



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:45 AM EDT

PDB ID : 6NKM / pdb_00006nkm
Title : Structure of PhqE D166N Reductase/Diels-Alderase from *Penicillium fellutanum* in complex with NADP⁺ and substrate
Authors : Newmister, S.A.; Dan, Q.; Smith, J.L.; Sherman, D.H.
Deposited on : 2019-01-07
Resolution : 1.90 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:

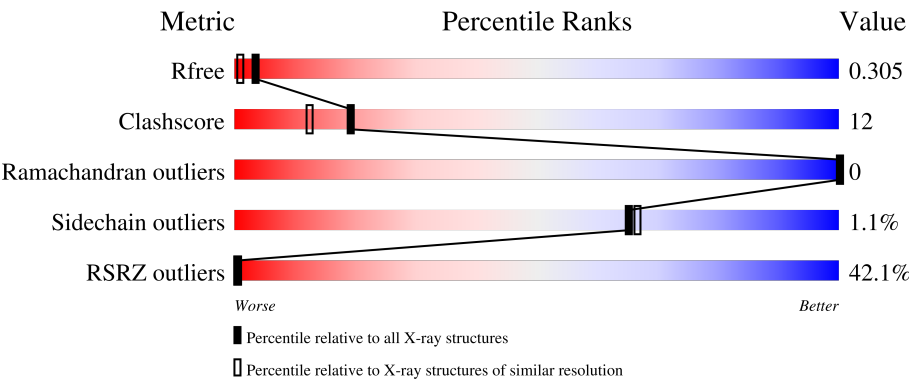
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 ≥ 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	265	14% 81%15%..
1	B	265	16% 80%16%.
1	C	265	29% 72%24%..
1	D	265	21% 78%17%..
1	E	265	77% 71%25%..

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Mol	Chain	Length	Quality of chain
1	F	265	89% 68% 28% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11701 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1866	1167	322	365	12			
1	B	257	Total	C	N	O	S	0	0	0
			1866	1167	322	365	12			
1	C	257	Total	C	N	O	S	0	0	0
			1866	1167	322	365	12			
1	D	257	Total	C	N	O	S	0	0	0
			1866	1167	322	365	12			
1	E	257	Total	C	N	O	S	0	0	0
			1866	1167	322	365	12			
1	F	257	Total	C	N	O	S	0	0	0
			1862	1165	321	364	12			

There are 6 discrepancies between the modelled and reference sequences:

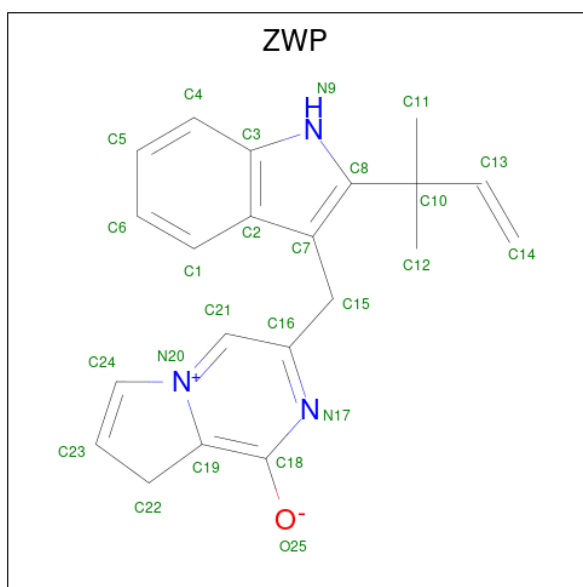
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ASN	ASP	conflict	UNP L0E2Z4
B	166	ASN	ASP	conflict	UNP L0E2Z4
C	166	ASN	ASP	conflict	UNP L0E2Z4
D	166	ASN	ASP	conflict	UNP L0E2Z4
E	166	ASN	ASP	conflict	UNP L0E2Z4
F	166	ASN	ASP	conflict	UNP L0E2Z4

- 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
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is 3-{[2-(2-methylbut-3-en-2-yl)-1H-indol-3-yl]methyl}-8H-pyrrolo[1,2-a]pyrazin-5-ium-1-olate (CCD ID: ZWP) (formula: C₂₁H₂₁N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	21	3	1		

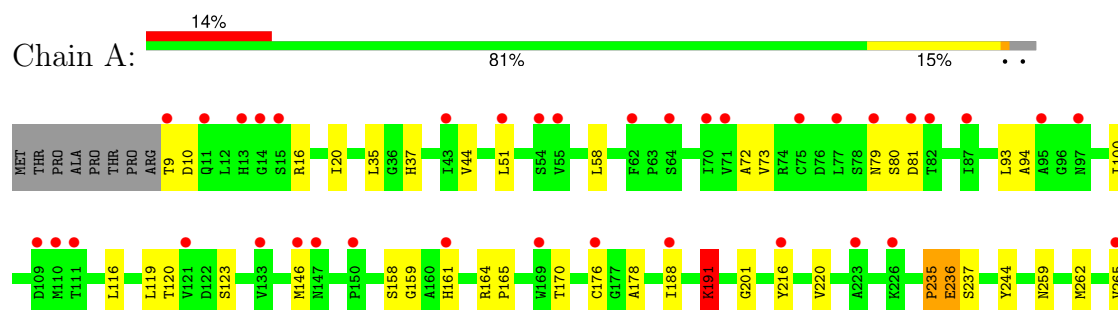
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	49	Total	O	0	0
			49	49		
4	C	40	Total	O	0	0
			40	40		
4	D	41	Total	O	0	0
			41	41		
4	E	5	Total	O	0	0
			5	5		
4	F	1	Total	O	0	0
			1	1		

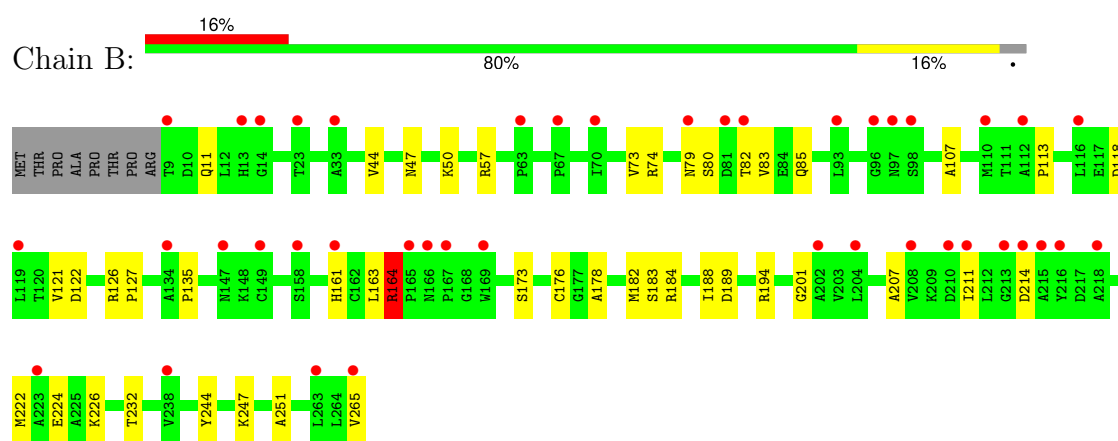
3 Residue-property plots

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.

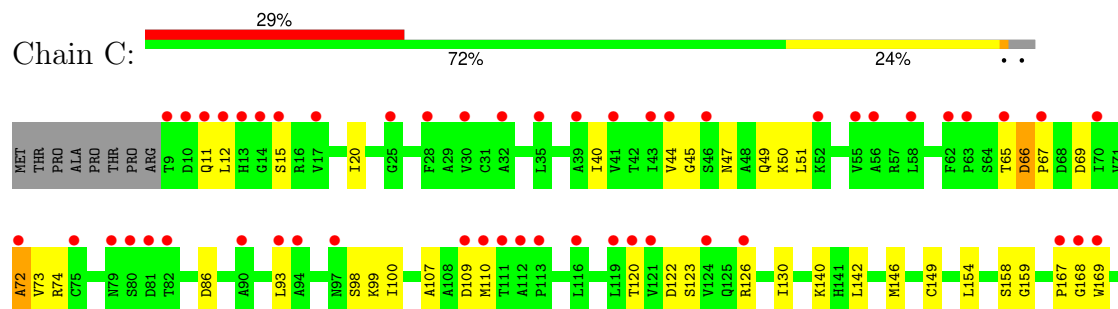
- Molecule 1: Short chain dehydrogenase

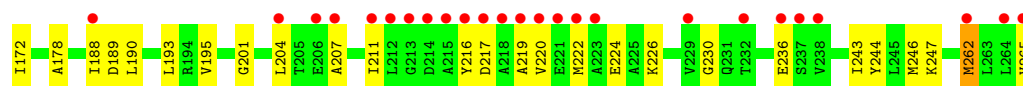


- Molecule 1: Short chain dehydrogenase

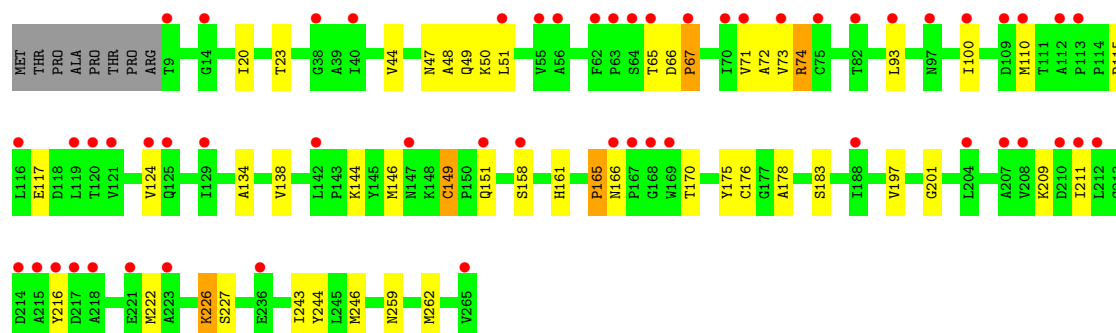
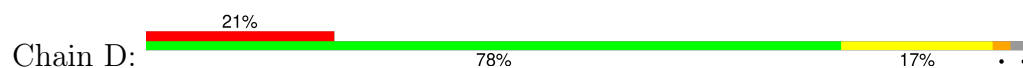


- Molecule 1: Short chain dehydrogenase

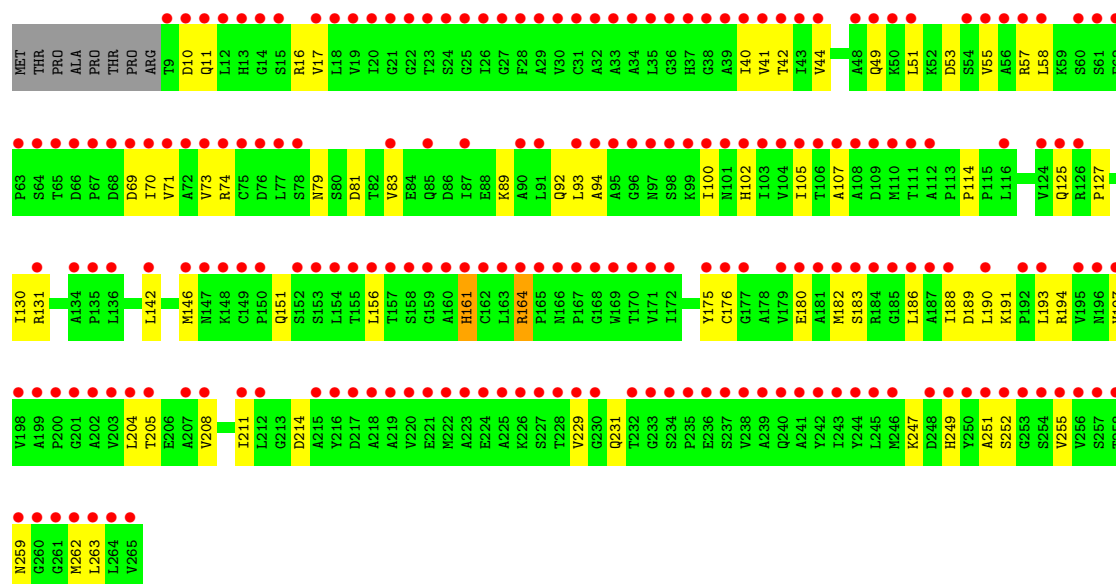
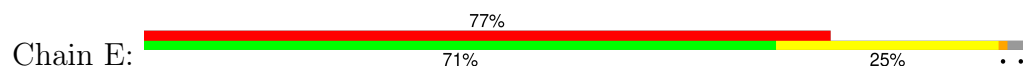




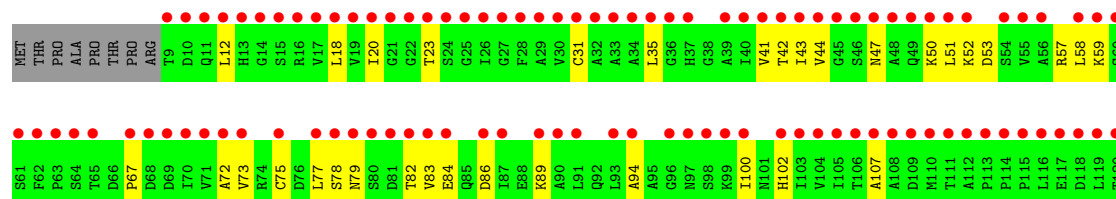
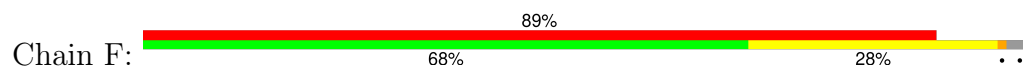
• Molecule 1: Short chain dehydrogenase

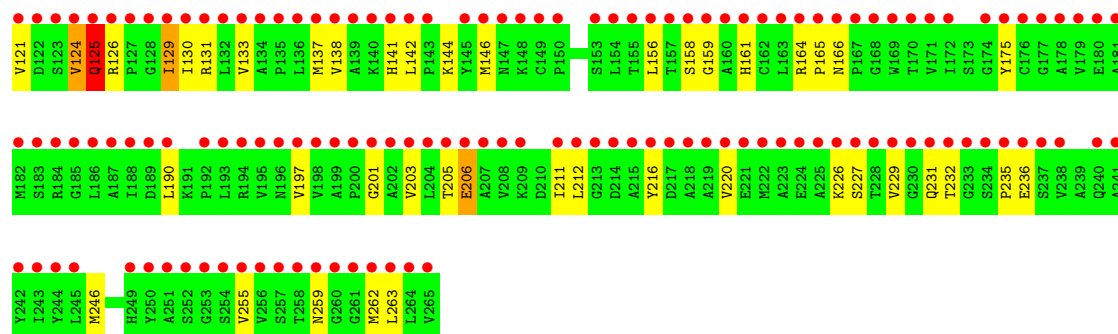


• Molecule 1: Short chain dehydrogenase



• Molecule 1: Short chain dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.48Å 117.19Å 63.73Å 90.00° 107.44° 90.00°	Depositor
Resolution (Å)	48.76 – 1.90 48.76 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.76-1.90) 97.1 (48.76-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.274 , 0.306 0.273 , 0.305	Depositor DCC
R_{free} test set	5570 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11701	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, ZWP

