



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:38 PM BST

PDB ID : 6NKM
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

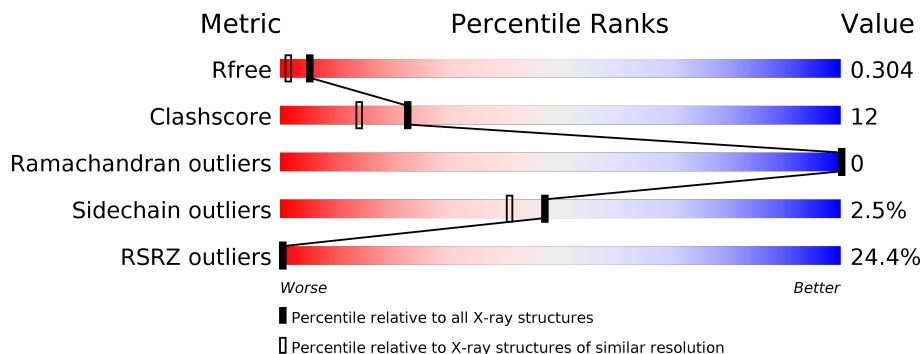
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	
1	B	265	
1	C	265	
1	D	265	
1	E	265	
1	F	265	

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.

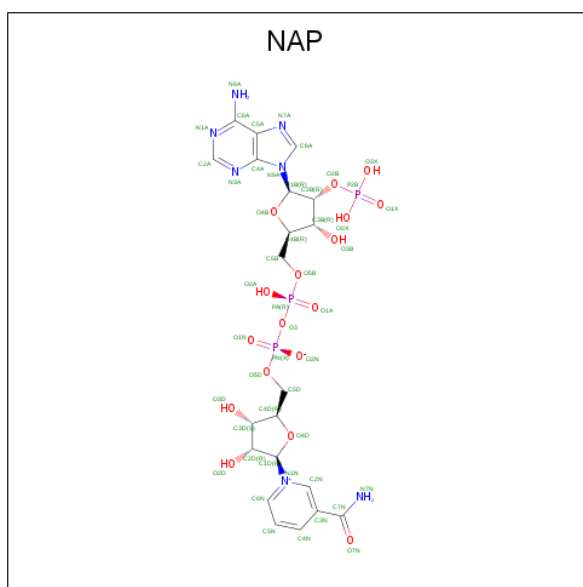
- Molecule 1 is a protein called Short chain dehydrogenase.

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

There are 6 discrepancies between the modelled and reference sequences:

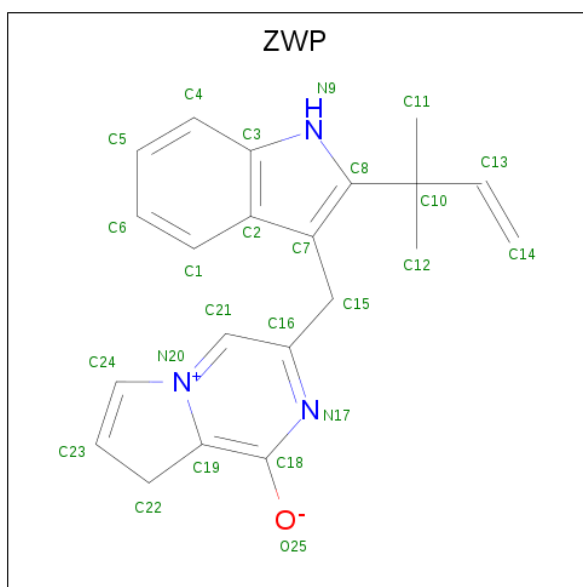
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ASN	ASP	conflict	UNP L0E2Z4
B	166	ASN	ASP	conflict	UNP L0E2Z4
C	166	ASN	ASP	conflict	UNP L0E2Z4
D	166	ASN	ASP	conflict	UNP L0E2Z4
E	166	ASN	ASP	conflict	UNP L0E2Z4
F	166	ASN	ASP	conflict	UNP L0E2Z4

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 48	21	7	17	3	0	0
2	B	1	Total 48	21	7	17	3	0	0
2	C	1	Total 48	21	7	17	3	0	0
2	D	1	Total 48	21	7	17	3	0	0
2	E	1	Total 48	21	7	17	3	0	0
2	F	1	Total 48	21	7	17	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 (three-letter code: ZWP) (formula: C₂₁H₂₁N₃O) (labeled as "Ligand of Interest" by author).



