	0.44
1:B:363:ARG:HB2	1:B:366:TYR:CD2	2.53	0.44
1:D:225:ARG:HD3	1:D:231:GLU:OE2	2.18	0.43
1:B:194:HIS:CE1	1:B:217:LYS:HD3	2.54	0.43
1:B:221:PHE:CE2	2:B:801:NAP:H2A	2.54	0.43
1:B:354:GLU:O	1:B:358:GLU:HG3	2.18	0.43
1:C:155:VAL:HG11	1:C:253:THR:HG21	1.99	0.43
1:A:225:ARG:HG2	1:A:231:GLU:OE1	2.19	0.43
1:B:99:PHE:CE2	1:B:337:THR:HB	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:TYR:CD1	1:D:17:PRO:HD2	2.53	0.43
1:A:246:VAL:HB	1:A:274:MET:HG2	2.00	0.43
1:D:227:PRO:HB2	1:D:230:VAL:CG2	2.38	0.43
1:D:227:PRO:O	1:D:230:VAL:HB	2.19	0.42
1:B:2:ALA:CB	1:B:69:HIS:ND1	2.78	0.42
1:C:11:ASP:OD2	1:C:55:SER:OG	2.31	0.42
1:C:184:VAL:HA	1:C:187:SER:HB3	2.00	0.42
1:C:291:ARG:O	1:C:295:VAL:HG23	2.19	0.42
1:B:151:VAL:HG21	2:B:801:NAP:C4N	2.50	0.42
1:B:155:VAL:HG11	1:B:253:THR:HG21	2.00	0.42
1:A:123:ILE:HD12	1:A:147:ASN:OD1	2.20	0.42
2:A:801:NAP:H8A	2:A:801:NAP:H2B	1.64	0.42
1:D:242:VAL:O	1:D:246:VAL:HG13	2.19	0.42
1:C:221:PHE:CE2	1:C:242:VAL:HB	2.55	0.42
1:B:16:TYR:CG	1:B:17:PRO:HD2	2.55	0.41
1:B:113:LYS:HA	1:B:113:LYS:HD3	1.89	0.41
1:A:80:GLU:HA	1:A:85:GLU:CD	2.45	0.41
1:A:107:GLU:H	1:A:107:GLU:CD	2.28	0.41
2:C:801:NAP:H8A	2:C:801:NAP:H2B	1.70	0.41
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.96	0.41
1:A:212:LYS:HE3	1:A:233:GLU:O	2.20	0.41
1:A:250:ASP:OD1	1:D:22:ARG:NH1	2.49	0.41
1:A:309:ASP:HB2	1:A:332:PRO:O	2.21	0.41
1:A:312:PHE:HA	1:A:313:PRO:HA	1.89	0.40
1:D:109:ILE:HD12	1:D:132:ALA:HB3	2.03	0.40
1:C:225:ARG:HD3	1:C:238:TYR:CG	2.56	0.40
1:B:281:VAL:HA	1:B:307:ALA:O	2.20	0.40
1:B:373:LYS:HB3	4:B:903:HOH:O	2.21	0.40
1:A:97:GLN:HB3	1:A:99[B]:PHE:CE2	2.57	0.40
1:A:223[A]:ARG:HB2	2:A:801:NAP:O2X	2.21	0.40
1:B:134:ILE:HG23	1:B:372:GLY:O	2.22	0.40
1:A:7:VAL:HA	1:A:74:THR:O	2.21	0.40
1:A:99[B]:PHE:CE2	1:A:337:THR:HB	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	387/386 (100%)	370 (96%)	16 (4%)	1 (0%)	36	34
1	B	385/386 (100%)	368 (96%)	17 (4%)	0	100	100
1	C	384/386 (100%)	370 (96%)	14 (4%)	0	100	100
1	D	374/386 (97%)	359 (96%)	15 (4%)	0	100	100
All	All	1530/1544 (99%)	1467 (96%)	62 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ALA

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	324/321 (101%)	322 (99%)	2 (1%)	78	84
1	B	322/321 (100%)	317 (98%)	5 (2%)	55	61
1	C	321/321 (100%)	321 (100%)	0	100	100
1	D	314/321 (98%)	309 (98%)	5 (2%)	55	61
All	All	1281/1284 (100%)	1269 (99%)	12 (1%)	78	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78[A]	GLU
1	B	78[B]	GLU
1	B	145[A]	TYR
1	B	145[B]	TYR
1	B	205	LEU
1	A	145[A]	TYR
1	A	145[B]	TYR
1	D	171[A]	GLN
1	D	171[B]	GLN
1	D	225	ARG
1	D	228	GLU
1	D	229	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	GLN
1	B	224	HIS
1	A	224	HIS
1	C	35	GLN
1	D	232	ASN
1	D	333	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	C	802	-	2,2,2	3.15	2 (100%)	0,1,1	-	-
3	AZI	B	802	-	2,2,2	3.32	2 (100%)	0,1,1	-	-
2	NAP	C	801	-	50,52,52	4.00	20 (40%)	71,80,80	2.43	16 (22%)
2	NAP	B	801	-	50,52,52	3.94	21 (42%)	71,80,80	2.39	15 (21%)
3	AZI	A	802	-	2,2,2	3.26	2 (100%)	0,1,1	-	-
2	NAP	A	801	-	50,52,52	4.05	20 (40%)	71,80,80	2.52	17 (23%)