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	0.56	4/1895 (0.2%)	0.63	0/2580
1	B	0.82	7/1895 (0.4%)	0.71	1/2580 (0.0%)
1	C	0.79	3/1895 (0.2%)	0.77	5/2580 (0.2%)
1	D	0.75	3/1895 (0.2%)	0.80	9/2580 (0.3%)
1	E	0.44	0/1895	0.92	12/2580 (0.5%)
1	F	0.55	2/1891 (0.1%)	0.95	10/2575 (0.4%)
All	All	0.67	19/11366 (0.2%)	0.80	37/15475 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	THR	C-N	-10.57	1.26	1.33
1	A	191	LYS	CA-C	-8.13	1.44	1.53
1	D	149	CYS	CA-C	-7.24	1.45	1.52
1	B	184	ARG	C-O	-6.73	1.16	1.24
1	B	224	GLU	C-O	-6.71	1.16	1.24
1	C	86	ASP	C-O	-6.54	1.16	1.24
1	B	222	MET	C-O	-6.49	1.16	1.24
1	B	164	ARG	C-O	-6.40	1.16	1.24
1	A	236	GLU	C-O	-6.30	1.16	1.24
1	A	235	PRO	C-O	-6.27	1.16	1.24
1	B	183	SER	C-O	-6.16	1.17	1.24
1	F	129	ILE	CG1-CD1	6.13	1.75	1.51
1	D	149	CYS	C-O	6.02	1.29	1.24
1	A	237	SER	C-O	-5.90	1.17	1.24
1	C	262	MET	C-O	-5.85	1.16	1.24
1	F	232	THR	C-N	5.78	1.37	1.33
1	D	227	SER	C-O	-5.28	1.17	1.23
1	B	113	PRO	CA-C	-5.15	1.47	1.52
1	C	72	ALA	C-O	-5.12	1.17	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	92	GLN	CA-C-N	-9.33	106.12	122.26
1	E	92	GLN	C-N-CA	-9.33	106.12	122.26
1	D	149	CYS	O-C-N	-8.85	116.04	121.71
1	F	125	GLN	N-CA-C	8.66	120.80	111.36
1	E	164	ARG	CD-NE-CZ	8.53	136.34	124.40
1	E	125	GLN	CA-CB-CG	-8.15	97.80	114.10
1	E	161	HIS	CB-CA-C	-8.05	92.59	110.21
1	E	89	LYS	CA-CB-CG	7.55	129.20	114.10
1	D	226	LYS	CB-CA-C	-7.13	102.30	111.50
1	C	66	ASP	N-CA-C	-7.05	99.32	109.48
1	E	164	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	D	166	ASN	CB-CA-C	6.84	116.94	110.17
1	E	164	ARG	CG-CD-NE	-6.69	97.28	112.00
1	F	226	LYS	CD-CE-NZ	-6.32	91.67	111.90
1	C	236	GLU	CB-CA-C	-6.21	100.87	110.81
1	E	164	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	F	235	PRO	CA-C-N	-5.91	111.33	120.31
1	F	235	PRO	C-N-CA	-5.91	111.33	120.31
1	F	226	LYS	CA-CB-CG	-5.91	102.29	114.10
1	C	149	CYS	O-C-N	5.88	125.47	121.71
1	E	161	HIS	N-CA-CB	5.74	120.77	110.32
1	B	85	GLN	N-CA-CB	5.69	118.58	110.16
1	C	66	ASP	CA-C-N	5.68	125.77	119.87
1	C	66	ASP	C-N-CA	5.68	125.77	119.87
1	D	49	GLN	CA-CB-CG	-5.55	103.00	114.10
1	F	236	GLU	CA-CB-CG	5.49	125.09	114.10
1	E	89	LYS	CB-CG-CD	-5.48	98.71	111.30
1	D	66	ASP	C-N-CD	-5.39	102.88	125.00
1	F	124	VAL	CA-C-N	5.39	127.94	120.29
1	F	124	VAL	C-N-CA	5.39	127.94	120.29
1	D	165	PRO	CA-C-N	5.30	130.98	121.76
1	D	165	PRO	C-N-CA	5.30	130.98	121.76
1	F	236	GLU	N-CA-CB	5.27	118.45	110.28
1	E	93	LEU	CA-CB-CG	5.27	134.73	116.30
1	F	226	LYS	CA-C-O	5.21	127.96	120.51
1	D	48	ALA	CA-C-N	-5.01	113.26	121.92
1	D	48	ALA	C-N-CA	-5.01	113.26	121.92

There are no chirality outliers.

There are no planarity outliers.

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	1866	0	1901	27	0
1	B	1866	0	1901	28	0
1	C	1866	0	1901	55	0
1	D	1866	0	1901	42	0
1	E	1866	0	1901	57	0
1	F	1862	0	1895	82	2
2	A	48	0	24	1	0
2	B	48	0	24	2	0
2	C	48	0	24	3	0
2	D	48	0	24	1	0
2	E	48	0	24	1	0
2	F	48	0	23	1	0
3	A	25	0	0	0	0
4	A	60	0	0	1	0
4	B	49	0	0	1	0
4	C	40	0	0	1	0
4	D	41	0	0	1	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
All	All	11701	0	11543	270	2

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 12.

All (270) 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:129:ILE:CD1	1:F:129:ILE:CG1	1.75	1.63
1:D:209:LYS:HG2	1:D:216:TYR:CE2	1.49	1.48
1:D:222:MET:HG2	1:D:226:LYS:NZ	1.35	1.40
1:C:11:GLN:CB	1:F:89:LYS:HE3	1.61	1.28
1:D:222:MET:CG	1:D:226:LYS:NZ	2.04	1.18
1:E:182:MET:O	1:E:186:LEU:HD23	1.47	1.14
1:C:11:GLN:HB2	1:F:89:LYS:CE	1.81	1.10
1:D:209:LYS:CG	1:D:216:TYR:CE2	2.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:THR:O	1:C:67:PRO:HD3	1.55	1.05
1:D:222:MET:CG	1:D:226:LYS:HZ1	1.67	1.03
1:E:161:HIS:HE1	1:E:176:CYS:CB	1.73	1.01
1:F:211:ILE:HD12	1:F:212:LEU:HG	1.41	0.99
1:D:209:LYS:HG2	1:D:216:TYR:CD2	1.97	0.97
1:B:79:ASN:HB3	1:B:82:THR:HG22	1.45	0.97
1:E:161:HIS:HE1	1:E:176:CYS:SG	1.87	0.96
1:D:74:ARG:HH11	1:D:74:ARG:HG2	1.28	0.95
1:E:161:HIS:CE1	1:E:176:CYS:SG	2.63	0.91
1:C:11:GLN:HB2	1:F:89:LYS:HE3	0.92	0.91
1:D:222:MET:HG2	1:D:226:LYS:HZ3	0.92	0.90
1:A:164:ARG:NH1	1:A:265:VAL:O	2.05	0.89
1:B:118:ASP:OD2	1:E:74:ARG:NH2	2.05	0.88
1:F:18:LEU:HD23	1:F:94:ALA:HB2	1.54	0.88
1:F:18:LEU:CD2	1:F:94:ALA:HB2	2.05	0.86
1:F:18:LEU:HD12	1:F:20:ILE:HG13	1.58	0.86
1:F:211:ILE:CD1	1:F:212:LEU:HG	2.07	0.85
1:C:110:MET:HG3	1:C:211:ILE:HD11	1.59	0.84
1:C:12:LEU:HA	1:C:15:SER:OG	1.77	0.84
1:C:120:THR:HG23	1:C:123:SER:H	1.41	0.84
1:F:131:ARG:HE	1:F:175:TYR:CB	1.93	0.81
1:F:107:ALA:HB1	1:F:130:ILE:HD11	1.63	0.80
1:C:122:ASP:OD2	1:C:126:ARG:NH2	2.15	0.79
1:A:119:LEU:HD13	4:A:931:HOH:O	1.83	0.79
1:E:182:MET:O	1:E:186:LEU:CD2	2.29	0.79
1:E:161:HIS:HE1	1:E:176:CYS:HB2	1.47	0.79
1:F:78:SER:HB2	1:F:126:ARG:HH12	1.47	0.78
1:E:161:HIS:CE1	1:E:176:CYS:HB2	2.18	0.78
1:D:100:ILE:HB	1:D:146:MET:HG2	1.66	0.77
1:D:74:ARG:HG2	1:D:74:ARG:NH1	1.95	0.77
1:E:161:HIS:CE1	1:E:176:CYS:CB	2.63	0.77
1:D:158:SER:HB2	1:D:197:VAL:HG11	1.66	0.77
1:F:102:HIS:CG	1:F:246:MET:HG2	2.21	0.76
1:E:164:ARG:NH1	1:E:262:MET:O	2.19	0.76
1:F:18:LEU:HD23	1:F:94:ALA:CB	2.16	0.76
1:F:79:ASN:HB3	1:F:82:THR:HG22	1.67	0.75
1:A:188:ILE:O	1:A:191:LYS:HG2	1.88	0.74
1:A:165:PRO:HG2	1:B:188:ILE:HD12	1.70	0.73
1:F:84:GLU:HG3	1:F:137:MET:HE2	1.68	0.73
1:C:11:GLN:CG	1:F:89:LYS:HE3	2.19	0.73
1:F:79:ASN:O	1:F:83:VAL:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:ILE:HA	1:F:44:VAL:HG22	1.70	0.73
1:F:44:VAL:HG12	1:F:73:VAL:HG22	1.71	0.72
1:F:161:HIS:HB3	1:F:165:PRO:HA	1.71	0.71
1:D:65:THR:O	1:D:67:PRO:HD3	1.92	0.69
1:F:129:ILE:CD1	1:F:129:ILE:CB	2.70	0.69
1:A:120:THR:HG23	1:A:123:SER:H	1.58	0.69
1:F:142:LEU:HD11	1:F:190:LEU:HD22	1.74	0.69
1:C:140:LYS:HE3	1:D:117:GLU:O	1.94	0.68
1:D:209:LYS:HG2	1:D:216:TYR:HE2	1.50	0.68
1:E:55:VAL:HG13	1:E:70:ILE:HG22	1.75	0.68
1:B:11:GLN:HE22	1:B:247:LYS:HA	1.58	0.67
1:C:11:GLN:CB	1:F:89:LYS:CE	2.52	0.67
1:E:208:VAL:HA	1:E:211:ILE:HD12	1.76	0.67
1:F:124:VAL:O	1:F:175:TYR:OH	2.09	0.66
1:F:259:ASN:O	1:F:262:MET:HG3	1.95	0.66
1:A:51:LEU:HD12	1:A:72:ALA:HB1	1.77	0.66
1:C:188:ILE:HD12	1:D:165:PRO:HG2	1.77	0.65
1:F:18:LEU:HD12	1:F:20:ILE:CG1	2.28	0.64
1:D:183:SER:OG	4:D:901:HOH:O	2.15	0.64
1:E:105:ILE:HG13	1:E:156:LEU:HA	1.79	0.64
1:D:161:HIS:NE2	1:D:176:CYS:SG	2.71	0.64
1:C:51:LEU:HD22	1:C:72:ALA:HB1	1.79	0.64
1:C:65:THR:O	1:C:67:PRO:CD	2.39	0.64
1:F:211:ILE:HD12	1:F:212:LEU:CG	2.24	0.64
1:B:214:ASP:OD2	1:E:57:ARG:HD3	1.98	0.63
1:F:20:ILE:HA	1:F:44:VAL:CG2	2.28	0.63
1:F:131:ARG:HE	1:F:175:TYR:HB2	1.64	0.63
1:E:51:LEU:O	1:E:55:VAL:CG2	2.47	0.62
1:E:51:LEU:O	1:E:55:VAL:HG23	1.98	0.62
1:D:222:MET:CG	1:D:226:LYS:HZ3	1.81	0.61
1:E:107:ALA:HB1	1:E:130:ILE:HD11	1.83	0.61
1:D:158:SER:HB2	1:D:197:VAL:CG1	2.31	0.60
1:A:16:ARG:NH1	1:A:94:ALA:O	2.34	0.60
1:F:18:LEU:HD22	1:F:94:ALA:HB2	1.83	0.60
1:C:109:ASP:OD1	1:C:130:ILE:HG21	2.02	0.60
1:E:182:MET:C	1:E:186:LEU:HD23	2.24	0.60
1:E:17:VAL:HG22	1:E:102:HIS:HB2	1.85	0.59
1:E:40:ILE:HG23	1:E:69:ASP:HA	1.84	0.59
1:C:47:ASN:HB3	1:C:50:LYS:HB2	1.83	0.59
1:E:194:ARG:HG2	1:E:252:SER:HB2	1.82	0.59
1:E:186:LEU:N	1:E:186:LEU:HD22	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:SER:OG	1:F:229:VAL:HG12	2.02	0.59
1:A:44:VAL:HG22	1:A:73:VAL:HG22	1.86	0.58
1:E:205:THR:O	1:E:208:VAL:HG12	2.04	0.58
1:C:122:ASP:OD2	1:C:126:ARG:CZ	2.52	0.58
1:B:161:HIS:NE2	1:B:176:CYS:SG	2.73	0.57
1:B:79:ASN:O	1:B:83:VAL:HG23	2.04	0.57
1:F:161:HIS:NE2	1:F:166:ASN:ND2	2.52	0.57
1:D:47:ASN:HB3	1:D:50:LYS:HB2	1.86	0.57
1:C:51:LEU:CD1	1:C:74:ARG:HB2	2.35	0.57
1:B:47:ASN:HB3	1:B:50:LYS:HB2	1.87	0.56
1:C:189:ASP:OD2	1:D:170:THR:OG1	2.15	0.56
1:F:161:HIS:HB3	1:F:164:ARG:O	2.05	0.56
1:F:35:LEU:HD12	1:F:58:LEU:HD22	1.87	0.56
1:F:59:LYS:HE3	1:F:67:PRO:HB3	1.88	0.56
1:E:42:THR:HG22	1:E:71:VAL:HG23	1.88	0.55
1:B:44:VAL:HG22	1:B:73:VAL:HG13	1.87	0.55
1:F:75:CYS:SG	1:F:86:ASP:HB3	2.47	0.55
1:D:149:CYS:SG	1:D:151:GLN:NE2	2.79	0.55
1:D:44:VAL:HG22	1:D:73:VAL:HG22	1.89	0.55
1:F:47:ASN:HB3	1:F:50:LYS:HB2	1.87	0.55
1:B:201:GLY:O	2:B:801:NAP:H4N	2.07	0.55
1:F:161:HIS:CD2	1:F:166:ASN:ND2	2.75	0.55
1:A:259:ASN:HB2	1:A:262:MET:HG2	1.88	0.55
1:B:164:ARG:NH2	1:B:265:VAL:O	2.28	0.54
1:C:219:ALA:HA	1:C:222:MET:HE3	1.88	0.54
1:F:53:ASP:O	1:F:57:ARG:HG2	2.07	0.54
1:B:122:ASP:OD2	1:B:126:ARG:NH2	2.39	0.54
1:D:110:MET:O	1:D:211:ILE:HD11	2.07	0.54
1:F:255:VAL:HG23	1:F:255:VAL:O	2.07	0.54
1:E:142:LEU:HD11	1:E:190:LEU:HD23	1.88	0.54
1:E:204:LEU:HA	1:E:208:VAL:HG11	1.89	0.54
1:C:220:VAL:O	1:C:224:GLU:HG3	2.08	0.53
1:D:201:GLY:O	2:D:801:NAP:H4N	2.07	0.53
1:C:110:MET:CG	1:C:211:ILE:HD11	2.37	0.52
1:F:82:THR:O	1:F:82:THR:OG1	2.27	0.52
1:D:209:LYS:HD2	1:D:216:TYR:CZ	2.44	0.52
1:A:80:SER:HB3	1:B:121:VAL:HG11	1.92	0.52
1:E:79:ASN:O	1:E:83:VAL:HG23	2.09	0.52
1:C:243:ILE:HD13	1:C:246:MET:HE2	1.91	0.52
1:E:182:MET:HG2	1:E:186:LEU:HD21	1.90	0.52
1:A:216:TYR:O	1:A:220:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:MET:HE3	1:F:137:MET:HA	1.92	0.51
1:F:133:VAL:O	1:F:137:MET:HG2	2.09	0.51
1:F:229:VAL:HG13	1:F:231:GLN:HB2	1.93	0.51
1:A:9:THR:O	1:A:9:THR:OG1	2.19	0.51
1:F:156:LEU:HB2	1:F:197:VAL:HG12	1.93	0.51
1:E:44:VAL:HG22	1:E:73:VAL:HG22	1.93	0.51
1:E:188:ILE:O	1:E:191:LYS:HG2	2.11	0.50
1:A:100:ILE:HB	1:A:146:MET:HG2	1.93	0.50
1:F:211:ILE:HD12	1:F:212:LEU:N	2.27	0.50
1:B:122:ASP:OD2	1:B:126:ARG:NE	2.41	0.50
1:E:10:ASP:OD1	1:E:247:LYS:NZ	2.45	0.50
1:E:131:ARG:HD3	1:E:175:TYR:HB3	1.94	0.50
1:F:82:THR:OG1	1:F:86:ASP:OD1	2.29	0.50
1:F:161:HIS:HB3	1:F:165:PRO:CA	2.40	0.50
1:C:65:THR:HG22	1:C:66:ASP:O	2.11	0.50
1:F:131:ARG:NE	1:F:175:TYR:CB	2.71	0.49
1:D:222:MET:HG3	1:D:226:LYS:NZ	2.14	0.49
1:A:201:GLY:O	2:A:801:NAP:H4N	2.12	0.49
1:A:10:ASP:OD2	1:A:37:HIS:HB3	2.13	0.49
1:D:259:ASN:HB2	1:D:262:MET:HG2	1.94	0.49
1:F:138:VAL:HG12	1:F:142:LEU:HD23	1.95	0.49
1:F:51:LEU:HD21	1:F:72:ALA:CB	2.43	0.49
1:A:161:HIS:CE1	1:A:176:CYS:SG	3.06	0.48
1:C:201:GLY:O	2:C:801:NAP:H4N	2.12	0.48
1:E:94:ALA:HB3	1:E:100:ILE:HD11	1.95	0.48
1:E:186:LEU:CD2	1:E:186:LEU:N	2.76	0.48
1:B:11:GLN:NE2	4:B:903:HOH:O	2.39	0.48
1:B:244:TYR:HB2	1:D:244:TYR:HB2	1.95	0.48
1:C:178:ALA:HB2	1:D:178:ALA:HB2	1.95	0.48
1:F:203:VAL:HG12	1:F:205:THR:HG23	1.95	0.48
1:A:170:THR:OG1	1:B:189:ASP:OD2	2.18	0.48
1:E:194:ARG:HD2	1:E:251:ALA:O	2.13	0.48
1:E:263:LEU:HD12	1:E:263:LEU:H	1.78	0.48
1:B:107:ALA:HA	2:B:801:NAP:O4B	2.14	0.48
1:E:259:ASN:HB2	1:E:262:MET:HG2	1.96	0.47
1:D:71:VAL:HG21	1:D:93:LEU:HD21	1.96	0.47
1:F:131:ARG:HE	1:F:175:TYR:HB3	1.75	0.47
1:B:57:ARG:HD2	1:E:214:ASP:OD2	2.14	0.47
1:E:107:ALA:HA	2:E:801:NAP:O4B	2.13	0.47
1:E:142:LEU:HD13	1:E:146:MET:HE2	1.96	0.47
1:F:121:VAL:O	1:F:124:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:HIS:O	1:B:173:SER:OG	2.29	0.47
1:C:11:GLN:HG3	1:F:89:LYS:HE3	1.93	0.47
1:C:158:SER:O	2:C:801:NAP:H6N	2.15	0.47
1:C:98:SER:OG	1:C:99:LYS:N	2.48	0.47
1:F:18:LEU:HD22	1:F:42:THR:HB	1.97	0.47
1:B:178:ALA:O	1:B:182:MET:HB2	2.15	0.46
1:E:42:THR:HA	1:E:71:VAL:O	2.15	0.46
1:E:79:ASN:OD1	1:E:81:ASP:OD2	2.34	0.46
1:E:229:VAL:HG12	1:E:231:GLN:HB2	1.96	0.46
1:C:100:ILE:HB	1:C:146:MET:HG2	1.97	0.46
1:F:77:LEU:HB2	1:F:130:ILE:HD12	1.98	0.46
1:F:201:GLY:O	2:F:801:NAP:H4N	2.15	0.46
1:A:178:ALA:HB2	1:B:178:ALA:HB2	1.96	0.46
1:C:107:ALA:HB1	1:C:130:ILE:HD11	1.97	0.46
1:C:169:TRP:HE3	1:C:172:ILE:HG13	1.80	0.46
1:E:197:VAL:HG22	1:E:255:VAL:HA	1.98	0.46
1:F:262:MET:HB2	1:F:263:LEU:HD12	1.98	0.46
1:A:161:HIS:HD1	1:A:161:HIS:H	1.64	0.46
1:C:120:THR:HG23	1:C:123:SER:N	2.20	0.46
1:C:142:LEU:HD13	1:C:146:MET:HE2	1.98	0.46
1:D:20:ILE:HA	1:D:44:VAL:HB	1.98	0.46
1:F:52:LYS:HA	1:F:52:LYS:HD3	1.49	0.46
1:F:102:HIS:CD2	1:F:246:MET:HG2	2.50	0.45
1:C:243:ILE:HD13	1:C:246:MET:CE	2.46	0.45
1:B:207:ALA:O	1:B:211:ILE:HG13	2.16	0.45
1:F:158:SER:OG	1:F:159:GLY:N	2.49	0.45
1:B:135:PRO:HB2	1:B:182:MET:HE1	1.99	0.45
1:D:51:LEU:HD22	1:D:72:ALA:HB1	1.98	0.45
1:E:49:GLN:NE2	1:E:53:ASP:OD1	2.50	0.45
1:F:131:ARG:HH21	1:F:175:TYR:HB2	1.81	0.45
1:F:216:TYR:O	1:F:220:VAL:HG23	2.17	0.45
1:D:144:LYS:HB2	1:D:144:LYS:HE2	1.83	0.45
1:F:141:HIS:HA	1:F:144:LYS:NZ	2.32	0.45
1:C:216:TYR:HD2	1:C:217:ASP:OD1	2.00	0.44
1:F:161:HIS:HB3	1:F:164:ARG:C	2.42	0.44
1:E:161:HIS:HA	1:E:164:ARG:O	2.17	0.44
1:F:18:LEU:CD1	1:F:20:ILE:CG1	2.94	0.44
1:A:244:TYR:HB2	1:C:244:TYR:HB2	2.00	0.44
1:F:23:THR:CG2	1:F:51:LEU:HA	2.48	0.44
1:C:66:ASP:HA	1:C:67:PRO:HD2	1.75	0.43
1:E:127:PRO:HB3	1:E:131:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ASN:O	1:E:262:MET:HE3	2.17	0.43
1:F:131:ARG:NE	1:F:175:TYR:HB3	2.32	0.43
1:A:20:ILE:HA	1:A:44:VAL:HB	2.00	0.43
1:B:164:ARG:HE	1:B:164:ARG:HB3	1.60	0.43
1:C:11:GLN:HB2	1:F:89:LYS:CD	2.44	0.43
1:C:50:LYS:NZ	2:C:801:NAP:O1X	2.49	0.43
1:C:73:VAL:CG1	1:C:93:LEU:HD22	2.49	0.43
1:F:211:ILE:CD1	1:F:212:LEU:CG	2.86	0.43
1:A:116:LEU:HD12	1:A:119:LEU:HD22	2.01	0.43
1:C:12:LEU:CA	1:C:15:SER:OG	2.57	0.43
1:E:58:LEU:HD23	1:E:58:LEU:HA	1.67	0.43
1:A:120:THR:CG2	1:A:123:SER:H	2.29	0.43
1:D:23:THR:HG22	1:D:51:LEU:HD23	2.01	0.43
1:C:40:ILE:HG12	1:C:69:ASP:CG	2.44	0.43
1:F:35:LEU:HG	1:F:41:VAL:HG21	2.01	0.43
1:C:226:LYS:C	1:C:265:VAL:HG21	2.43	0.43
1:F:100:ILE:O	1:F:146:MET:HG2	2.18	0.43
1:B:194:ARG:HD2	1:B:251:ALA:O	2.19	0.43
1:C:45:GLY:O	1:C:74:ARG:HA	2.19	0.43
1:D:134:ALA:O	1:D:138:VAL:HG23	2.19	0.43
1:C:224:GLU:O	1:C:230:GLY:HA2	2.19	0.42
1:D:124:VAL:O	1:D:175:TYR:OH	2.25	0.42
1:F:211:ILE:CD1	1:F:212:LEU:CD2	2.97	0.42
1:C:20:ILE:HA	1:C:44:VAL:HB	2.02	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.89	0.42
1:B:126:ARG:HB3	1:B:127:PRO:HD3	2.01	0.42
1:F:52:LYS:HZ3	1:F:72:ALA:HB3	1.83	0.42
1:C:216:TYR:CD2	1:C:217:ASP:OD1	2.73	0.42
1:F:43:ILE:HB	1:F:72:ALA:CB	2.50	0.42
1:C:11:GLN:NE2	1:C:247:LYS:HA	2.34	0.42
1:D:74:ARG:HH11	1:D:74:ARG:CG	2.11	0.42
1:F:12:LEU:HD21	1:F:246:MET:HB3	2.01	0.42
1:D:209:LYS:CG	1:D:216:TYR:HE2	2.13	0.42
1:F:31:CYS:SG	1:F:43:ILE:HD13	2.60	0.41
1:F:44:VAL:HG12	1:F:73:VAL:CG2	2.46	0.41
1:E:16:ARG:HA	1:E:40:ILE:O	2.20	0.41
1:E:17:VAL:O	1:E:41:VAL:HA	2.21	0.41
1:B:74:ARG:NH2	1:E:114:PRO:HB3	2.35	0.41
1:C:154:LEU:O	1:C:195:VAL:HA	2.21	0.41
1:C:207:ALA:O	1:C:211:ILE:HG13	2.21	0.41
1:E:180:GLU:O	1:E:183:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD12	1:A:58:LEU:HD22	2.02	0.41
1:A:79:ASN:ND2	1:A:81:ASP:HB2	2.35	0.41
1:C:190:LEU:O	1:C:193:LEU:HB3	2.21	0.41
1:D:243:ILE:HA	1:D:246:MET:HE2	2.03	0.41
1:E:11:GLN:HE21	1:E:249:HIS:CE1	2.39	0.41
1:E:189:ASP:HB2	1:E:190:LEU:HD12	2.03	0.41
1:F:52:LYS:NZ	1:F:72:ALA:HB3	2.35	0.41
1:C:167:PRO:HA	1:C:168:GLY:HA2	1.67	0.40
1:E:193:LEU:HD12	1:E:194:ARG:H	1.86	0.40
1:D:50:LYS:HE3	1:D:50:LYS:HB3	1.83	0.40
1:D:73:VAL:CG1	1:D:93:LEU:HD22	2.51	0.40
1:F:82:THR:O	1:F:83:VAL:C	2.64	0.40
1:C:158:SER:OG	1:C:159:GLY:N	2.54	0.40
1:C:204:LEU:HB2	4:C:903:HOH:O	2.21	0.40
1:E:151:GLN:HG3	1:E:249:HIS:CE1	2.56	0.40
1:A:158:SER:OG	1:A:159:GLY:N	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:GLU:OE2	1:F:206:GLU:OE2[2_555]	1.68	0.52
1:F:125:GLN:OE1	1:F:125:GLN:OE1[2_556]	2.11	0.09