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

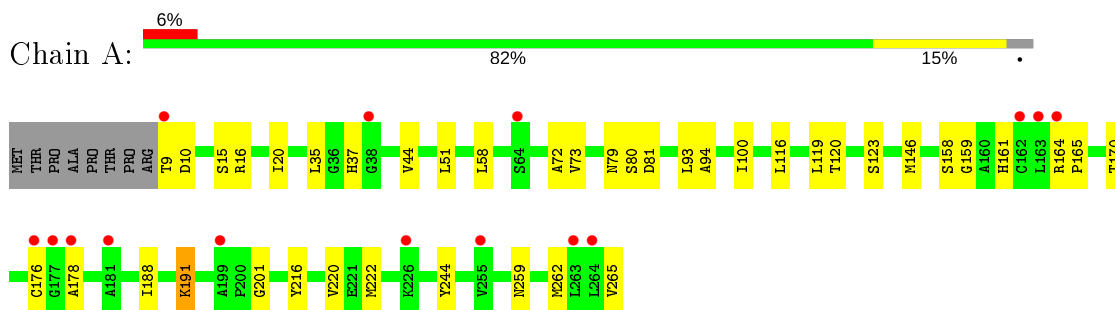
- Molecule 4 is water.

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		

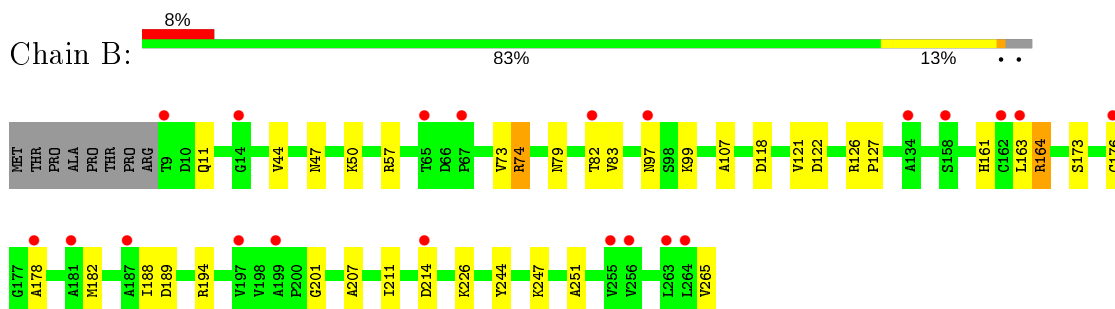
3 Residue-property plots [i](#)

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.