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	801	-	-	6/35/67/67	0/5/5/5
2	NAP	B	801	-	-	5/35/67/67	0/5/5/5
2	NAP	A	801	-	-	4/35/67/67	0/5/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	NAP	C3B-C4B	-10.46	1.26	1.53
2	A	801	NAP	C3B-C4B	-10.35	1.26	1.53
2	C	801	NAP	C2B-C1B	-10.27	1.27	1.53
2	B	801	NAP	C2B-C1B	-10.22	1.27	1.53
2	B	801	NAP	C3B-C4B	-10.21	1.27	1.53
2	A	801	NAP	O4D-C1D	-10.15	1.27	1.40
2	A	801	NAP	C2B-C1B	-10.15	1.28	1.53
2	B	801	NAP	O4D-C1D	-10.01	1.27	1.40
2	C	801	NAP	O4D-C1D	-9.81	1.28	1.40
2	A	801	NAP	PA-O3	9.19	1.69	1.59
2	C	801	NAP	PA-O3	8.43	1.68	1.59
2	A	801	NAP	PN-O3	8.35	1.68	1.59
2	C	801	NAP	C3D-C4D	-8.20	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	C3D-C4D	-8.17	1.32	1.53
2	B	801	NAP	C3D-C4D	-8.09	1.32	1.53
2	C	801	NAP	PN-O3	8.05	1.68	1.59
2	B	801	NAP	PA-O3	7.84	1.68	1.59
2	C	801	NAP	O4D-C4D	7.57	1.61	1.45
2	A	801	NAP	O4D-C4D	7.57	1.61	1.45
2	B	801	NAP	O4D-C4D	7.56	1.61	1.45
2	B	801	NAP	PN-O3	7.52	1.67	1.59
2	B	801	NAP	C3B-C2B	5.87	1.65	1.53
2	A	801	NAP	C6A-N6A	5.86	1.49	1.34
2	C	801	NAP	C6A-N6A	5.84	1.49	1.34
2	A	801	NAP	C3B-C2B	5.80	1.65	1.53
2	B	801	NAP	C6A-N6A	5.80	1.49	1.34
2	C	801	NAP	C3B-C2B	5.79	1.65	1.53
2	B	801	NAP	C7N-N7N	4.97	1.42	1.33
2	C	801	NAP	C7N-N7N	4.92	1.42	1.33
2	A	801	NAP	C7N-N7N	4.78	1.41	1.33
2	C	801	NAP	O4B-C1B	4.75	1.53	1.42
2	A	801	NAP	O4B-C1B	4.61	1.52	1.42
2	C	801	NAP	O4B-C4B	4.50	1.55	1.45
2	A	801	NAP	O4B-C4B	4.49	1.55	1.45
2	B	801	NAP	O4B-C4B	4.39	1.54	1.45
2	B	801	NAP	O4B-C1B	4.38	1.52	1.42
2	A	801	NAP	P2B-O2B	3.52	1.65	1.59
2	B	801	NAP	P2B-O2B	3.48	1.65	1.59
3	B	802	AZI	N3-N2	-3.37	1.16	1.23
2	C	801	NAP	P2B-O2B	3.33	1.65	1.59
3	A	802	AZI	N1-N2	-3.31	1.16	1.23
3	B	802	AZI	N1-N2	-3.28	1.16	1.23
3	A	802	AZI	N3-N2	-3.20	1.16	1.23
2	B	801	NAP	O3D-C3D	3.17	1.50	1.43
3	C	802	AZI	N3-N2	-3.17	1.16	1.23
3	C	802	AZI	N1-N2	-3.13	1.16	1.23
2	A	801	NAP	O3D-C3D	3.03	1.50	1.43
2	C	801	NAP	C8A-N7A	2.98	1.37	1.31
2	C	801	NAP	O3D-C3D	2.98	1.50	1.43
2	B	801	NAP	C8A-N7A	2.90	1.37	1.31
2	A	801	NAP	C8A-N7A	2.80	1.37	1.31
2	C	801	NAP	C1B-N9A	2.75	1.53	1.46
2	A	801	NAP	C1B-N9A	2.70	1.53	1.46
2	B	801	NAP	C4A-N9A	-2.58	1.32	1.37
2	B	801	NAP	C1B-N9A	2.42	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	C2A-N1A	2.38	1.38	1.33
2	C	801	NAP	C2A-N1A	2.37	1.38	1.33
2	B	801	NAP	C2A-N1A	2.35	1.38	1.33
2	B	801	NAP	C5A-C4A	-2.30	1.35	1.39
2	C	801	NAP	O3B-C3B	2.21	1.48	1.43
2	B	801	NAP	O3B-C3B	2.17	1.48	1.43
2	A	801	NAP	O3B-C3B	2.13	1.48	1.43
2	A	801	NAP	C4N-C3N	-2.13	1.36	1.39
2	A	801	NAP	C5A-C4A	-2.12	1.35	1.39
2	C	801	NAP	C4A-N9A	-2.08	1.33	1.37
2	C	801	NAP	C5A-C4A	-2.06	1.35	1.39
2	B	801	NAP	C4N-C3N	-2.01	1.36	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	C1B-N9A-C8A	-11.72	101.08	127.09
2	C	801	NAP	C1B-N9A-C8A	-10.80	103.12	127.09
2	B	801	NAP	C1B-N9A-C8A	-10.48	103.83	127.09
2	A	801	NAP	C4A-N9A-C1B	9.52	148.91	126.63
2	C	801	NAP	C4A-N9A-C1B	8.66	146.89	126.63
2	B	801	NAP	C4A-N9A-C1B	8.09	145.56	126.63
2	B	801	NAP	N3A-C2A-N1A	-6.07	119.40	128.58
2	C	801	NAP	N3A-C2A-N1A	-6.06	119.41	128.58
2	A	801	NAP	N3A-C2A-N1A	-6.00	119.50	128.58
2	B	801	NAP	N9A-C8A-N7A	-5.96	105.49	113.94
2	C	801	NAP	N9A-C8A-N7A	-5.65	105.92	113.94
2	A	801	NAP	N9A-C8A-N7A	-5.55	106.06	113.94
2	B	801	NAP	C4B-O4B-C1B	-4.93	98.58	109.47
2	A	801	NAP	C4B-O4B-C1B	-4.67	99.15	109.47
2	B	801	NAP	C4A-N9A-C8A	4.62	110.58	105.74
2	C	801	NAP	C4B-O4B-C1B	-4.35	99.86	109.47
2	A	801	NAP	C4A-N9A-C8A	4.06	110.00	105.74
2	C	801	NAP	C4A-N9A-C8A	4.01	109.94	105.74
2	B	801	NAP	C2B-C1B-N9A	3.71	119.86	113.75
2	C	801	NAP	C4D-O4D-C1D	-3.70	106.53	109.92
2	C	801	NAP	C2B-C1B-N9A	3.64	119.74	113.75
2	A	801	NAP	C5A-C4A-N3A	-3.55	121.82	126.72
2	B	801	NAP	C4D-O4D-C1D	-3.28	106.92	109.92
2	C	801	NAP	C5A-N7A-C8A	3.24	108.54	103.45
2	A	801	NAP	C4D-O4D-C1D	-3.23	106.97	109.92
2	A	801	NAP	C2A-N3A-C4A	3.22	119.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAP	C5A-N7A-C8A	3.17	108.42	103.45
2	A	801	NAP	C5A-N7A-C8A	3.16	108.42	103.45
2	C	801	NAP	C2A-N3A-C4A	3.14	119.50	111.83
2	A	801	NAP	C2B-C1B-N9A	3.06	118.78	113.75
2	C	801	NAP	C5A-C4A-N3A	-3.01	122.57	126.72
2	B	801	NAP	C2A-N3A-C4A	2.88	118.87	111.83
2	C	801	NAP	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	801	NAP	C4A-C5A-N7A	-2.72	107.47	110.58
2	C	801	NAP	C2B-C3B-C4B	2.65	107.69	101.99
2	A	801	NAP	C2B-C3B-C4B	2.63	107.65	101.99
2	C	801	NAP	O2B-C2B-C3B	-2.59	102.39	111.68
2	A	801	NAP	C5A-C6A-N6A	-2.53	117.03	123.29
2	A	801	NAP	C4A-C5A-N7A	-2.52	107.70	110.58
2	B	801	NAP	C2B-C3B-C4B	2.50	107.37	101.99
2	B	801	NAP	C5A-C6A-N6A	-2.35	117.46	123.29
2	B	801	NAP	C5A-C4A-N3A	-2.35	123.48	126.72
2	C	801	NAP	C5A-C6A-N6A	-2.25	117.72	123.29
2	C	801	NAP	C5A-C4A-N9A	2.19	108.20	105.81
2	A	801	NAP	O2B-C2B-C3B	-2.09	104.16	111.68
2	A	801	NAP	N6A-C6A-N1A	2.03	122.90	118.38
2	B	801	NAP	C5A-C4A-N9A	2.03	108.02	105.81
2	A	801	NAP	O7N-C7N-N7N	-2.02	119.70	122.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