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	255/265 (96%)	252 (99%)	3 (1%)	0	100	100
1	B	255/265 (96%)	249 (98%)	6 (2%)	0	100	100
1	C	255/265 (96%)	248 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	255/265 (96%)	250 (98%)	5 (2%)	0	100	100
1	E	255/265 (96%)	250 (98%)	5 (2%)	0	100	100
1	F	255/265 (96%)	248 (97%)	7 (3%)	0	100	100
All	All	1530/1590 (96%)	1497 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	204/211 (97%)	201 (98%)	3 (2%)	57	56
1	B	204/211 (97%)	200 (98%)	4 (2%)	48	46
1	C	204/211 (97%)	202 (99%)	2 (1%)	68	70
1	D	204/211 (97%)	201 (98%)	3 (2%)	57	56
1	E	204/211 (97%)	204 (100%)	0	100	100
1	F	203/211 (96%)	201 (99%)	2 (1%)	68	70
All	All	1223/1266 (97%)	1209 (99%)	14 (1%)	65	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
1	A	235	PRO
1	A	236	GLU
1	B	80	SER
1	B	163	LEU
1	B	164	ARG
1	B	226	LYS
1	C	49	GLN
1	C	262	MET
1	D	67	PRO

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Mol	Chain	Res	Type
1	D	74	ARG
1	D	115	PRO
1	F	125	GLN
1	F	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	79	ASN
1	A	92	GLN
1	A	147	ASN
1	A	161	HIS
1	A	240	GLN
1	B	11	GLN
1	B	13	HIS
1	B	166	ASN
1	C	13	HIS
1	C	85	GLN
1	D	151	GLN
1	E	11	GLN
1	E	147	ASN
1	E	161	HIS
1	F	13	HIS
1	F	166	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

7 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	ZWP	A	802	-	25,28,28	1.51	4 (16%)	29,42,42	1.67	7 (24%)
2	NAP	C	801	-	50,52,52	4.16	23 (46%)	71,80,80	1.79	17 (23%)
2	NAP	F	801	-	50,52,52	4.18	22 (44%)	71,80,80	1.81	17 (23%)
2	NAP	D	801	-	50,52,52	4.15	22 (44%)	71,80,80	1.82	17 (23%)
2	NAP	B	801	-	50,52,52	4.11	22 (44%)	71,80,80	1.81	17 (23%)
2	NAP	E	801	-	50,52,52	4.16	23 (46%)	71,80,80	1.76	15 (21%)
2	NAP	A	801	-	50,52,52	4.11	23 (46%)	71,80,80	1.90	16 (22%)

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
3	ZWP	A	802	-	-	4/13/19/19	0/4/4/4
2	NAP	C	801	-	-	2/35/67/67	0/5/5/5
2	NAP	F	801	-	-	2/35/67/67	0/5/5/5
2	NAP	D	801	-	-	4/35/67/67	0/5/5/5
2	NAP	B	801	-	-	4/35/67/67	0/5/5/5
2	NAP	E	801	-	-	2/35/67/67	0/5/5/5
2	NAP	A	801	-	-	3/35/67/67	0/5/5/5