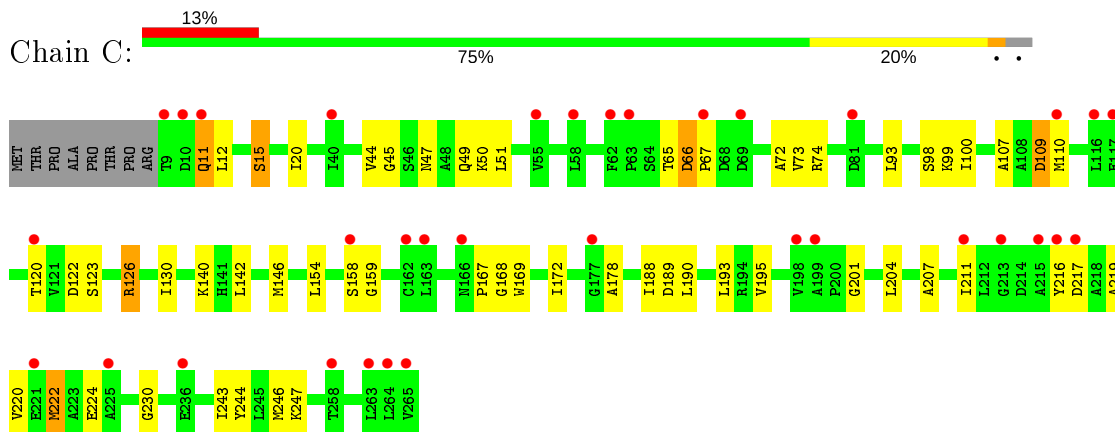
- Molecule 1: Short chain dehydrogenase



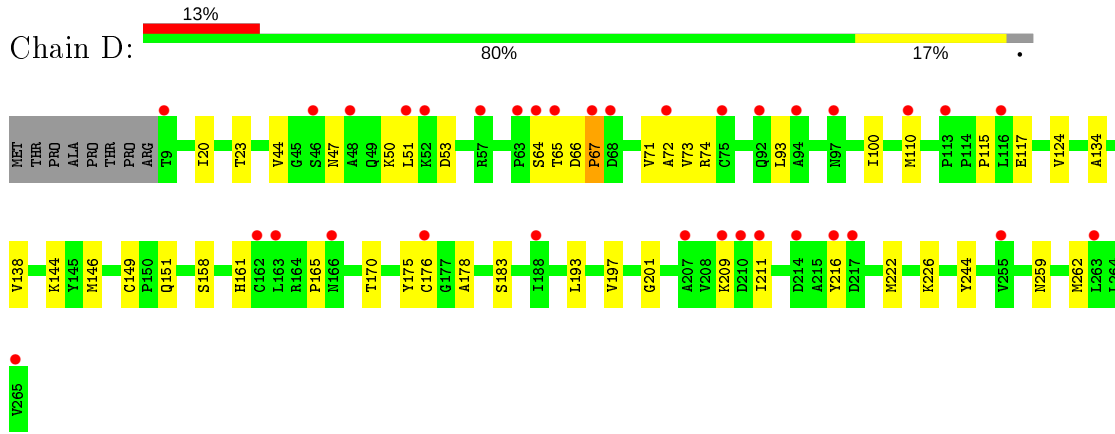
- Molecule 1: Short chain dehydrogenase



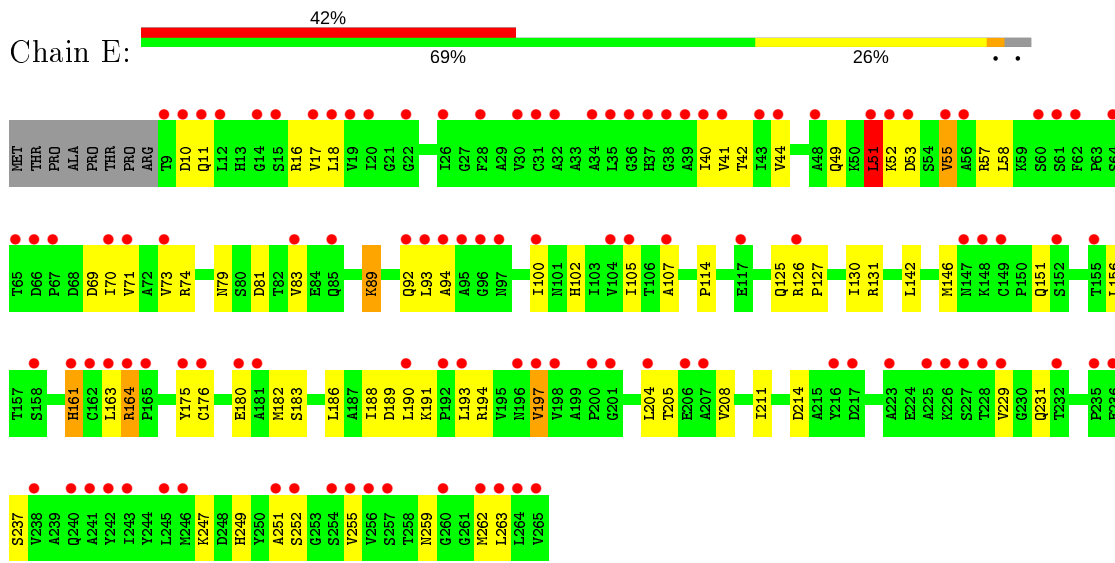
- Molecule 1: Short chain dehydrogenase



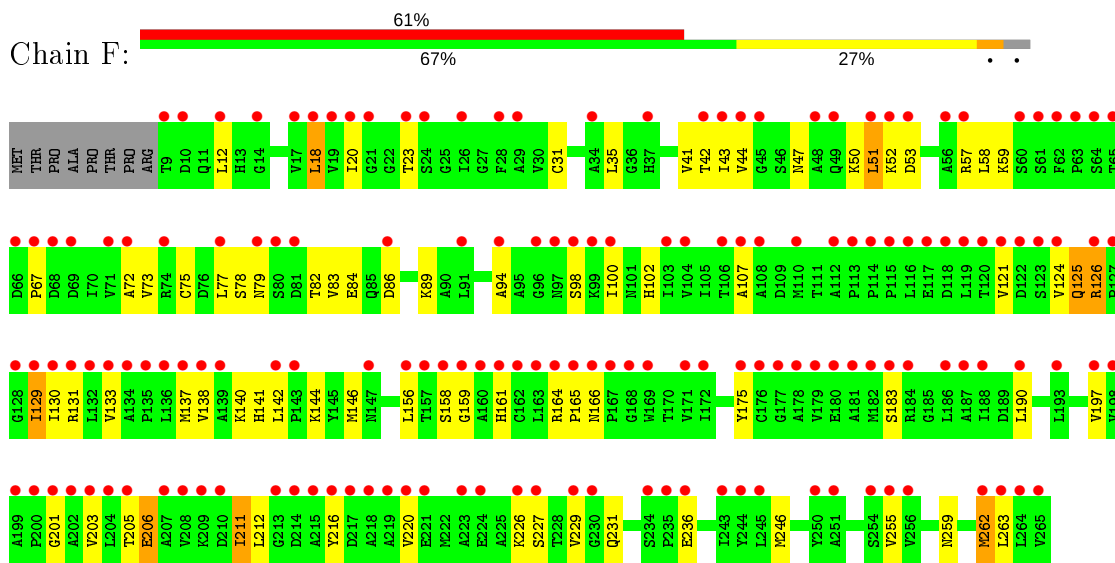
- Molecule 1: Short chain dehydrogenase



• 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)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.274 , 0.306 0.272 , 0.304	Depositor DCC
R_{free} test set	5561 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for -h-2*1,-k,l	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/1895	0.64	0/2580
1	B	0.62	0/1895	0.68	0/2580
1	C	0.63	1/1895 (0.1%)	0.71	1/2580 (0.0%)
1	D	0.61	0/1895	0.71	1/2580 (0.0%)
1	E	0.45	0/1895	1.03	21/2580 (0.8%)
1	F	0.50	0/1891	0.91	7/2575 (0.3%)
All	All	0.55	1/11366 (0.0%)	0.79	30/15475 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	SER	CB-OG	5.05	1.48	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	164	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	E	164	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	E	126	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	E	126	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	E	164	ARG	CD-NE-CZ	9.10	136.34	123.60