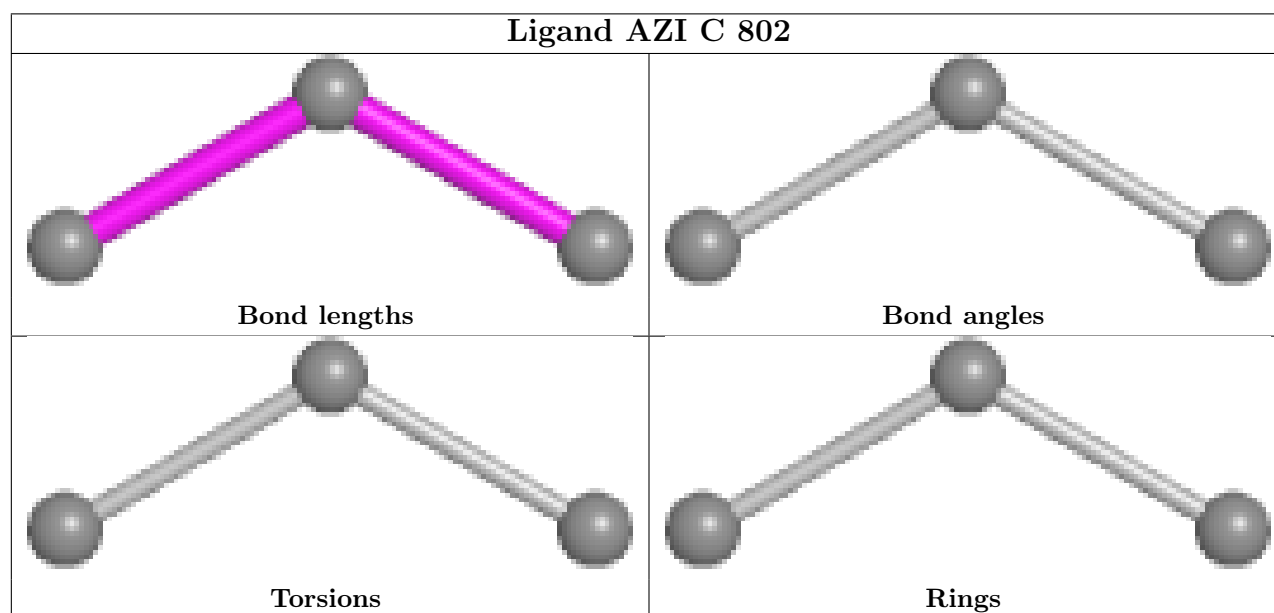
Mol	Chain	Res	Type	Atoms
2	B	801	NAP	O4D-C1D-N1N-C6N
2	A	801	NAP	O4D-C1D-N1N-C6N
2	C	801	NAP	PN-O3-PA-O5B
2	C	801	NAP	O4D-C1D-N1N-C6N
2	B	801	NAP	PN-O3-PA-O5B
2	A	801	NAP	PN-O3-PA-O5B
2	B	801	NAP	C3B-C4B-C5B-O5B
2	A	801	NAP	C5D-O5D-PN-O1N
2	C	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	O4B-C4B-C5B-O5B
2	B	801	NAP	O4D-C1D-N1N-C2N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	C	801	NAP	O4D-C1D-N1N-C2N
2	C	801	NAP	O4B-C4B-C5B-O5B
2	C	801	NAP	C3B-C4B-C5B-O5B