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O4D-C1D	17.15	1.63	1.40
2	D	801	NAP	O4D-C1D	17.15	1.63	1.40
2	E	801	NAP	O4D-C1D	16.96	1.63	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	O4D-C1D	16.84	1.63	1.40
2	B	801	NAP	O4D-C1D	16.82	1.63	1.40
2	C	801	NAP	O4D-C1D	16.44	1.62	1.40
2	F	801	NAP	C2B-C1B	-9.31	1.30	1.53
2	B	801	NAP	C2B-C1B	-9.24	1.30	1.53
2	D	801	NAP	C2B-C1B	-9.22	1.30	1.53
2	C	801	NAP	C2B-C1B	-9.12	1.30	1.53
2	E	801	NAP	C2B-C1B	-9.06	1.30	1.53
2	A	801	NAP	C2B-C1B	-9.05	1.30	1.53
2	C	801	NAP	PN-O3	9.01	1.69	1.59
2	D	801	NAP	O4B-C1B	8.74	1.62	1.42
2	F	801	NAP	O4B-C1B	8.65	1.62	1.42
2	C	801	NAP	O4B-C1B	8.63	1.62	1.42
2	F	801	NAP	PN-O3	8.56	1.68	1.59
2	B	801	NAP	PN-O3	8.24	1.68	1.59
2	A	801	NAP	O4B-C1B	8.22	1.61	1.42
2	E	801	NAP	O4B-C1B	8.11	1.60	1.42
2	D	801	NAP	PN-O3	7.84	1.68	1.59
2	A	801	NAP	PN-O3	7.83	1.68	1.59
2	D	801	NAP	C7N-N7N	7.81	1.47	1.33
2	E	801	NAP	PN-O3	7.79	1.67	1.59
2	B	801	NAP	O4B-C1B	7.78	1.60	1.42
2	A	801	NAP	C7N-N7N	7.76	1.47	1.33
2	B	801	NAP	C7N-N7N	7.74	1.47	1.33
2	E	801	NAP	C7N-N7N	7.61	1.47	1.33
2	F	801	NAP	C7N-N7N	7.58	1.46	1.33
2	C	801	NAP	C7N-N7N	7.47	1.46	1.33
2	E	801	NAP	O4D-C4D	-6.90	1.29	1.45
2	C	801	NAP	O4D-C4D	-6.50	1.30	1.45
2	A	801	NAP	O4B-C4B	-6.48	1.30	1.45
2	B	801	NAP	O4D-C4D	-6.42	1.30	1.45
2	D	801	NAP	O4D-C4D	-6.38	1.30	1.45
2	F	801	NAP	C3N-C7N	6.33	1.60	1.50
2	C	801	NAP	C3N-C7N	6.17	1.59	1.50
2	F	801	NAP	O4D-C4D	-6.17	1.31	1.45
2	E	801	NAP	C3N-C7N	6.14	1.59	1.50
2	B	801	NAP	O4B-C4B	-6.14	1.31	1.45
2	A	801	NAP	O4D-C4D	-6.08	1.31	1.45
2	D	801	NAP	C3N-C7N	6.05	1.59	1.50
2	C	801	NAP	PA-O3	6.04	1.66	1.59
2	E	801	NAP	PA-O3	5.85	1.65	1.59
2	D	801	NAP	O4B-C4B	-5.82	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	NAP	O4B-C4B	-5.78	1.32	1.45
2	C	801	NAP	O4B-C4B	-5.70	1.32	1.45
2	F	801	NAP	O4B-C4B	-5.60	1.32	1.45
2	A	801	NAP	C3N-C7N	5.59	1.58	1.50
2	A	801	NAP	PA-O3	5.41	1.65	1.59
2	B	801	NAP	C3N-C7N	5.34	1.58	1.50
2	B	801	NAP	PA-O3	5.26	1.65	1.59
2	F	801	NAP	PA-O3	4.96	1.64	1.59
2	D	801	NAP	PA-O3	4.84	1.64	1.59
2	C	801	NAP	C6A-N6A	4.56	1.45	1.34
3	A	802	ZWP	C24-C23	4.51	1.53	1.34
2	D	801	NAP	C6A-N6A	4.46	1.45	1.34
2	E	801	NAP	C6A-N6A	4.42	1.45	1.34
2	F	801	NAP	C6A-N6A	4.38	1.45	1.34
2	A	801	NAP	C6A-N6A	4.22	1.45	1.34
2	B	801	NAP	C5A-N7A	-4.22	1.31	1.39
2	F	801	NAP	C5A-N7A	-4.19	1.31	1.39
2	C	801	NAP	C5A-N7A	-4.18	1.31	1.39
2	B	801	NAP	C6A-N6A	4.10	1.44	1.34
2	E	801	NAP	C5A-N7A	-4.10	1.31	1.39
2	D	801	NAP	C5A-N7A	-4.10	1.31	1.39
2	A	801	NAP	C5A-N7A	-4.04	1.31	1.39
2	E	801	NAP	O3D-C3D	-3.93	1.33	1.43
2	D	801	NAP	O3D-C3D	-3.81	1.33	1.43
2	C	801	NAP	O3D-C3D	-3.80	1.33	1.43
2	B	801	NAP	O3D-C3D	-3.80	1.33	1.43
2	A	801	NAP	O3D-C3D	-3.77	1.33	1.43
2	F	801	NAP	O3D-C3D	-3.74	1.33	1.43
2	E	801	NAP	O7N-C7N	-3.63	1.17	1.24
2	F	801	NAP	O2D-C2D	3.53	1.51	1.43
2	C	801	NAP	O2D-C2D	3.51	1.51	1.43
2	E	801	NAP	O2D-C2D	3.48	1.51	1.43
2	B	801	NAP	O7N-C7N	-3.46	1.17	1.24
2	A	801	NAP	O2D-C2D	3.43	1.51	1.43
2	B	801	NAP	O2D-C2D	3.38	1.51	1.43
2	D	801	NAP	O7N-C7N	-3.31	1.18	1.24
2	D	801	NAP	O2D-C2D	3.28	1.51	1.43
2	A	801	NAP	O7N-C7N	-3.22	1.18	1.24
2	F	801	NAP	O7N-C7N	-3.12	1.18	1.24
2	C	801	NAP	O7N-C7N	-2.99	1.18	1.24
3	A	802	ZWP	C2-C7	-2.80	1.39	1.44
2	B	801	NAP	C5N-C4N	-2.78	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	NAP	P2B-O2B	2.69	1.64	1.59
2	F	801	NAP	PA-O5B	2.67	1.69	1.59
2	F	801	NAP	O3B-C3B	-2.66	1.36	1.43
2	A	801	NAP	C8A-N7A	2.65	1.36	1.31
2	C	801	NAP	PA-O5B	2.56	1.69	1.59
2	A	801	NAP	P2B-O2B	2.55	1.64	1.59
2	E	801	NAP	C4A-N9A	-2.53	1.32	1.37
2	D	801	NAP	P2B-O2B	2.49	1.63	1.59
2	D	801	NAP	C8A-N9A	-2.48	1.33	1.37
2	E	801	NAP	C8A-N9A	-2.47	1.33	1.37
2	B	801	NAP	C4N-C3N	-2.47	1.35	1.39
2	E	801	NAP	O3B-C3B	-2.46	1.36	1.43
2	A	801	NAP	PN-O5D	2.43	1.68	1.59
2	A	801	NAP	C4N-C3N	-2.43	1.35	1.39
2	E	801	NAP	PA-O5B	2.41	1.68	1.59
2	B	801	NAP	C4A-N9A	-2.39	1.32	1.37
2	B	801	NAP	PA-O5B	2.36	1.68	1.59
2	A	801	NAP	O3B-C3B	-2.36	1.37	1.43
2	D	801	NAP	O3B-C3B	-2.34	1.37	1.43
2	F	801	NAP	C8A-N9A	-2.32	1.33	1.37
2	E	801	NAP	C4N-C3N	-2.32	1.35	1.39
2	C	801	NAP	O3B-C3B	-2.31	1.37	1.43
2	B	801	NAP	C8A-N9A	-2.27	1.33	1.37
2	F	801	NAP	P2B-O2B	2.26	1.63	1.59
3	A	802	ZWP	C21-N20	-2.26	1.33	1.35
2	B	801	NAP	O3B-C3B	-2.25	1.37	1.43
2	D	801	NAP	C4N-C3N	-2.25	1.36	1.39
2	F	801	NAP	C5N-C4N	-2.25	1.35	1.38
2	E	801	NAP	P2B-O2B	2.24	1.63	1.59
2	E	801	NAP	PN-O5D	2.24	1.68	1.59
2	C	801	NAP	C4N-C3N	-2.23	1.36	1.39
3	A	802	ZWP	C19-N20	-2.23	1.32	1.36
2	F	801	NAP	C4N-C3N	-2.21	1.36	1.39
2	C	801	NAP	C8A-N9A	-2.21	1.33	1.37
2	C	801	NAP	C4A-N9A	-2.16	1.33	1.37
2	B	801	NAP	C5A-C4A	-2.16	1.35	1.39
2	F	801	NAP	C4A-N9A	-2.15	1.33	1.37
2	A	801	NAP	C8A-N9A	-2.14	1.33	1.37
2	C	801	NAP	C5N-C4N	-2.14	1.35	1.38
2	D	801	NAP	PA-O5B	2.13	1.67	1.59
2	E	801	NAP	C5N-C4N	-2.12	1.35	1.38
2	E	801	NAP	C5A-C4A	-2.09	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	PA-O5B	2.08	1.67	1.59
2	C	801	NAP	PN-O5D	2.06	1.67	1.59
2	B	801	NAP	PN-O5D	2.06	1.67	1.59
2	A	801	NAP	C5N-C4N	-2.05	1.35	1.38
2	D	801	NAP	C4A-N9A	-2.05	1.33	1.37
2	A	801	NAP	C5A-C4A	-2.04	1.35	1.39
2	F	801	NAP	PN-O5D	2.03	1.67	1.59
2	D	801	NAP	C5B-C4B	2.03	1.57	1.51
2	C	801	NAP	O2B-C2B	2.02	1.51	1.44
2	D	801	NAP	C5N-C4N	-2.01	1.35	1.38

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	NAP	N3A-C2A-N1A	-5.84	119.75	128.58
2	D	801	NAP	N3A-C2A-N1A	-5.73	119.90	128.58
2	C	801	NAP	N3A-C2A-N1A	-5.61	120.08	128.58
2	B	801	NAP	N3A-C2A-N1A	-5.53	120.22	128.58
2	A	801	NAP	N3A-C2A-N1A	-5.40	120.40	128.58
2	E	801	NAP	N3A-C2A-N1A	-5.37	120.46	128.58
2	A	801	NAP	C4D-O4D-C1D	-5.36	105.02	109.92
2	D	801	NAP	C5A-C4A-N3A	-5.35	119.35	126.72
2	A	801	NAP	C5A-C4A-N3A	-5.25	119.48	126.72
2	C	801	NAP	C5A-C4A-N3A	-5.25	119.48	126.72
2	F	801	NAP	C5A-C4A-N3A	-5.22	119.53	126.72
2	A	801	NAP	N6A-C6A-N1A	-5.10	107.02	118.38
2	B	801	NAP	C5A-C4A-N3A	-5.03	119.79	126.72
2	C	801	NAP	N6A-C6A-N1A	-4.90	107.47	118.38
2	E	801	NAP	C5A-C4A-N3A	-4.72	120.21	126.72
2	D	801	NAP	N6A-C6A-N1A	-4.58	108.18	118.38
2	A	801	NAP	N9A-C8A-N7A	-4.58	107.44	113.94
2	E	801	NAP	N6A-C6A-N1A	-4.53	108.29	118.38
2	E	801	NAP	N9A-C8A-N7A	-4.41	107.68	113.94
3	A	802	ZWP	C10-C8-N9	-4.40	113.31	120.15
2	B	801	NAP	N9A-C8A-N7A	-4.37	107.74	113.94
2	F	801	NAP	N9A-C8A-N7A	-4.26	107.89	113.94
2	D	801	NAP	N9A-C8A-N7A	-4.15	108.05	113.94
2	F	801	NAP	N6A-C6A-N1A	-4.04	109.38	118.38
2	F	801	NAP	C4D-O4D-C1D	-4.01	106.25	109.92
2	C	801	NAP	C5A-C6A-N6A	3.90	132.95	123.29
2	A	801	NAP	C5A-C6A-N6A	3.79	132.66	123.29
2	C	801	NAP	N9A-C8A-N7A	-3.61	108.82	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAP	N6A-C6A-N1A	-3.57	110.43	118.38
2	D	801	NAP	C2A-N3A-C4A	3.56	120.52	111.83
2	A	801	NAP	C2A-N3A-C4A	3.52	120.44	111.83
2	C	801	NAP	C2A-N3A-C4A	3.50	120.38	111.83
2	E	801	NAP	C5A-C6A-N6A	3.47	131.87	123.29
2	F	801	NAP	C2A-N3A-C4A	3.46	120.28	111.83
2	D	801	NAP	C5A-C6A-N6A	3.37	131.62	123.29
2	B	801	NAP	C2B-C1B-N9A	-3.32	108.29	113.75
2	B	801	NAP	C2A-N3A-C4A	3.31	119.92	111.83
2	B	801	NAP	N3A-C4A-N9A	3.30	132.77	127.17
2	F	801	NAP	N3A-C4A-N9A	3.28	132.75	127.17
2	E	801	NAP	C2A-N3A-C4A	3.26	119.80	111.83
2	B	801	NAP	C4D-O4D-C1D	-3.26	106.94	109.92
2	A	801	NAP	C5A-N7A-C8A	3.22	108.52	103.45
3	A	802	ZWP	C15-C16-N17	3.19	121.08	115.78
2	D	801	NAP	N3A-C4A-N9A	3.17	132.55	127.17
2	B	801	NAP	P2B-O2B-C2B	-3.15	115.01	123.43
2	B	801	NAP	C3N-C7N-N7N	3.11	121.57	117.74
2	E	801	NAP	C5A-N7A-C8A	3.06	108.26	103.45
2	E	801	NAP	C3N-C7N-N7N	3.06	121.51	117.74
2	D	801	NAP	C5A-N7A-C8A	3.03	108.21	103.45
2	F	801	NAP	C5A-C6A-N6A	3.03	130.78	123.29
2	F	801	NAP	C5A-N7A-C8A	3.01	108.18	103.45
3	A	802	ZWP	C4-C3-C2	-2.96	119.32	122.19
2	C	801	NAP	C5A-N7A-C8A	2.85	107.94	103.45
2	A	801	NAP	C2B-C1B-N9A	-2.78	109.17	113.75
3	A	802	ZWP	C15-C16-C21	-2.76	117.92	121.35
2	C	801	NAP	N3A-C4A-N9A	2.76	131.86	127.17
2	C	801	NAP	C4D-O4D-C1D	-2.75	107.40	109.92
2	F	801	NAP	C5B-C4B-C3B	-2.73	105.40	115.21
2	B	801	NAP	C5A-N7A-C8A	2.72	107.72	103.45
2	A	801	NAP	C5A-C4A-N9A	2.70	108.76	105.81
2	A	801	NAP	N3A-C4A-N9A	2.70	131.75	127.17
2	C	801	NAP	C6N-N1N-C2N	-2.65	119.62	121.88
2	E	801	NAP	C4A-N9A-C1B	-2.64	120.45	126.63
2	E	801	NAP	C5B-C4B-C3B	-2.63	105.75	115.21
2	A	801	NAP	C4A-C5A-N7A	-2.63	107.58	110.58
2	D	801	NAP	C6N-N1N-C2N	-2.63	119.64	121.88
2	E	801	NAP	N3A-C4A-N9A	2.62	131.63	127.17
2	C	801	NAP	C5A-C4A-N9A	2.61	108.66	105.81
2	D	801	NAP	C2B-C1B-N9A	-2.59	109.48	113.75
2	C	801	NAP	C4A-C5A-N7A	-2.58	107.63	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	ZWP	C1-C2-C3	2.54	121.48	118.84
2	B	801	NAP	C5A-C6A-N6A	2.52	129.52	123.29
2	B	801	NAP	C4A-N9A-C8A	2.50	108.36	105.74
2	D	801	NAP	C4D-O4D-C1D	-2.47	107.66	109.92
2	E	801	NAP	C4A-C5A-N7A	-2.47	107.76	110.58
2	F	801	NAP	P2B-O2B-C2B	-2.44	116.92	123.43
2	B	801	NAP	C6A-C5A-C4A	2.40	120.46	117.18
2	A	801	NAP	C5D-C4D-C3D	-2.40	106.58	115.21
2	D	801	NAP	C4A-C5A-N7A	-2.38	107.86	110.58
2	E	801	NAP	C4A-N9A-C8A	2.30	108.15	105.74
3	A	802	ZWP	C1-C2-C7	-2.29	129.82	133.73
2	A	801	NAP	C4A-N9A-C1B	-2.26	121.35	126.63
2	B	801	NAP	C4A-N9A-C1B	-2.25	121.36	126.63
2	F	801	NAP	C6A-C5A-C4A	2.23	120.23	117.18
2	C	801	NAP	O7N-C7N-N7N	-2.22	119.41	122.62
2	D	801	NAP	O4B-C1B-N9A	2.20	112.32	108.09
2	F	801	NAP	C4A-N9A-C8A	2.19	108.04	105.74
2	F	801	NAP	C4A-N9A-C1B	-2.18	121.54	126.63
2	C	801	NAP	O4B-C1B-N9A	2.16	112.25	108.09
2	E	801	NAP	C5A-C4A-N9A	2.15	108.15	105.81
2	D	801	NAP	C6A-C5A-C4A	2.13	120.09	117.18
2	F	801	NAP	C3N-C7N-N7N	2.13	120.36	117.74
2	A	801	NAP	C6A-C5A-C4A	2.12	120.07	117.18
2	C	801	NAP	C6A-C5A-C4A	2.12	120.07	117.18
2	E	801	NAP	P2B-O2B-C2B	-2.12	117.78	123.43
2	F	801	NAP	C4A-C5A-N7A	-2.10	108.18	110.58
2	D	801	NAP	C5A-C4A-N9A	2.10	108.10	105.81
2	B	801	NAP	C2N-C3N-C4N	2.10	120.70	118.26
2	A	801	NAP	C5B-C4B-C3B	-2.10	107.66	115.21
2	C	801	NAP	C4A-N9A-C1B	-2.09	121.74	126.63
2	F	801	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
2	B	801	NAP	O7N-C7N-C3N	-2.08	117.06	119.60
2	D	801	NAP	C5D-C4D-C3D	-2.06	107.81	115.21
3	A	802	ZWP	C3-C2-C7	2.05	108.70	106.84
2	C	801	NAP	C3N-C7N-N7N	2.04	120.25	117.74
2	D	801	NAP	C4A-N9A-C1B	-2.03	121.88	126.63