1	E	161	HIS	CB-CA-C	-8.91	92.59	110.40
1	E	93	LEU	CB-CG-CD1	-8.79	96.05	111.00
1	F	226	LYS	CD-CE-NZ	-8.71	91.67	111.70
1	E	51	LEU	CB-CG-CD2	8.50	125.45	111.00
1	E	93	LEU	CA-CB-CG	8.45	134.73	115.30
1	D	66	ASP	C-N-CD	-8.05	102.88	120.60
1	E	93	LEU	CB-CG-CD2	8.04	124.67	111.00
1	E	89	LYS	CA-CB-CG	7.18	129.20	113.40
1	E	18	LEU	CA-CB-CG	7.12	131.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	GLN	CA-CB-CG	-7.09	97.80	113.40
1	E	164	ARG	CG-CD-NE	-6.92	97.28	111.80
1	F	18	LEU	CB-CG-CD2	6.77	122.50	111.00
1	E	51	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	E	18	LEU	CB-CG-CD2	-6.40	100.11	111.00
1	E	92	GLN	C-N-CA	-6.23	106.12	121.70
1	C	66	ASP	C-N-CD	-6.06	107.26	120.60
1	F	129	ILE	CG1-CB-CG2	-6.00	98.20	111.40
1	F	262	MET	CA-CB-CG	5.90	123.33	113.30
1	E	55	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	F	211	ILE	CG1-CB-CG2	-5.75	98.75	111.40
1	E	161	HIS	N-CA-CB	5.65	120.77	110.60
1	F	236	GLU	CA-CB-CG	5.31	125.09	113.40
1	E	197	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	E	18	LEU	CB-CG-CD1	5.16	119.78	111.00
1	F	226	LYS	CA-CB-CG	-5.05	102.29	113.40