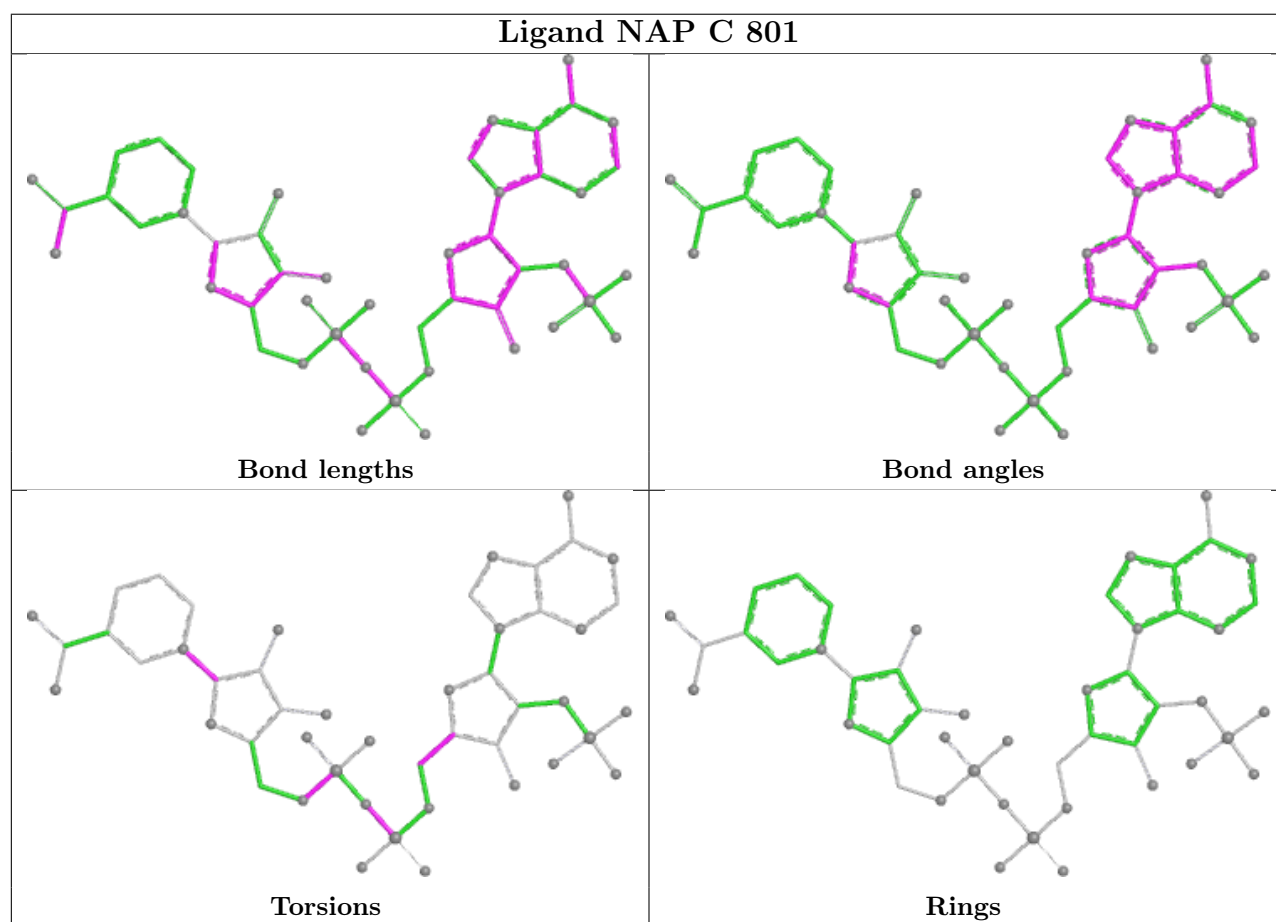
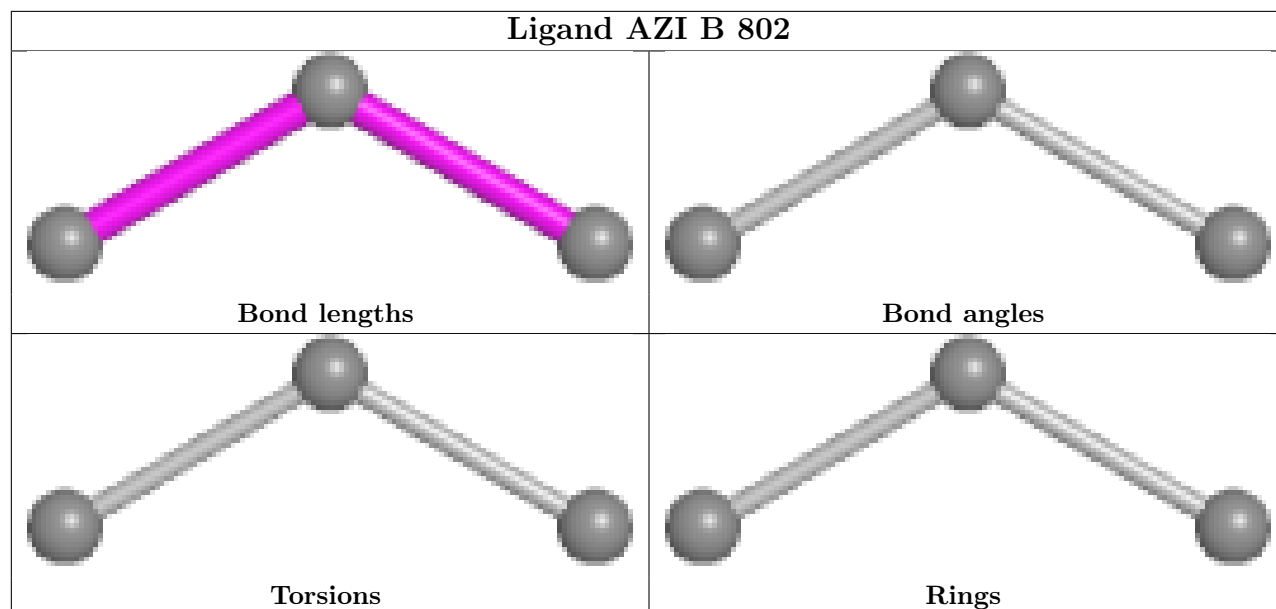
There are no ring outliers.