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	801	NAP	O4D-C1D-N1N-C2N
2	D	801	NAP	O4D-C1D-N1N-C2N
3	A	802	ZWP	C8-C10-C13-C14
3	A	802	ZWP	C11-C10-C13-C14
2	A	801	NAP	PA-O3-PN-O2N
2	B	801	NAP	PA-O3-PN-O2N
2	C	801	NAP	PA-O3-PN-O2N
2	D	801	NAP	PA-O3-PN-O2N
2	E	801	NAP	PA-O3-PN-O2N
3	A	802	ZWP	C12-C10-C13-C14
2	F	801	NAP	PA-O3-PN-O2N
2	A	801	NAP	O4D-C1D-N1N-C6N
2	B	801	NAP	O4D-C1D-N1N-C6N
2	D	801	NAP	O4D-C1D-N1N-C6N
2	B	801	NAP	PA-O3-PN-O1N
2	C	801	NAP	PA-O3-PN-O1N
2	D	801	NAP	PA-O3-PN-O1N
2	F	801	NAP	PA-O3-PN-O1N
3	A	802	ZWP	C12-C10-C8-N9
2	E	801	NAP	O4B-C4B-C5B-O5B

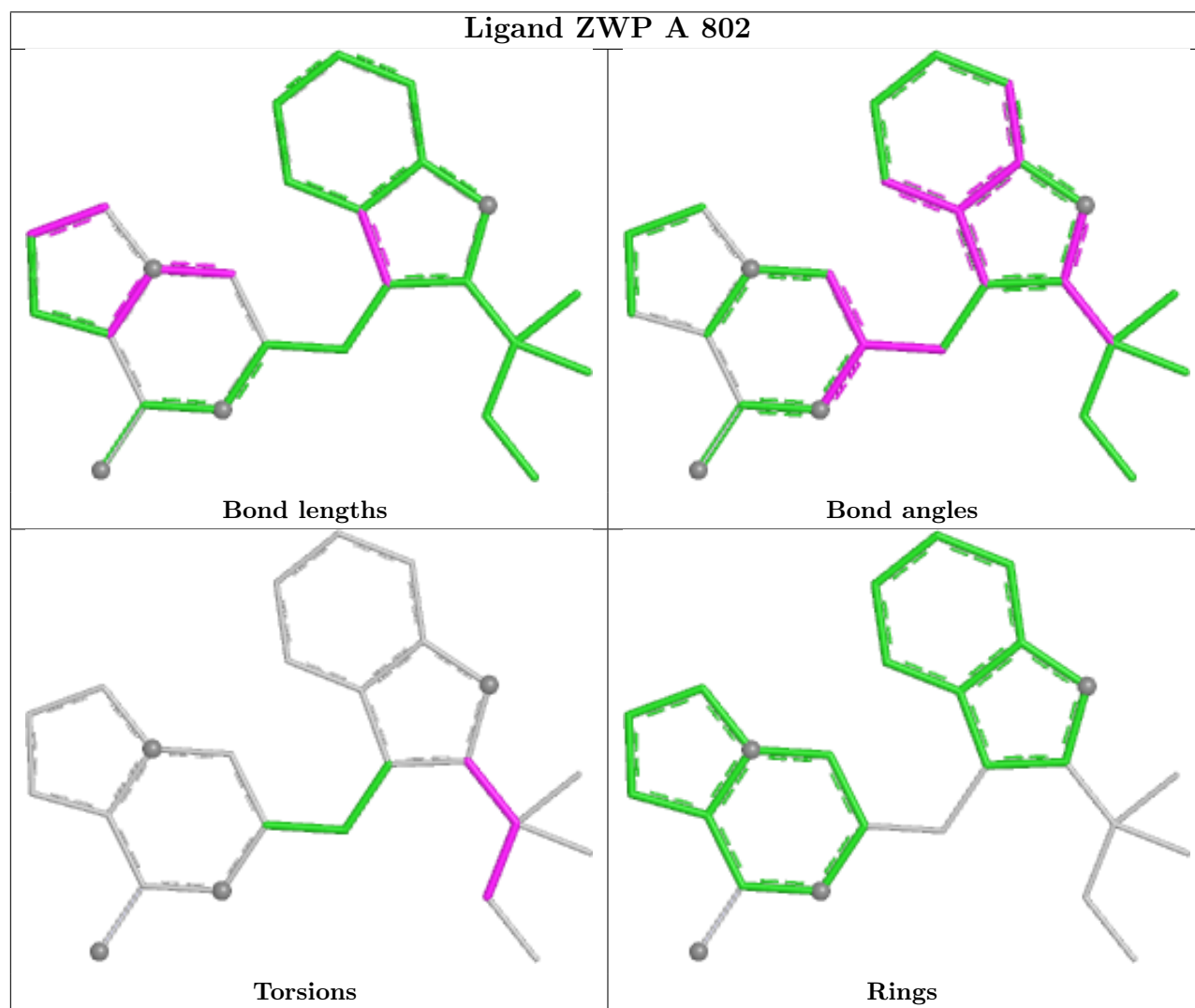
There are no ring outliers.

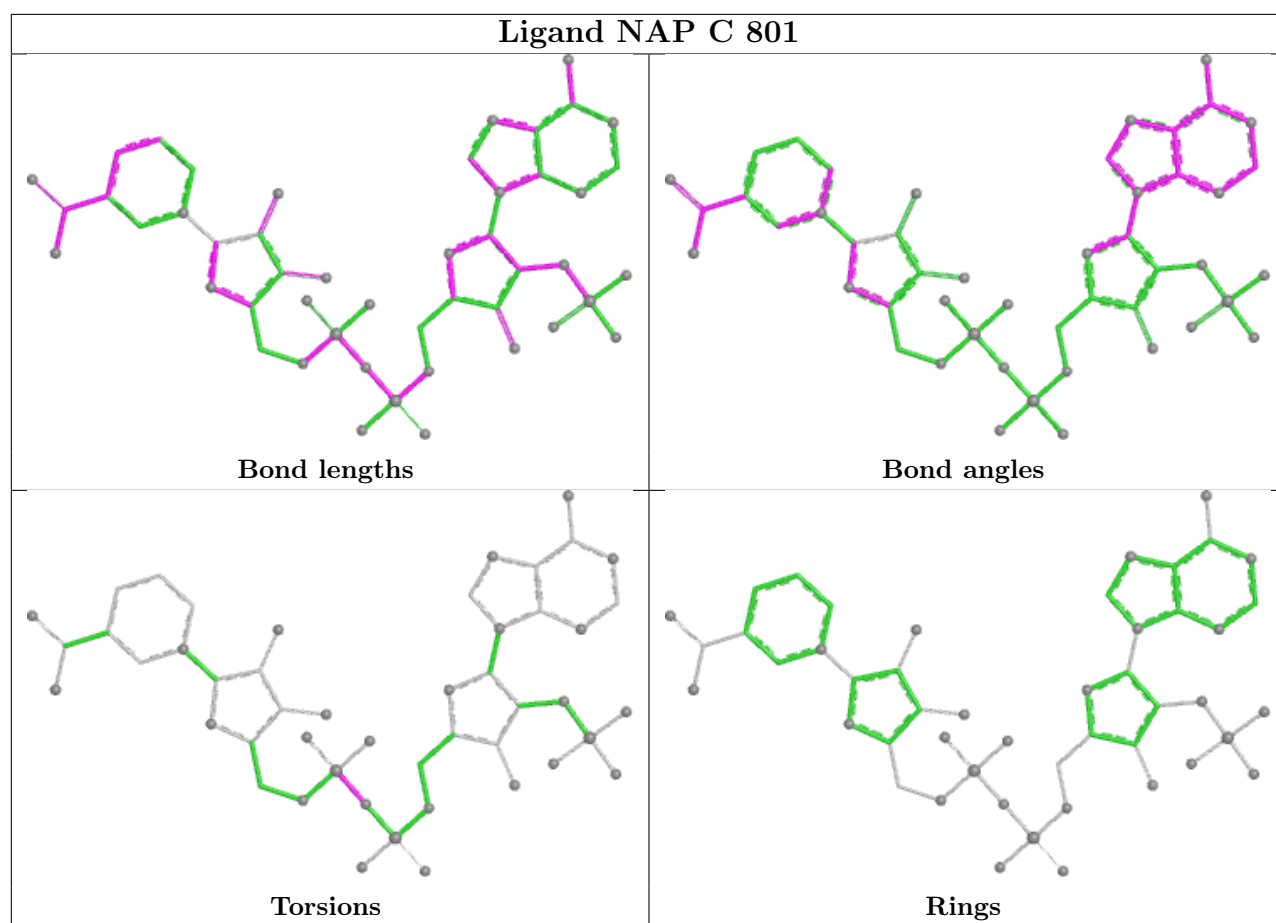
6 monomers are involved in 9 short contacts:

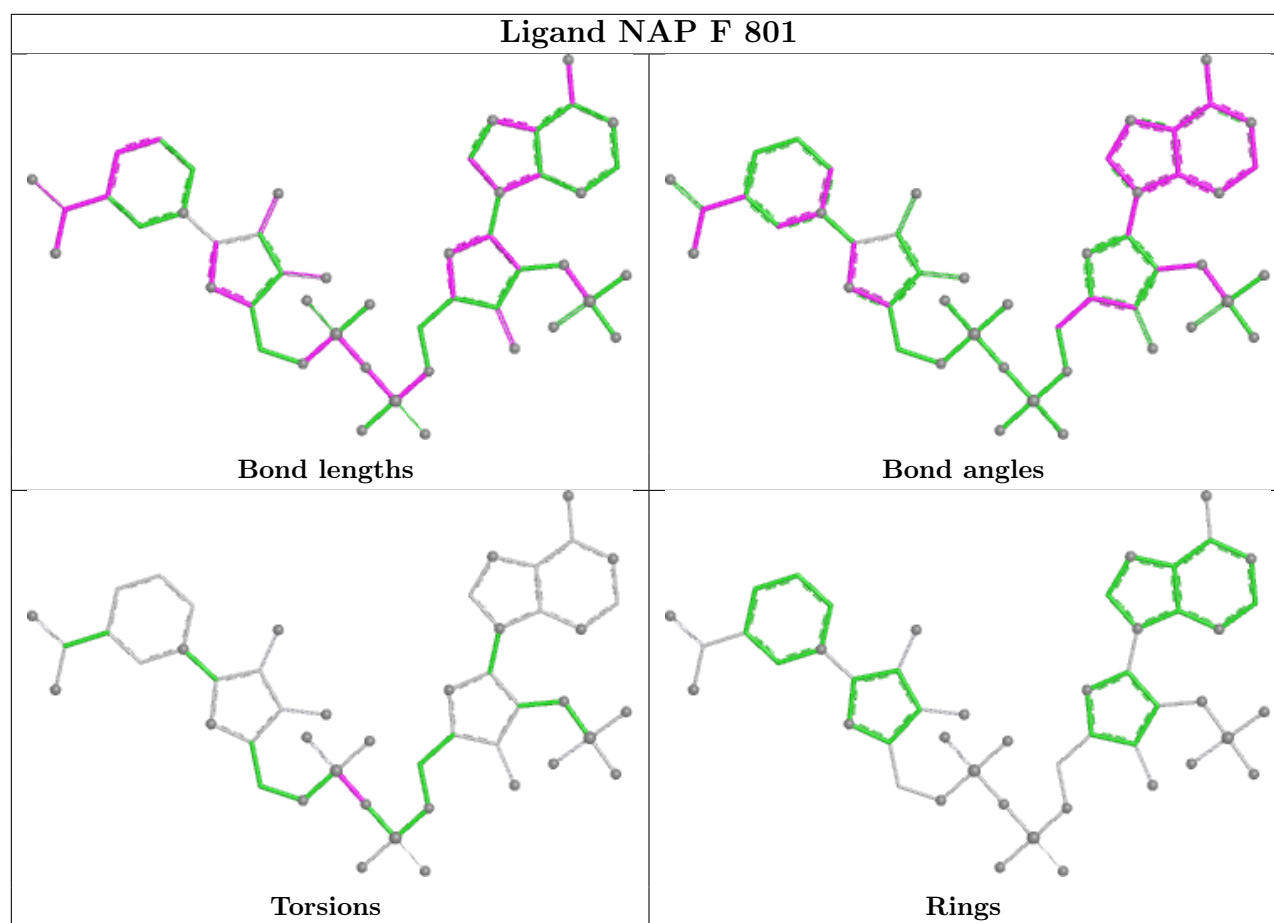
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	NAP	3	0
2	F	801	NAP	1	0
2	D	801	NAP	1	0
2	B	801	NAP	2	0
2	E	801	NAP	1	0
2	A	801	NAP	1	0

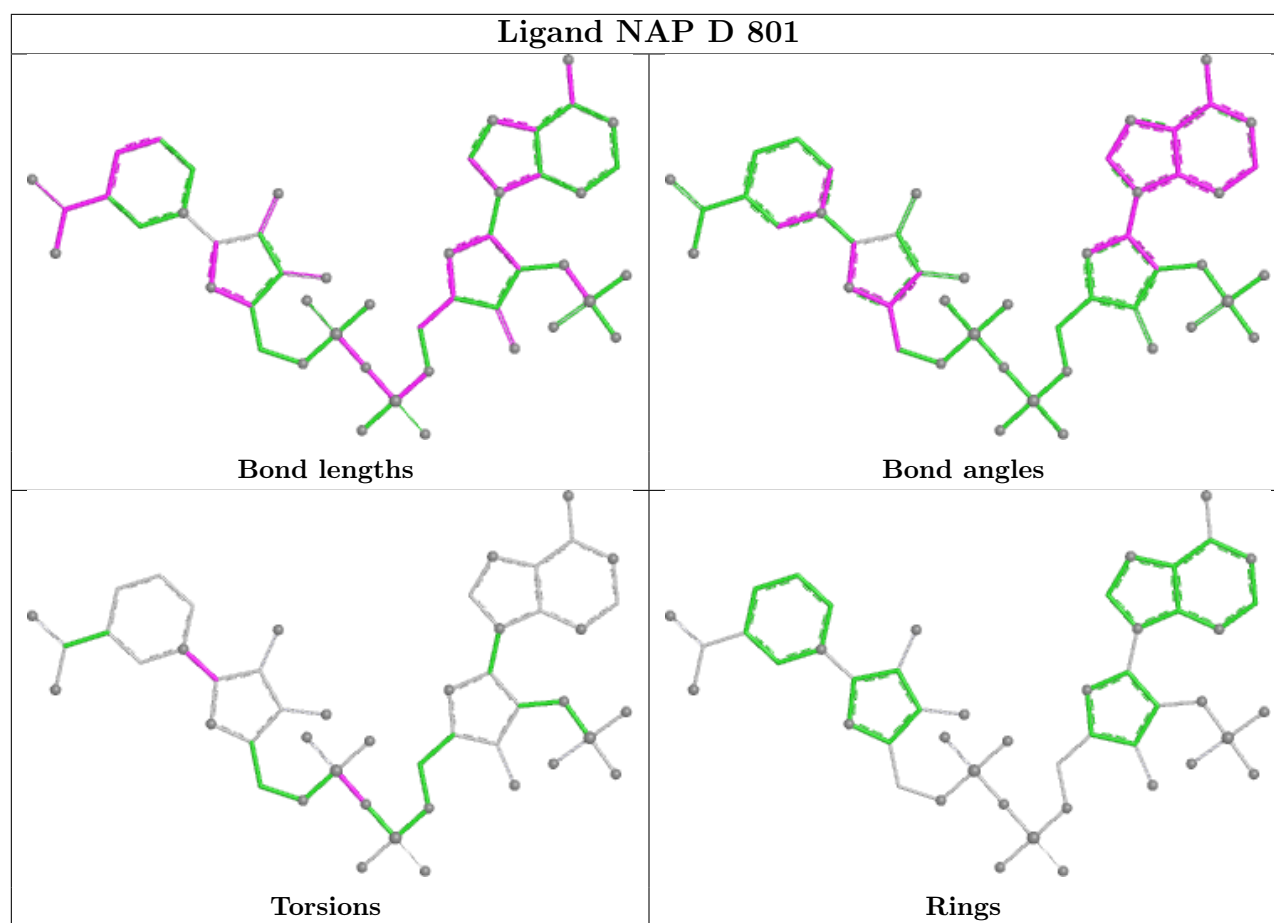
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