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	27	0
1	C	1866	0	1901	53	0
1	D	1866	0	1901	41	0
1	E	1866	0	1901	57	0
1	F	1862	0	1895	81	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	265	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 (265) 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:CG1	1:F:129:ILE:CD1	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
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:HG2	1:D:74:ARG:HH11	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:120:THR:HG23	1:C:123:SER:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HA	1:C:15:SER:OG	1.77	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:NH1	1:D:74:ARG:HG2	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:137:MET:HE3	1:F:140:LYS:HD2	1.68	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: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
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:CB	1:F:129:ILE:CD1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:124:VAL:O	1:F:175:TYR:OH	2.09	0.62
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: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
1:F:84:GLU:HG3	1:F:137:MET:HE2	1.84	0.59
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:F:255:VAL:O	1:F:255:VAL:HG23	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG22	1:D:73:VAL:HG22	1.89	0.55
1:E:182:MET:C	1:E:186:LEU:HD23	2.24	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:243:ILE:HD13	1:C:246:MET:HE2	1.89	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: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:219:ALA:HA	1:C:222:MET:HE3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:LEU:N	1:E:186:LEU:CD2	2.76	0.48
1:E:94:ALA:HB3	1:E:100:ILE:HD11	1.95	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:H	1:E:263:LEU:HD12	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:F:121:VAL:O	1:F:124:VAL:HG22	2.14	0.47
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:262:MET:HE3	1:F:262:MET:HB3	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE2	1:D:144:LYS:HB2	1.83	0.45
1:E:262:MET:HE2	1:E:262:MET:HB3	1.70	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: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
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:HB3	1:B:164:ARG:HE	1.60	0.43
1:C:11:GLN:HB2	1:F:89:LYS:CD	2.44	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:F:35:LEU:HG	1:F:41:VAL:HG21	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:D:74:ARG:HH11	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:C:50:LYS:NZ	2:C:801:NAP:O1X	2.49	0.41
1:E:16:ARG:HA	1:E:40:ILE:O	2.20	0.41
1:E:142:LEU:HD13	1:E:146:MET:HE2	2.02	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
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: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:A:35:LEU:HD12	1:A:58:LEU:HD22	2.02	0.41
1:C:142:LEU:HD13	1:C:146:MET:HE2	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: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
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/211 (97%)	201 (98%)	3 (2%)	65	62
1	B	204/211 (97%)	198 (97%)	6 (3%)	42	35
1	C	204/211 (97%)	199 (98%)	5 (2%)	47	41
1	D	204/211 (97%)	199 (98%)	5 (2%)	47	41
1	E	204/211 (97%)	199 (98%)	5 (2%)	47	41
1	F	203/211 (96%)	197 (97%)	6 (3%)	41	33
All	All	1223/1266 (97%)	1193 (98%)	30 (2%)	47	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	191	LYS
1	A	222	MET
1	B	74	ARG
1	B	97	ASN
1	B	99	LYS
1	B	163	LEU
1	B	164	ARG
1	B	226	LYS
1	C	11	GLN
1	C	49	GLN
1	C	109	ASP
1	C	126	ARG
1	C	222	MET
1	D	53	ASP
1	D	64	SER
1	D	67	PRO
1	D	115	PRO
1	D	193	LEU
1	E	51	LEU
1	E	52	LYS
1	E	89	LYS
1	E	163	LEU
1	E	237	SER
1	F	51	LEU
1	F	98	SER
1	F	125	GLN
1	F	126	ARG
1	F	183	SER
1	F	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	92	GLN
1	A	161	HIS
1	B	11	GLN
1	C	85	GLN
1	D	151	GLN
1	E	11	GLN