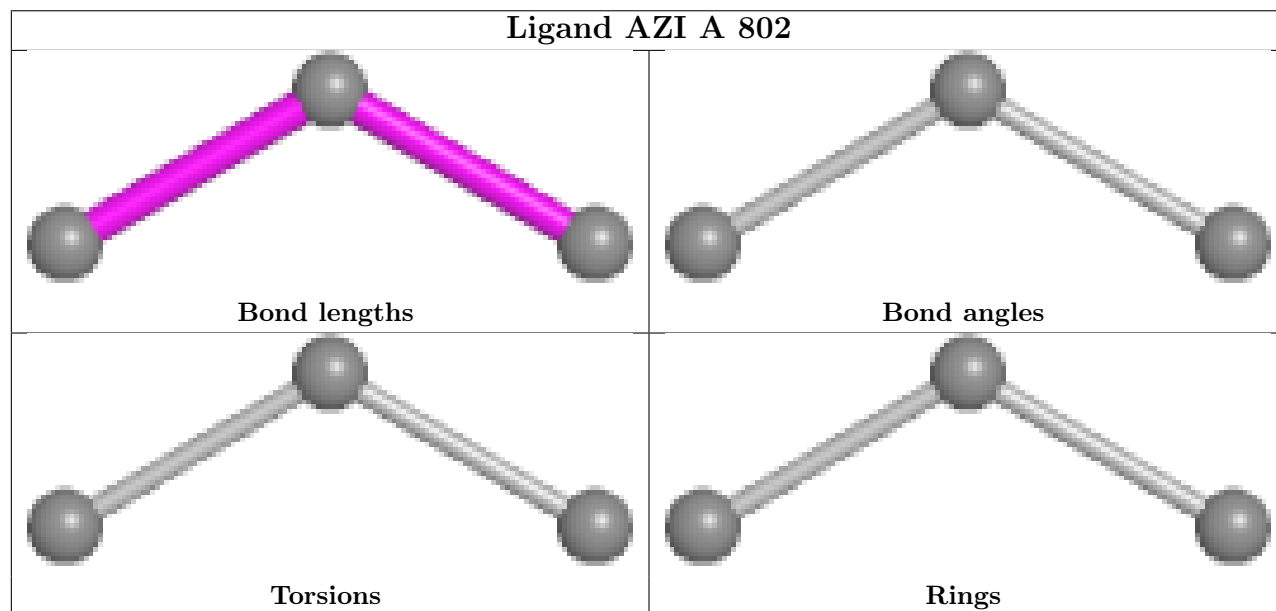
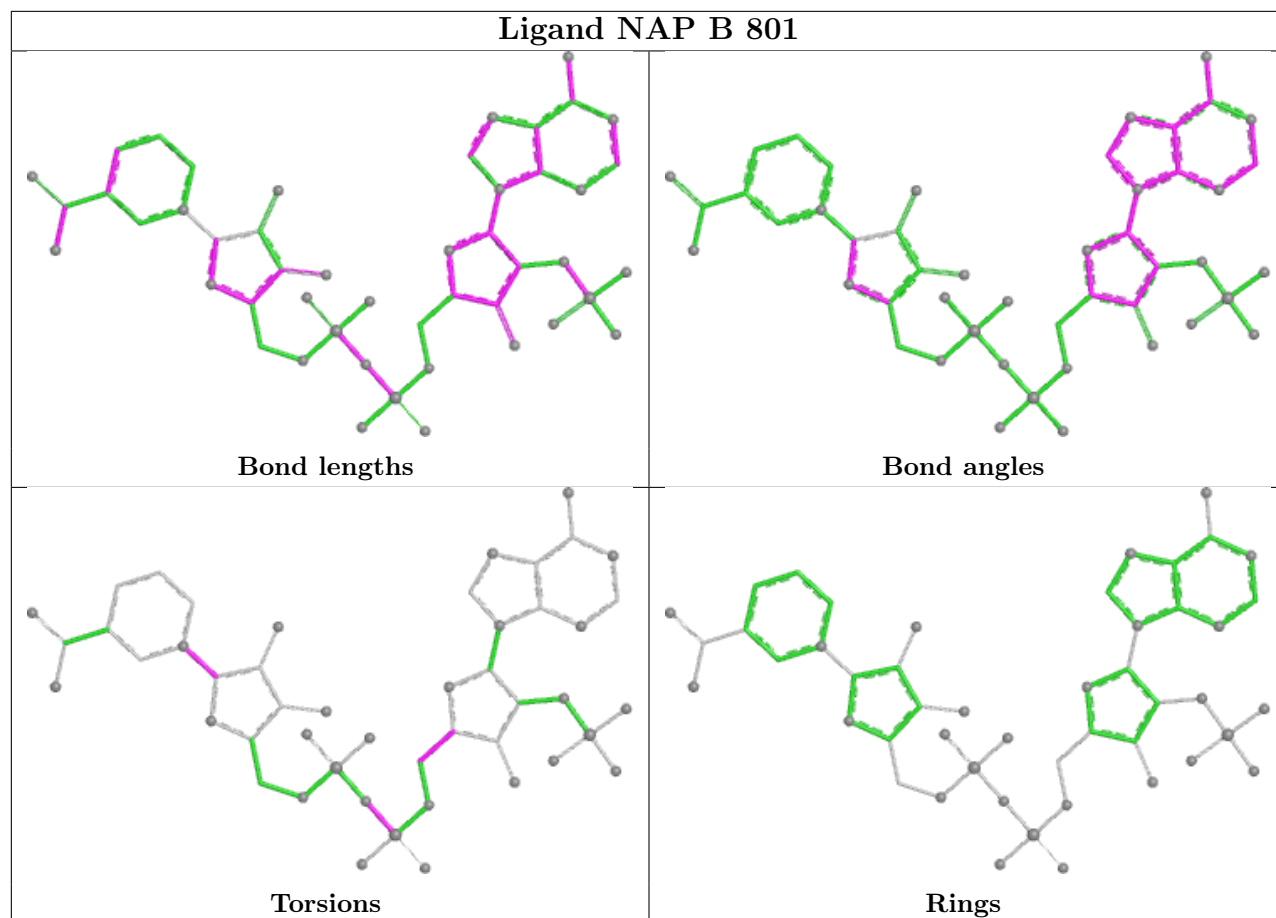
3 monomers are involved in 10 short contacts:

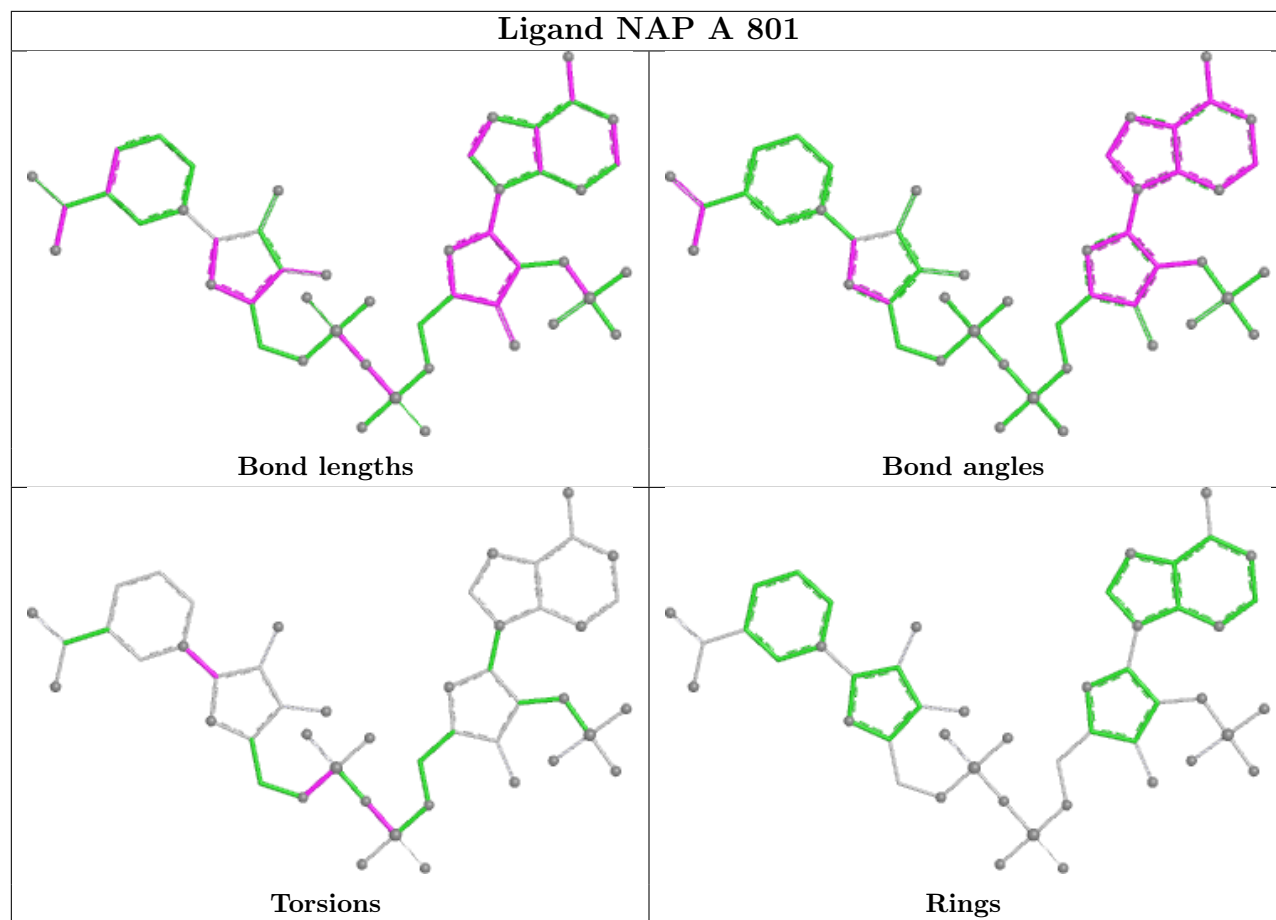
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	NAP	3	0
2	B	801	NAP	2	0
2	A	801	NAP	5	0