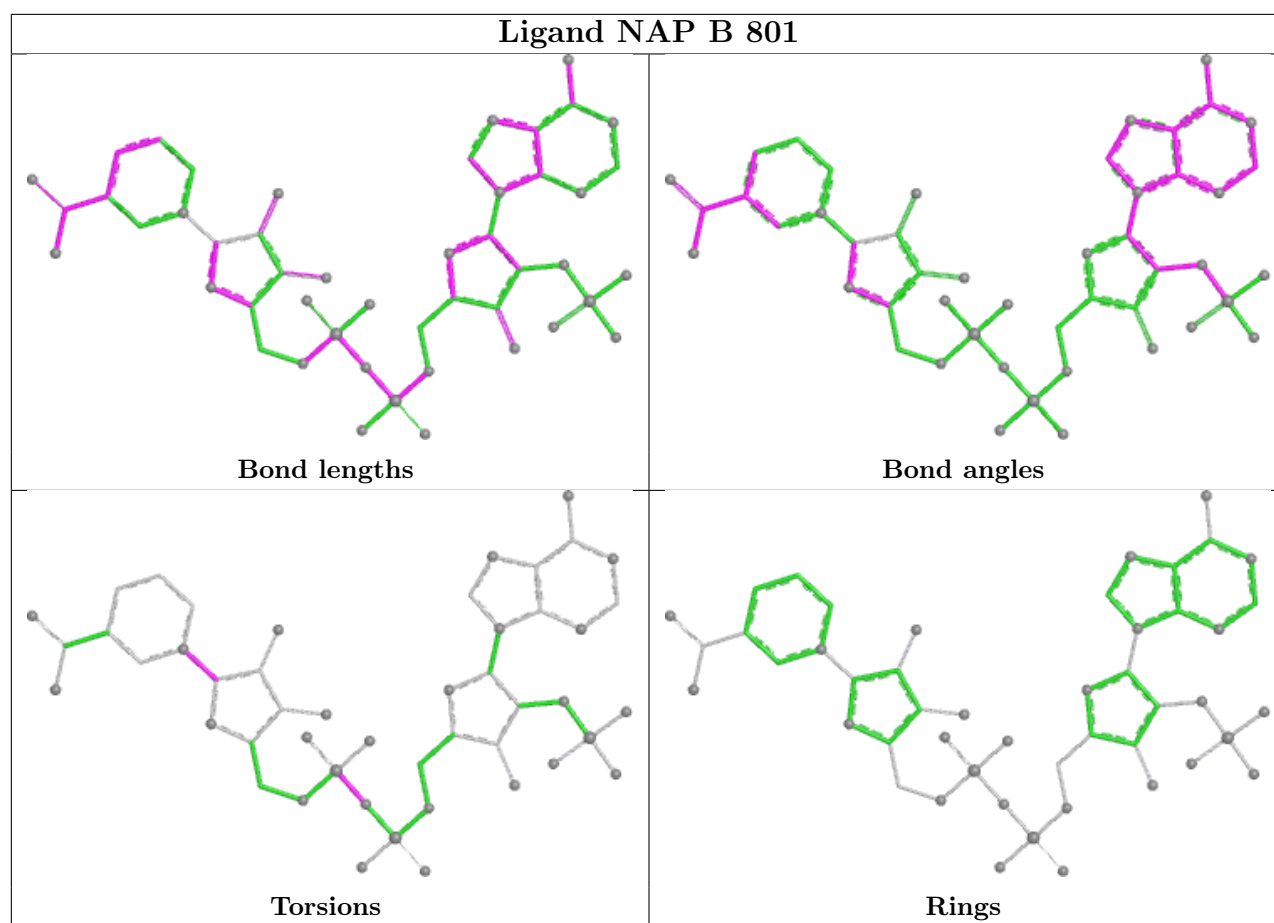
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

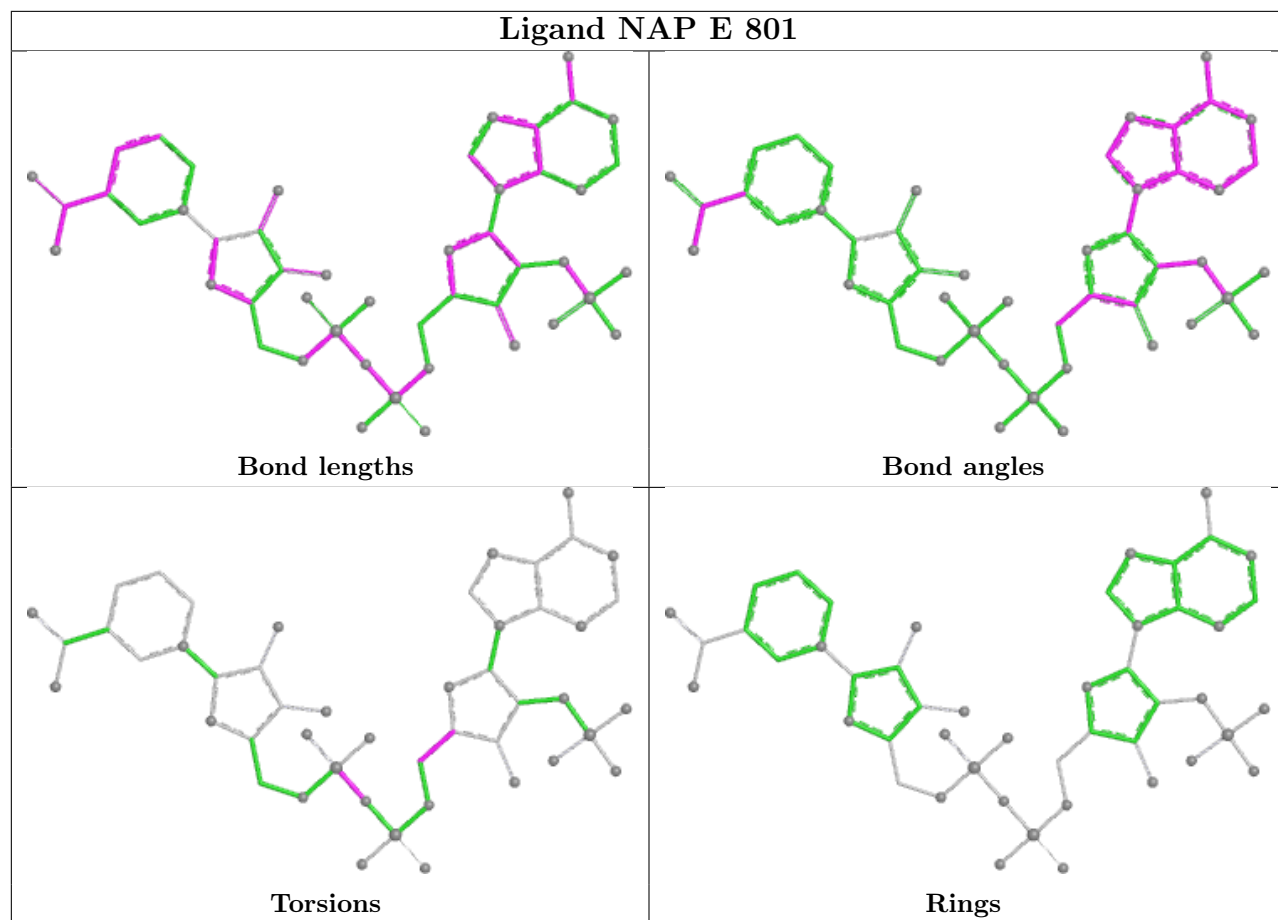


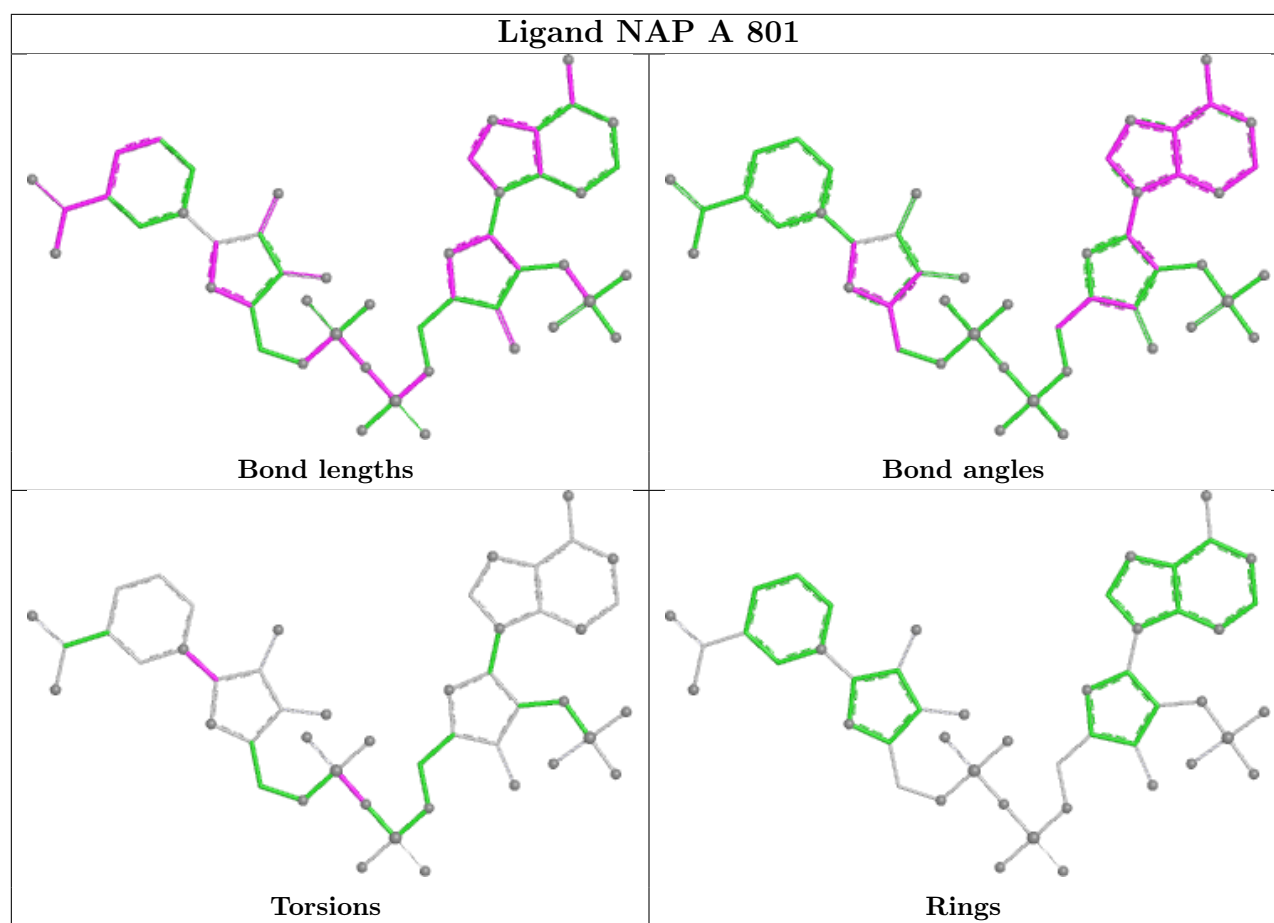












5.7 Other polymers [i](#)

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	257/265 (96%)	1.13	37 (14%) 6 6	34, 49, 73, 132	0
1	B	257/265 (96%)	1.10	42 (16%) 4 4	33, 50, 79, 122	0
1	C	257/265 (96%)	1.52	76 (29%) 1 1	33, 57, 109, 194	0
1	D	257/265 (96%)	1.37	55 (21%) 2 2	34, 55, 100, 133	0
1	E	257/265 (96%)	3.10	203 (78%) 0 0	52, 83, 131, 177	0
1	F	257/265 (96%)	3.82	236 (91%) 0 0	57, 84, 145, 173	0
All	All	1542/1590 (96%)	2.01	649 (42%) 0 0	33, 63, 118, 194	0