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Mol	Chain	Res	Type
1	E	147	ASN
1	E	161	HIS
1	F	166	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	NAP	F	801	-	45,52,52	4.66	16 (35%)	56,80,80	1.69	8 (14%)
2	NAP	C	801	-	45,52,52	4.58	17 (37%)	56,80,80	1.85	8 (14%)
2	NAP	E	801	-	45,52,52	4.64	18 (40%)	56,80,80	1.83	8 (14%)
2	NAP	B	801	-	45,52,52	4.53	19 (42%)	56,80,80	1.65	9 (16%)
2	NAP	A	801	-	45,52,52	4.66	19 (42%)	56,80,80	1.77	6 (10%)
3	ZWP	A	802	-	22,28,28	1.37	3 (13%)	25,42,42	1.75	7 (28%)
2	NAP	D	801	-	45,52,52	4.67	16 (35%)	56,80,80	1.71	5 (8%)

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	F	801	-	-	4/31/67/67	0/5/5/5
2	NAP	C	801	-	-	5/31/67/67	0/5/5/5
2	NAP	E	801	-	-	4/31/67/67	0/5/5/5
2	NAP	B	801	-	-	5/31/67/67	0/5/5/5
2	NAP	A	801	-	-	4/31/67/67	0/5/5/5
3	ZWP	A	802	-	-	5/11/19/19	0/4/4/4
2	NAP	D	801	-	-	5/31/67/67	0/5/5/5