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	383/386 (99%)	0.20	11 (2%) 53 57	9, 24, 42, 56	6 (1%)
1	B	383/386 (99%)	0.02	3 (0%) 82 84	7, 20, 38, 58	4 (1%)
1	C	383/386 (99%)	0.31	23 (6%) 27 31	9, 24, 50, 71	3 (0%)
1	D	374/386 (96%)	0.17	18 (4%) 35 40	11, 24, 50, 84	2 (0%)
All	All	1523/1544 (98%)	0.18	55 (3%) 46 50	7, 23, 45, 84	15 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223[A]	ARG	5.2
1	C	228	GLU	4.0
1	A	384	VAL	3.7
1	C	373	LYS	3.7
1	D	230	VAL	3.5
1	C	378	GLY	3.5
1	C	312	PHE	3.4
1	C	383	THR	3.4
1	C	376	GLY	3.4
1	D	79	GLY	3.4
1	C	384	VAL	3.3
1	D	222	ALA	3.3
1	B	359	GLU	3.1
1	D	261	GLY	3.1
1	C	380	HIS	3.0
1	C	379	ALA	3.0
1	D	312	PHE	3.0
1	D	226	LEU	2.9
1	A	371	GLY	2.9
1	A	364[A]	GLU	2.8
1	D	224	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	78[A]	GLU	2.7
1	D	80	GLU	2.7
1	C	135	LYS	2.7
1	C	224	HIS	2.6
1	A	228	GLU	2.6
1	A	360	ARG	2.5
1	B	384	VAL	2.5
1	C	222	ALA	2.5
1	D	260	PRO	2.5
1	C	130[A]	LEU	2.5
1	C	238	TYR	2.4
1	C	243	GLU	2.4
1	D	225	ARG	2.4
1	A	361	PRO	2.4
1	C	226	LEU	2.4
1	C	240	PRO	2.3
1	D	228	GLU	2.3
1	C	382	TYR	2.3
1	D	238	TYR	2.3
1	A	223[A]	ARG	2.3
1	C	221	PHE	2.3
1	D	240	PRO	2.3
1	C	261	GLY	2.3
1	B	78[A]	GLU	2.2
1	C	244	ASP	2.1
1	A	90	ASP	2.1
1	C	372	GLY	2.1
1	A	67	LEU	2.1
1	D	78	GLU	2.0
1	D	229	SER	2.1
1	C	374	LEU	2.0
1	A	232	ASN	2.0
1	D	259	HIS	2.0
1	D	227	PRO	2.0

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

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](#)

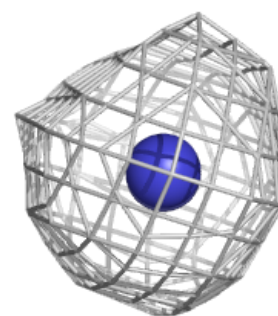
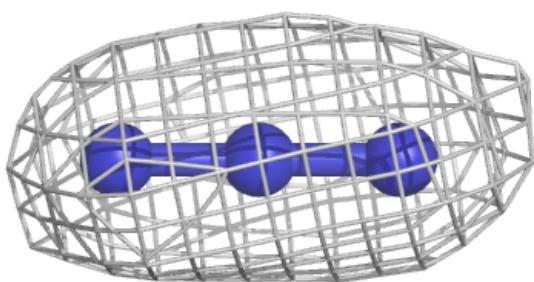
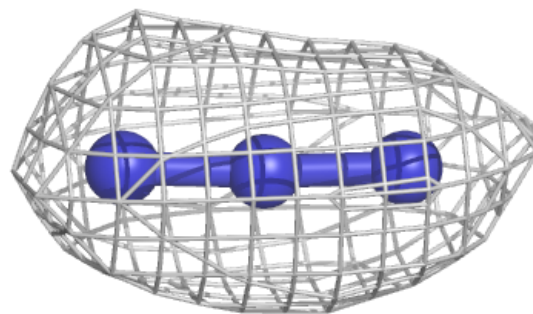
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AZI	C	802	3/3	0.92	0.11	18,18,19,19	0
2	NAP	C	801	48/48	0.96	0.09	11,22,45,60	0
2	NAP	A	801	48/48	0.96	0.07	13,21,35,39	0
3	AZI	B	802	3/3	0.97	0.07	13,13,16,18	0
2	NAP	B	801	48/48	0.97	0.06	6,14,26,30	0
3	AZI	A	802	3/3	0.98	0.07	14,14,15,16	0

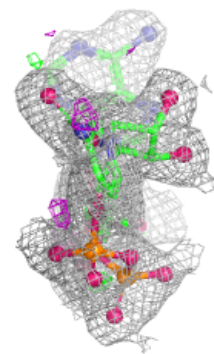
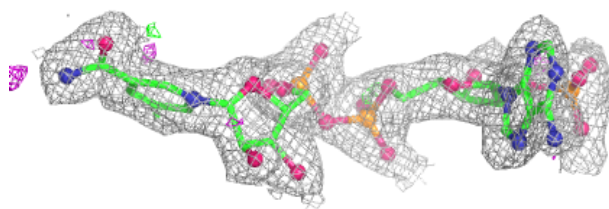
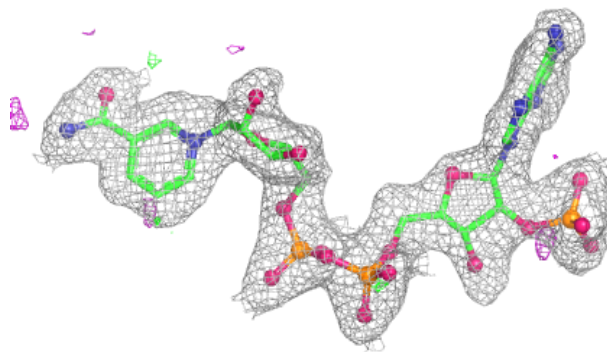
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AZI C 802:

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

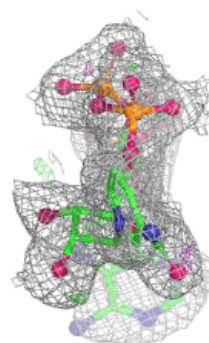
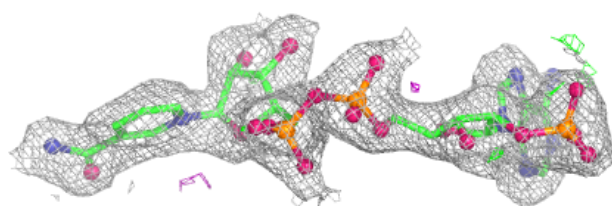
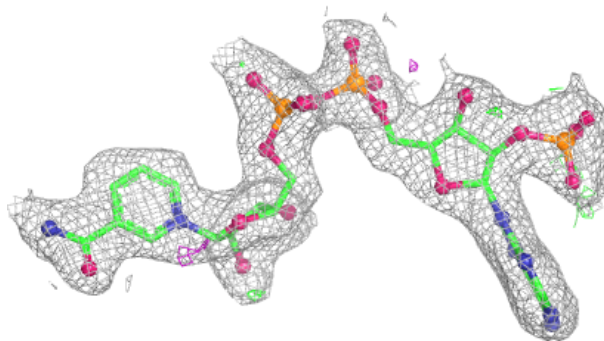
**Electron density around NAP C 801:**

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

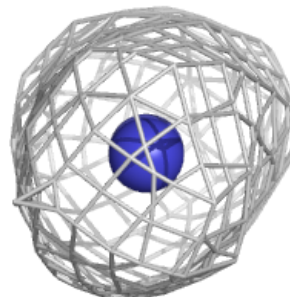
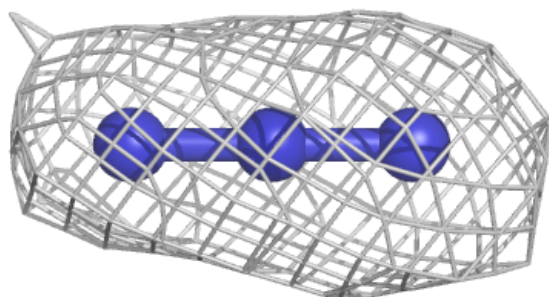
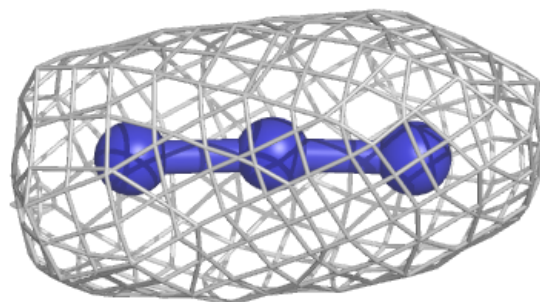


Electron density around NAP A 801:

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

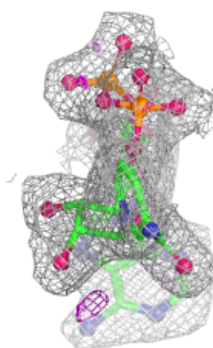
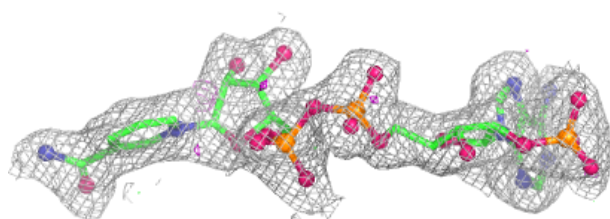
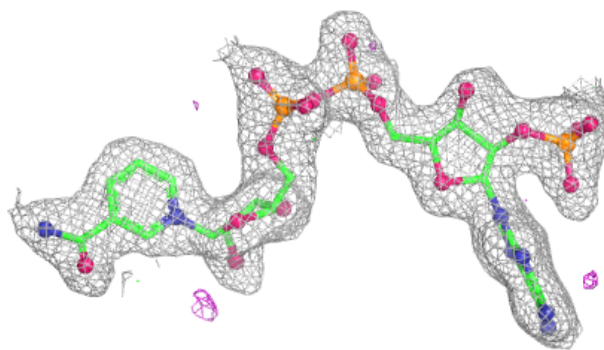
**Electron density around AZI B 802:**

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

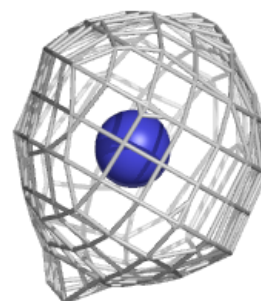
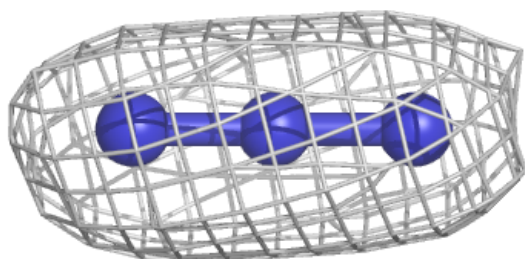
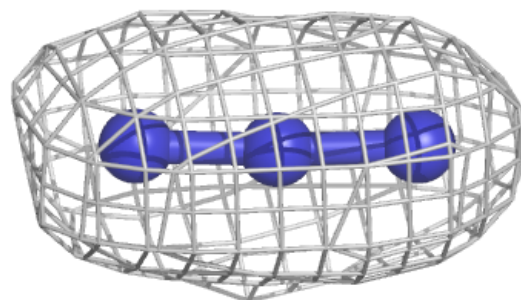


Electron density around NAP B 801:

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

**Electron density around AZI A 802:**

$2mF_o - DF_c$ (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.