All (649) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	263	LEU	10.1
1	E	263	LEU	10.1
1	F	197	VAL	9.2
1	F	223	ALA	9.0
1	B	263	LEU	8.1
1	E	256	VAL	7.9
1	F	116	LEU	7.7
1	F	255	VAL	7.6
1	F	71	VAL	7.5
1	F	121	VAL	7.4
1	F	130	ILE	7.4
1	F	163	LEU	7.3
1	F	182	MET	7.3
1	F	135	PRO	7.2
1	F	129	ILE	7.2
1	E	197	VAL	7.0
1	F	245	LEU	6.9
1	F	133	VAL	6.7
1	E	242	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	F	176	CYS	6.6
1	F	104	VAL	6.6
1	F	265	VAL	6.6
1	F	34	ALA	6.5
1	F	44	VAL	6.5
1	E	163	LEU	6.5
1	F	256	VAL	6.5
1	E	264	LEU	6.4
1	F	158	SER	6.4
1	E	255	VAL	6.4
1	E	70	ILE	6.2
1	E	39	ALA	6.2
1	F	244	TYR	6.2
1	F	12	LEU	6.1
1	F	201	GLY	6.1
1	F	19	VAL	6.1
1	F	124	VAL	6.1
1	E	198	VAL	6.0
1	F	250	TYR	6.0
1	F	203	VAL	6.0
1	F	188	ILE	6.0
1	F	207	ALA	5.9
1	F	131	ARG	5.8
1	E	235	PRO	5.8
1	C	215	ALA	5.8
1	F	190	LEU	5.7
1	F	162	CYS	5.7
1	C	116	LEU	5.7
1	D	62	PHE	5.7
1	F	198	VAL	5.7
1	F	77	LEU	5.7
1	C	216	TYR	5.7
1	F	18	LEU	5.6
1	F	157	THR	5.6
1	E	192	PRO	5.5
1	F	238	VAL	5.5
1	F	160	ALA	5.5
1	F	202	ALA	5.5
1	F	110	MET	5.5
1	E	245	LEU	5.5
1	E	41	VAL	5.5
1	E	28	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	229	VAL	5.4
1	E	31	CYS	5.4
1	F	156	LEU	5.4
1	E	94	ALA	5.4
1	E	32	ALA	5.3
1	F	134	ALA	5.3
1	F	138	VAL	5.2
1	F	179	VAL	5.2
1	F	193	LEU	5.2
1	F	204	LEU	5.2
1	F	262	MET	5.2
1	F	106	THR	5.2
1	C	211	ILE	5.1
1	E	17	VAL	5.1
1	F	208	VAL	5.1
1	E	100	ILE	5.1
1	E	176	CYS	5.1
1	E	257	SER	5.1
1	F	119	LEU	5.1
1	F	229	VAL	5.1
1	F	264	LEU	5.1
1	F	132	LEU	5.0
1	F	136	LEU	5.0
1	F	165	PRO	5.0
1	F	20	ILE	5.0
1	F	169	TRP	5.0
1	F	112	ALA	4.9
1	E	161	HIS	4.9
1	F	39	ALA	4.9
1	F	200	PRO	4.9
1	E	243	ILE	4.9
1	F	254	SER	4.8
1	E	260	GLY	4.8
1	F	215	ALA	4.8
1	E	203	VAL	4.8
1	F	220	VAL	4.8
1	F	235	PRO	4.8
1	E	35	LEU	4.8
1	F	23	THR	4.8
1	F	177	GLY	4.8
1	E	62	PHE	4.8
1	F	199	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	45	GLY	4.8
1	F	128	GLY	4.8
1	F	70	ILE	4.7
1	E	26	ILE	4.7
1	F	26	ILE	4.7
1	E	238	VAL	4.7
1	F	43	ILE	4.7
1	F	103	ILE	4.7
1	E	67	PRO	4.6
1	E	246	MET	4.6
1	F	48	ALA	4.6
1	E	9	THR	4.6
1	F	186	LEU	4.6
1	E	65	THR	4.6
1	F	171	VAL	4.6
1	E	105	ILE	4.6
1	F	172	ILE	4.6
1	E	190	LEU	4.6
1	F	228	THR	4.5
1	C	62	PHE	4.5
1	F	161	HIS	4.5
1	E	14	GLY	4.5
1	F	155	THR	4.5
1	F	183	SER	4.5
1	F	218	ALA	4.5
1	F	35	LEU	4.5
1	E	216	TYR	4.5
1	F	167	PRO	4.5
1	E	187	ALA	4.5
1	F	55	VAL	4.4
1	E	51	LEU	4.4
1	C	264	LEU	4.4
1	E	55	VAL	4.4
1	F	14	GLY	4.4
1	F	168	GLY	4.4
1	F	114	PRO	4.4
1	A	9	THR	4.3
1	E	225	ALA	4.3
1	F	219	ALA	4.3
1	E	265	VAL	4.2
1	F	222	MET	4.2
1	D	216	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	80	SER	4.2
1	F	107	ALA	4.2
1	F	181	ALA	4.2
1	E	12	LEU	4.2
1	F	142	LEU	4.2
1	E	188	ILE	4.2
1	E	27	GLY	4.2
1	F	28	PHE	4.2
1	F	21	GLY	4.2
1	F	137	MET	4.2
1	F	143	PRO	4.2
1	C	212	LEU	4.2
1	E	18	LEU	4.2
1	C	14	GLY	4.1
1	C	204	LEU	4.1
1	E	34	ALA	4.1
1	E	95	ALA	4.1
1	E	251	ALA	4.1
1	E	200	PRO	4.1
1	E	11	GLN	4.1
1	F	149	CYS	4.1
1	E	19	VAL	4.0
1	F	83	VAL	4.0
1	F	178	ALA	4.0
1	C	55	VAL	4.0
1	E	199	ALA	4.0
1	E	239	ALA	4.0
1	E	104	VAL	4.0
1	F	108	ALA	4.0
1	F	123	SER	4.0
1	E	29	ALA	4.0
1	F	29	ALA	4.0
1	C	265	VAL	4.0
1	E	30	VAL	4.0
1	E	40	ILE	4.0
1	F	243	ILE	4.0
1	E	250	TYR	3.9
1	F	216	TYR	3.9
1	E	93	LEU	3.9
1	F	100	ILE	3.9
1	F	257	SER	3.9
1	B	67	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	67	PRO	3.9
1	F	32	ALA	3.9
1	E	96	GLY	3.9
1	E	71	VAL	3.9
1	F	17	VAL	3.9
1	F	30	VAL	3.9
1	C	52	LYS	3.9
1	C	217	ASP	3.9
1	E	64	SER	3.9
1	E	158	SER	3.9
1	E	202	ALA	3.9
1	E	241	ALA	3.9
1	F	73	VAL	3.9
1	E	262	MET	3.9
1	F	212	LEU	3.8
1	E	33	ALA	3.8
1	E	230	GLY	3.8
1	D	211	ILE	3.8
1	E	73	VAL	3.8
1	C	15	SER	3.8
1	C	12	LEU	3.8
1	E	58	LEU	3.8
1	C	213	GLY	3.8
1	E	228	THR	3.8
1	F	251	ALA	3.8
1	E	103	ILE	3.8
1	F	180	GLU	3.8
1	F	51	LEU	3.8
1	F	65	THR	3.8
1	E	180	GLU	3.8
1	E	227	SER	3.8
1	E	193	LEU	3.7
1	C	56	ALA	3.7
1	F	33	ALA	3.7
1	F	72	ALA	3.7
1	E	254	SER	3.7
1	F	126	ARG	3.7
1	F	211	ILE	3.7
1	E	165	PRO	3.7
1	C	120	THR	3.7
1	E	37	HIS	3.7
1	E	258	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	9	THR	3.7
1	F	91	LEU	3.7
1	F	184	ARG	3.7
1	E	219	ALA	3.7
1	D	109	ASP	3.7
1	F	196	ASN	3.7
1	E	91	LEU	3.6
1	E	181	ALA	3.6
1	F	109	ASP	3.6
1	B	70	ILE	3.6
1	F	41	VAL	3.6
1	F	195	VAL	3.6
1	F	120	THR	3.6
1	F	78	SER	3.6
1	C	58	LEU	3.6
1	E	90	ALA	3.6
1	E	244	TYR	3.6
1	E	201	GLY	3.6
1	B	211	ILE	3.6
1	E	232	THR	3.6
1	F	221	GLU	3.6
1	F	159	GLY	3.6
1	F	105	ILE	3.6
1	E	13	HIS	3.6
1	E	233	GLY	3.5
1	E	43	ILE	3.5
1	D	55	VAL	3.5
1	B	97	ASN	3.5
1	B	119	LEU	3.5
1	F	96	GLY	3.5
1	D	110	MET	3.5
1	E	152	SER	3.5
1	E	252	SER	3.5
1	F	187	ALA	3.5
1	E	56	ALA	3.5
1	E	160	ALA	3.5
1	F	81	ASP	3.5
1	F	122	ASP	3.5
1	E	106	THR	3.4
1	A	43	ILE	3.4
1	E	177	GLY	3.4
1	F	67	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	205	THR	3.4
1	E	226	LYS	3.4
1	A	55	VAL	3.4
1	E	223	ALA	3.4
1	E	156	LEU	3.4
1	F	146	MET	3.4
1	E	220	VAL	3.4
1	C	169	TRP	3.4
1	D	169	TRP	3.4
1	E	112	ALA	3.4
1	B	9	THR	3.4
1	E	155	THR	3.4
1	F	175	TYR	3.3
1	B	14	GLY	3.3
1	F	153	SER	3.3
1	D	218	ALA	3.3
1	E	204	LEU	3.3
1	E	102	HIS	3.3
1	C	214	ASP	3.3
1	F	15	SER	3.3
1	F	87	ILE	3.3
1	E	208	VAL	3.3
1	E	22	GLY	3.3
1	D	70	ILE	3.3
1	E	222	MET	3.3
1	C	90	ALA	3.3
1	C	220	VAL	3.3
1	F	62	PHE	3.3
1	D	166	ASN	3.3
1	E	168	GLY	3.3
1	E	149	CYS	3.3
1	E	162	CYS	3.3
1	E	207	ALA	3.2
1	E	164	ARG	3.2
1	F	154	LEU	3.2
1	E	211	ILE	3.2
1	F	94	ALA	3.2
1	D	265	VAL	3.2
1	F	111	THR	3.2
1	E	261	GLY	3.2
1	E	20	ILE	3.2
1	E	111	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	110	MET	3.2
1	C	168	GLY	3.2
1	F	185	GLY	3.2
1	E	157	THR	3.1
1	F	145	TYR	3.1
1	A	51	LEU	3.1
1	E	10	ASP	3.1
1	F	97	ASN	3.1
1	E	175	TYR	3.1
1	D	214	ASP	3.1
1	D	64	SER	3.1
1	E	218	ALA	3.1
1	E	237	SER	3.1
1	C	43	ILE	3.1
1	F	117	GLU	3.1
1	C	93	LEU	3.1
1	D	116	LEU	3.1
1	F	227	SER	3.1
1	E	63	PRO	3.1
1	C	11	GLN	3.0
1	F	242	TYR	3.0
1	F	259	ASN	3.0
1	E	60	SER	3.0
1	A	176	CYS	3.0
1	E	150	PRO	3.0
1	F	113	PRO	3.0
1	D	56	ALA	3.0
1	E	142	LEU	3.0
1	E	101	ASN	3.0
1	E	196	ASN	3.0
1	A	265	VAL	3.0
1	C	221	GLU	3.0
1	C	236	GLU	3.0
1	D	167	PRO	3.0
1	E	38	GLY	3.0
1	F	230	GLY	3.0
1	A	71	VAL	3.0
1	B	13	HIS	3.0
1	E	15	SER	3.0
1	C	167	PRO	3.0
1	B	265	VAL	2.9
1	E	24	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	234	SER	2.9
1	C	9	THR	2.9
1	E	131	ARG	2.9
1	F	42	THR	2.9
1	F	82	THR	2.9
1	E	97	ASN	2.9
1	E	259	ASN	2.9
1	B	215	ALA	2.9
1	D	207	ALA	2.9
1	D	223	ALA	2.9
1	F	141	HIS	2.9
1	E	98	SER	2.9
1	E	148	LYS	2.9
1	F	22	GLY	2.9
1	D	215	ALA	2.9
1	A	161	HIS	2.9
1	F	40	ILE	2.9
1	C	35	LEU	2.9
1	E	159	GLY	2.9
1	F	139	ALA	2.9
1	E	61	SER	2.9
1	F	64	SER	2.9
1	D	82	THR	2.8
1	F	166	ASN	2.8
1	E	249	HIS	2.8
1	E	48	ALA	2.8
1	B	169	TRP	2.8
1	C	119	LEU	2.8
1	E	186	LEU	2.8
1	F	27	GLY	2.8
1	F	261	GLY	2.8
1	F	13	HIS	2.8
1	F	115	PRO	2.8
1	F	118	ASP	2.8
1	A	54	SER	2.8
1	E	110	MET	2.8
1	E	240	GLN	2.8
1	F	174	GLY	2.8
1	F	56	ALA	2.8
1	F	225	ALA	2.8
1	F	75	CYS	2.8
1	F	125	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	168	GLY	2.8
1	B	116	LEU	2.8
1	D	204	LEU	2.8
1	A	81	ASP	2.8
1	D	217	ASP	2.8
1	E	69	ASP	2.8
1	F	214	ASP	2.8
1	B	98	SER	2.7
1	B	158	SER	2.7
1	C	218	ALA	2.7
1	D	112	ALA	2.7
1	E	72	ALA	2.7
1	A	13	HIS	2.7
1	E	253	GLY	2.7
1	C	232	THR	2.7
1	D	9	THR	2.7
1	F	189	ASP	2.7
1	F	49	GLN	2.7
1	E	215	ALA	2.7
1	D	65	THR	2.7
1	F	170	THR	2.7
1	D	113	PRO	2.7
1	E	54	SER	2.7
1	E	126	ARG	2.7
1	F	226	LYS	2.7
1	E	109	ASP	2.7
1	C	82	THR	2.7
1	F	98	SER	2.7
1	E	87	ILE	2.7
1	E	147	ASN	2.7
1	C	219	ALA	2.6
1	C	223	ALA	2.6
1	F	253	GLY	2.6
1	A	110	MET	2.6
1	A	169	TRP	2.6
1	F	31	CYS	2.6
1	E	23	THR	2.6
1	D	63	PRO	2.6
1	D	51	LEU	2.6
1	E	154	LEU	2.6
1	A	109	ASP	2.6
1	C	32	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	107	ALA	2.6
1	A	216	TYR	2.6
1	C	65	THR	2.6
1	F	234	SER	2.6
1	F	63	PRO	2.6
1	D	142	LEU	2.6
1	A	14	GLY	2.6
1	C	109	ASP	2.6
1	F	36	GLY	2.6
1	D	71	VAL	2.6
1	F	90	ALA	2.6
1	B	82	THR	2.6
1	F	54	SER	2.6
1	F	79	ASN	2.6
1	F	164	ARG	2.6
1	E	36	GLY	2.6
1	F	50	LYS	2.6
1	B	112	ALA	2.6
1	E	124	VAL	2.6
1	E	179	VAL	2.6
1	F	61	SER	2.6
1	E	42	THR	2.6
1	F	224	GLU	2.5
1	B	81	ASP	2.5
1	E	21	GLY	2.5
1	F	148	LYS	2.5
1	F	213	GLY	2.5
1	F	260	GLY	2.5
1	E	108	ALA	2.5
1	F	241	ALA	2.5
1	D	208	VAL	2.5
1	F	68	ASP	2.5
1	E	172	ILE	2.5
1	C	30	VAL	2.5
1	C	206	GLU	2.5
1	E	236	GLU	2.5
1	C	10	ASP	2.5
1	C	79	ASN	2.5
1	F	236	GLU	2.5
1	A	146	MET	2.5
1	B	238	VAL	2.5
1	E	44	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	195	VAL	2.5
1	F	89	LYS	2.5
1	F	16	ARG	2.4
1	E	166	ASN	2.4
1	F	58	LEU	2.4
1	D	125	GLN	2.4
1	F	11	GLN	2.4
1	C	207	ALA	2.4
1	F	232	THR	2.4
1	C	81	ASP	2.4
1	F	69	ASP	2.4
1	A	133	VAL	2.4
1	D	67	PRO	2.4
1	E	135	PRO	2.4
1	F	127	PRO	2.4
1	B	96	GLY	2.4
1	E	185	GLY	2.4
1	C	80	SER	2.4
1	C	222	MET	2.4
1	C	70	ILE	2.4
1	C	126	ARG	2.4
1	F	194	ARG	2.4
1	D	73	VAL	2.4
1	E	83	VAL	2.4
1	D	151	GLN	2.4
1	E	85	GLN	2.4
1	F	240	GLN	2.4
1	F	25	GLY	2.4
1	E	146	MET	2.4
1	A	64	SER	2.4
1	F	209	LYS	2.4
1	F	147	ASN	2.4
1	C	13	HIS	2.4
1	C	41	VAL	2.4
1	F	24	SER	2.4
1	F	237	SER	2.4
1	E	99	LYS	2.4
1	E	184	ARG	2.3
1	E	212	LEU	2.3
1	F	102	HIS	2.3
1	F	249	HIS	2.3
1	E	182	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	17	VAL	2.3
1	D	124	VAL	2.3
1	A	11	GLN	2.3
1	A	77	LEU	2.3
1	D	119	LEU	2.3
1	A	97	ASN	2.3
1	D	147	ASN	2.3
1	A	87	ILE	2.3
1	C	262	MET	2.3
1	D	188	ILE	2.3
1	F	192	PRO	2.3
1	C	25	GLY	2.3
1	D	38	GLY	2.3
1	F	233	GLY	2.3
1	B	210	ASP	2.3
1	C	238	VAL	2.3
1	E	248	ASP	2.3
1	F	86	ASP	2.3
1	F	206	GLU	2.3
1	E	205	THR	2.3
1	A	226	LYS	2.3
1	C	28	PHE	2.3
1	A	223	ALA	2.3
1	B	134	ALA	2.3
1	F	150	PRO	2.3
1	A	15	SER	2.3
1	F	252	SER	2.3
1	F	217	ASP	2.3
1	F	47	ASN	2.3
1	B	93	LEU	2.3
1	C	111	THR	2.3
1	F	59	LYS	2.3
1	B	202	ALA	2.2
1	C	112	ALA	2.2
1	E	153	SER	2.2
1	A	79	ASN	2.2
1	D	97	ASN	2.2
1	C	75	CYS	2.2
1	E	57	ARG	2.2
1	D	93	LEU	2.2
1	D	212	LEU	2.2
1	E	77	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	218	ALA	2.2
1	C	94	ALA	2.2
1	E	217	ASP	2.2
1	B	166	ASN	2.2
1	D	75	CYS	2.2
1	F	60	SER	2.2
1	B	216	TYR	2.2
1	B	161	HIS	2.2
1	F	140	LYS	2.2
1	C	121	VAL	2.2
1	E	125	GLN	2.2
1	E	75	CYS	2.2
1	F	46	SER	2.2
1	B	213	GLY	2.2
1	B	167	PRO	2.2
1	C	113	PRO	2.2
1	A	70	ILE	2.1
1	C	188	ILE	2.1
1	D	129	ILE	2.1
1	B	23	THR	2.1
1	B	208	VAL	2.1
1	E	171	VAL	2.1
1	C	237	SER	2.1
1	D	14	GLY	2.1
1	A	75	CYS	2.1
1	B	165	PRO	2.1
1	C	63	PRO	2.1
1	E	116	LEU	2.1
1	B	147	ASN	2.1
1	C	97	ASN	2.1
1	A	62	PHE	2.1
1	E	49	GLN	2.1
1	F	231	GLN	2.1
1	D	210	ASP	2.1
1	E	68	ASP	2.1
1	E	76	ASP	2.1
1	C	46	SER	2.1
1	D	121	VAL	2.1
1	E	50	LYS	2.1
1	D	236	GLU	2.1
1	F	84	GLU	2.1
1	A	150	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	93	LEU	2.1
1	F	10	ASP	2.1
1	E	183	SER	2.1
1	A	82	THR	2.1
1	E	170	THR	2.1
1	E	224	GLU	2.1
1	F	52	LYS	2.1
1	E	25	GLY	2.1
1	E	169	TRP	2.1
1	F	37	HIS	2.1
1	C	44	VAL	2.1
1	C	124	VAL	2.1
1	C	229	VAL	2.1
1	E	167	PRO	2.1
1	A	95	ALA	2.1
1	B	223	ALA	2.1
1	C	39	ALA	2.1
1	D	40	ILE	2.0
1	E	221	GLU	2.0
1	F	99	LYS	2.0
1	C	110	MET	2.0
1	D	120	THR	2.0
1	A	147	ASN	2.0
1	B	79	ASN	2.0
1	B	63	PRO	2.0
1	B	149	CYS	2.0
1	B	204	LEU	2.0
1	E	136	LEU	2.0
1	B	33	ALA	2.0
1	C	72	ALA	2.0
1	E	134	ALA	2.0
1	B	214	ASP	2.0
1	E	66	ASP	2.0
1	E	74	ARG	2.0
1	D	221	GLU	2.0
1	D	158	SER	2.0
1	E	78	SER	2.0
1	A	188	ILE	2.0
1	D	100	ILE	2.0
1	A	111	THR	2.0
1	F	258	THR	2.0
1	A	121	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](#)