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O4D-C1D	16.00	1.63	1.41
2	D	801	NAP	O4D-C1D	15.99	1.63	1.41
2	E	801	NAP	O4D-C1D	15.81	1.63	1.41
2	A	801	NAP	O4D-C1D	15.71	1.63	1.41
2	B	801	NAP	O4D-C1D	15.69	1.63	1.41
2	A	801	NAP	C2D-C1D	-15.50	1.30	1.53
2	C	801	NAP	O4D-C1D	15.32	1.62	1.41
2	D	801	NAP	O4B-C1B	15.14	1.62	1.41
2	E	801	NAP	C2D-C1D	-15.07	1.30	1.53
2	F	801	NAP	O4B-C1B	14.99	1.62	1.41
2	C	801	NAP	O4B-C1B	14.96	1.62	1.41
2	D	801	NAP	C2D-C1D	-14.59	1.31	1.53
2	B	801	NAP	C2D-C1D	-14.58	1.31	1.53
2	F	801	NAP	C2D-C1D	-14.56	1.31	1.53
2	A	801	NAP	O4B-C1B	14.27	1.61	1.41
2	C	801	NAP	C2D-C1D	-14.19	1.32	1.53
2	E	801	NAP	O4B-C1B	14.09	1.60	1.41
2	B	801	NAP	O4B-C1B	13.54	1.60	1.41
2	D	801	NAP	C7N-N7N	7.53	1.47	1.33
2	A	801	NAP	C7N-N7N	7.48	1.47	1.33
2	B	801	NAP	C7N-N7N	7.47	1.47	1.33
2	E	801	NAP	C7N-N7N	7.34	1.47	1.33
2	F	801	NAP	C7N-N7N	7.31	1.46	1.33
2	C	801	NAP	C7N-N7N	7.20	1.46	1.33
2	E	801	NAP	O4D-C4D	-6.87	1.29	1.45
2	C	801	NAP	O4D-C4D	-6.47	1.30	1.45
2	A	801	NAP	O4B-C4B	-6.45	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAP	O4D-C4D	-6.39	1.30	1.45
2	D	801	NAP	O4D-C4D	-6.35	1.30	1.45
2	F	801	NAP	C3N-C7N	6.28	1.60	1.50
2	F	801	NAP	O4D-C4D	-6.14	1.31	1.45
2	C	801	NAP	C3N-C7N	6.13	1.59	1.50
2	B	801	NAP	O4B-C4B	-6.11	1.31	1.45
2	E	801	NAP	C3N-C7N	6.10	1.59	1.50
2	A	801	NAP	O4D-C4D	-6.05	1.31	1.45
2	D	801	NAP	C3N-C7N	6.01	1.59	1.50
2	D	801	NAP	O4B-C4B	-5.79	1.32	1.45
2	E	801	NAP	O4B-C4B	-5.75	1.32	1.45
2	C	801	NAP	O4B-C4B	-5.67	1.32	1.45
2	F	801	NAP	O4B-C4B	-5.57	1.32	1.45
2	A	801	NAP	C3N-C7N	5.55	1.58	1.50
2	B	801	NAP	C3N-C7N	5.30	1.58	1.50
2	E	801	NAP	O3D-C3D	-4.14	1.33	1.43
2	D	801	NAP	O3D-C3D	-4.01	1.33	1.43
2	C	801	NAP	O3D-C3D	-4.00	1.33	1.43
2	B	801	NAP	O3D-C3D	-4.00	1.33	1.43
2	A	801	NAP	O3D-C3D	-3.97	1.33	1.43
2	F	801	NAP	O3D-C3D	-3.95	1.33	1.43
3	A	802	ZWP	C24-C23	3.90	1.53	1.34
2	F	801	NAP	O2D-C2D	3.70	1.51	1.43
2	C	801	NAP	O2D-C2D	3.69	1.51	1.43
2	E	801	NAP	O2D-C2D	3.65	1.51	1.43
2	A	801	NAP	O2D-C2D	3.60	1.51	1.43
2	E	801	NAP	O7N-C7N	-3.54	1.17	1.24
2	B	801	NAP	O2D-C2D	3.54	1.51	1.43
2	D	801	NAP	O2D-C2D	3.44	1.51	1.43
2	B	801	NAP	O7N-C7N	-3.37	1.17	1.24
2	C	801	NAP	C6A-N6A	3.24	1.45	1.34
2	D	801	NAP	O7N-C7N	-3.22	1.18	1.24
2	D	801	NAP	C6A-N6A	3.17	1.45	1.34
2	E	801	NAP	C6A-N6A	3.14	1.45	1.34
2	A	801	NAP	O7N-C7N	-3.14	1.18	1.24
2	F	801	NAP	C6A-N6A	3.11	1.45	1.34
2	F	801	NAP	O7N-C7N	-3.04	1.18	1.24
2	A	801	NAP	C6A-N6A	3.00	1.45	1.34
2	F	801	NAP	C2A-N3A	2.93	1.36	1.32
2	D	801	NAP	C2A-N3A	2.93	1.36	1.32
2	C	801	NAP	O7N-C7N	-2.92	1.18	1.24