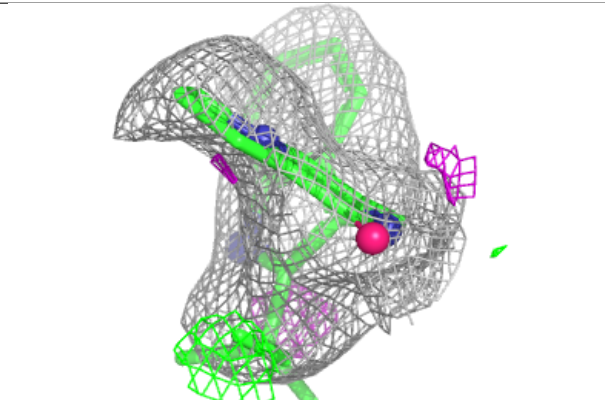
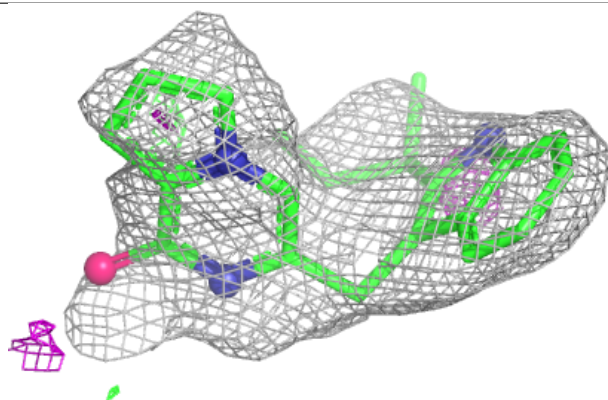
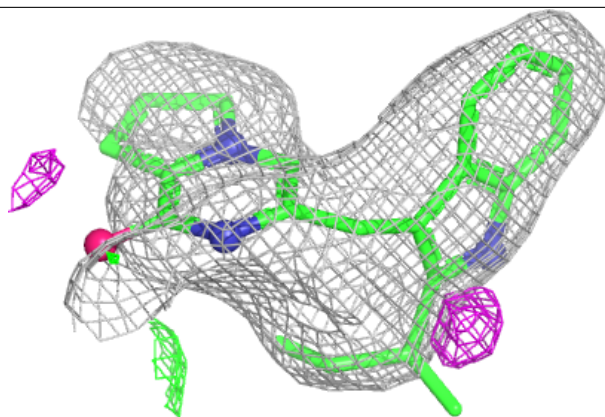
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZWP	A	802	25/25	0.75	0.21	65,76,80,82	0
2	NAP	F	801	48/48	0.78	0.16	55,71,80,83	0
2	NAP	E	801	48/48	0.85	0.14	63,76,85,89	0
2	NAP	B	801	48/48	0.93	0.10	44,51,67,90	0
2	NAP	C	801	48/48	0.93	0.09	48,54,63,68	0
2	NAP	D	801	48/48	0.93	0.09	47,53,60,62	0
2	NAP	A	801	48/48	0.94	0.09	37,46,51,58	0

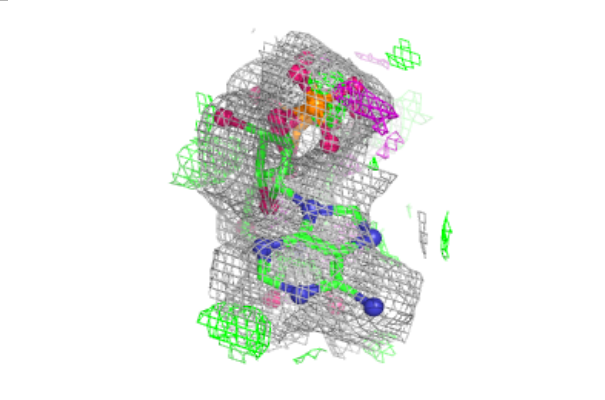
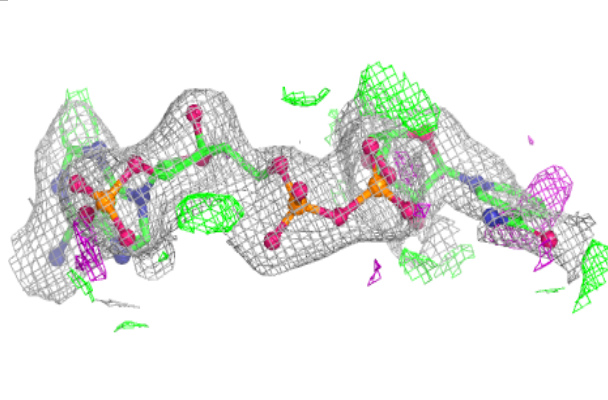
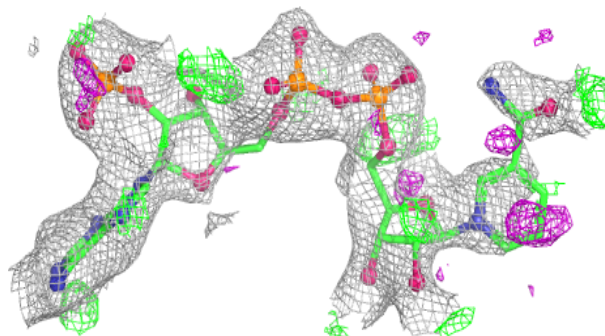
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZWP 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)

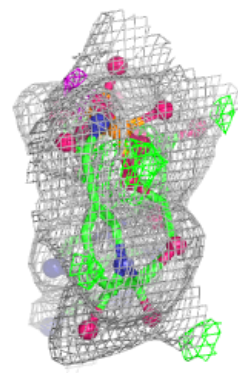
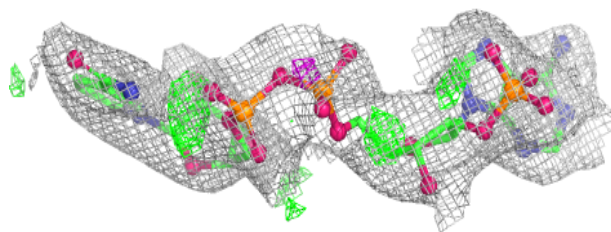
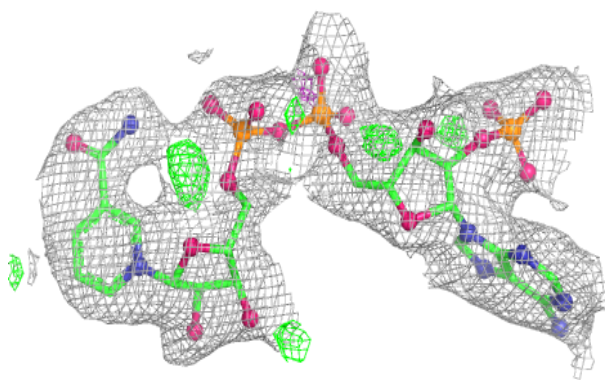
**Electron density around NAP F 801:**

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

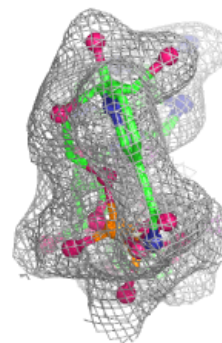
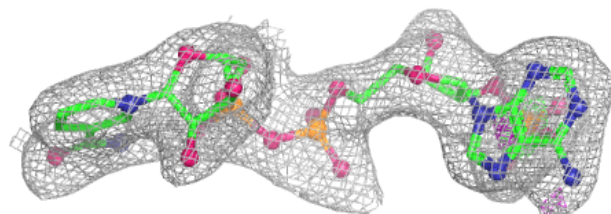
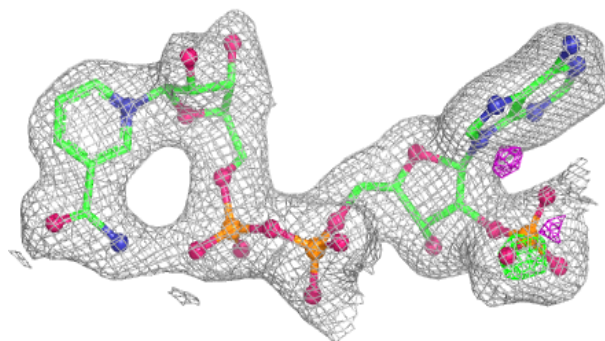


Electron density around NAP E 801:

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

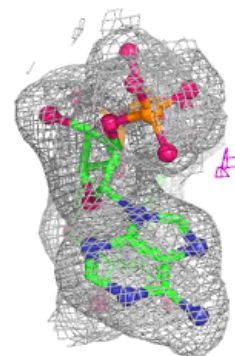
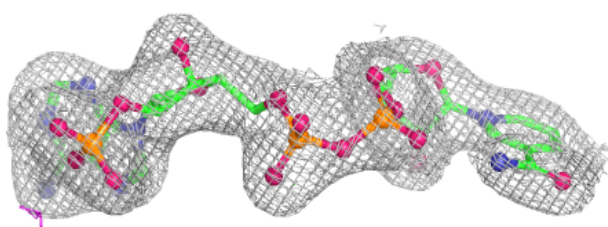
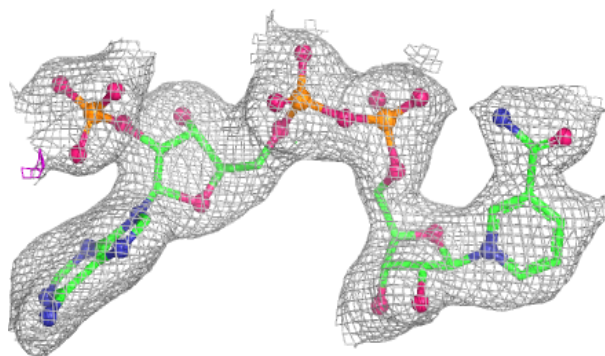
**Electron density around NAP B 801:**

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

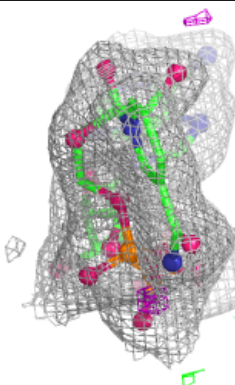
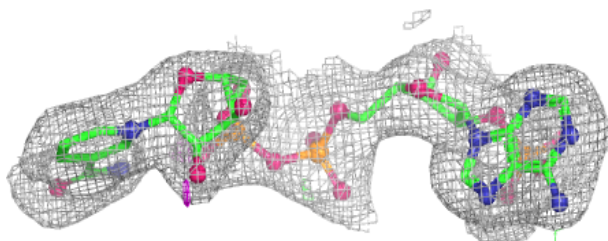
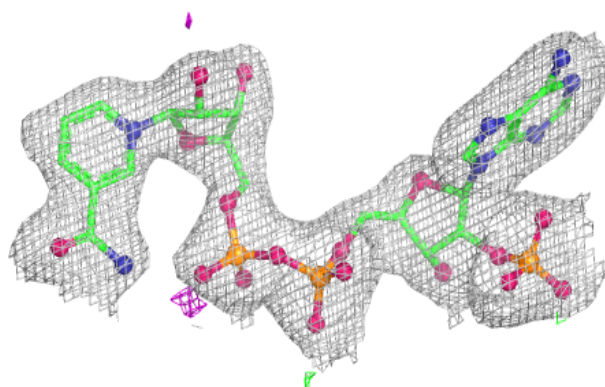


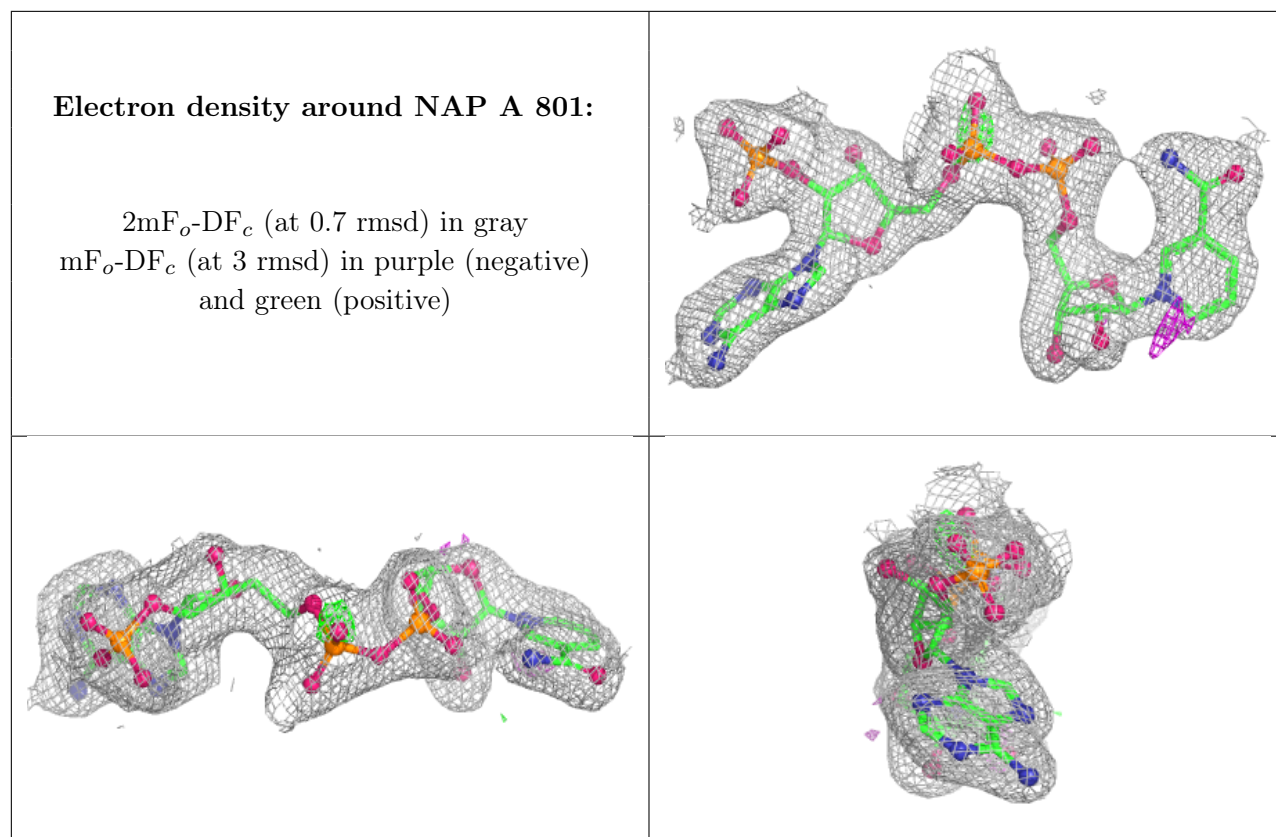
Electron density around NAP C 801:

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

**Electron density around NAP D 801:**

$2mF_o-DF_c$ (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.