2	B	801	NAP	C6A-N6A	2.92	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O3B-C3B	-2.81	1.36	1.43
2	C	801	NAP	C2A-N3A	2.72	1.36	1.32
2	B	801	NAP	C2A-N3A	2.67	1.36	1.32
2	A	801	NAP	C2A-N3A	2.65	1.36	1.32
2	C	801	NAP	P2B-O2B	2.62	1.64	1.59
2	F	801	NAP	PA-O5B	2.61	1.69	1.59
2	E	801	NAP	O3B-C3B	-2.60	1.36	1.43
2	C	801	NAP	PA-O5B	2.50	1.69	1.59
2	A	801	NAP	O3B-C3B	-2.49	1.37	1.43
2	A	801	NAP	P2B-O2B	2.48	1.64	1.59
2	D	801	NAP	O3B-C3B	-2.46	1.37	1.43
2	E	801	NAP	C2A-N3A	2.46	1.36	1.32
2	C	801	NAP	O3B-C3B	-2.44	1.37	1.43
2	D	801	NAP	P2B-O2B	2.43	1.63	1.59
2	B	801	NAP	O3B-C3B	-2.38	1.37	1.43
2	A	801	NAP	PN-O5D	2.38	1.68	1.59
2	E	801	NAP	PA-O5B	2.36	1.68	1.59
2	B	801	NAP	PA-O5B	2.31	1.68	1.59
2	B	801	NAP	C5A-N7A	-2.30	1.31	1.39
2	F	801	NAP	C5A-N7A	-2.29	1.31	1.39
2	C	801	NAP	C5A-N7A	-2.28	1.31	1.39
2	B	801	NAP	C5N-C4N	-2.27	1.34	1.38
2	E	801	NAP	C5A-N7A	-2.24	1.31	1.39
2	D	801	NAP	C5A-N7A	-2.24	1.31	1.39
2	F	801	NAP	P2B-O2B	2.21	1.63	1.59
2	A	801	NAP	C5A-N7A	-2.21	1.31	1.39
3	A	802	ZWP	C19-N20	-2.21	1.32	1.36
2	E	801	NAP	P2B-O2B	2.20	1.63	1.59
2	E	801	NAP	PN-O5D	2.19	1.68	1.59
2	B	801	NAP	C5A-C4A	-2.15	1.35	1.40
2	B	801	NAP	C4N-C3N	-2.11	1.35	1.39
2	E	801	NAP	C5A-C4A	-2.10	1.35	1.40
2	D	801	NAP	PA-O5B	2.09	1.67	1.59
2	A	801	NAP	C4N-C3N	-2.08	1.35	1.39
2	A	801	NAP	C5A-C4A	-2.07	1.35	1.40
2	A	801	NAP	PA-O5B	2.03	1.67	1.59
3	A	802	ZWP	C24-N20	2.03	1.46	1.41
2	C	801	NAP	PN-O5D	2.02	1.67	1.59
2	B	801	NAP	PN-O5D	2.01	1.67	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NAP	C5A-C6A-N6A	8.29	132.95	120.35
2	A	801	NAP	C5A-C6A-N6A	8.10	132.66	120.35
2	E	801	NAP	C5A-C6A-N6A	7.58	131.87	120.35
2	D	801	NAP	C5A-C6A-N6A	7.41	131.62	120.35
2	F	801	NAP	C5A-C6A-N6A	6.86	130.78	120.35
2	B	801	NAP	C5A-C6A-N6A	6.03	129.52	120.35
2	F	801	NAP	N3A-C2A-N1A	-5.71	119.75	128.68
2	D	801	NAP	N3A-C2A-N1A	-5.61	119.90	128.68
2	A	801	NAP	N6A-C6A-N1A	-5.57	107.02	118.57
2	C	801	NAP	N3A-C2A-N1A	-5.50	120.08	128.68
2	B	801	NAP	N3A-C2A-N1A	-5.41	120.22	128.68
2	C	801	NAP	N6A-C6A-N1A	-5.35	107.47	118.57
2	A	801	NAP	N3A-C2A-N1A	-5.29	120.40	128.68
2	E	801	NAP	N3A-C2A-N1A	-5.26	120.46	128.68
2	D	801	NAP	N6A-C6A-N1A	-5.01	108.18	118.57
2	E	801	NAP	N6A-C6A-N1A	-4.95	108.29	118.57
3	A	802	ZWP	C7-C15-C16	-4.60	106.19	114.09
2	F	801	NAP	N6A-C6A-N1A	-4.43	109.38	118.57
2	B	801	NAP	N6A-C6A-N1A	-3.92	110.43	118.57
2	E	801	NAP	PN-O3-PA	-3.55	120.65	132.83
2	E	801	NAP	C1B-N9A-C4A	-3.52	120.45	126.64
2	B	801	NAP	C3N-C7N-N7N	3.18	121.57	117.75
2	E	801	NAP	C3N-C7N-N7N	3.13	121.51	117.75
2	C	801	NAP	O4D-C1D-C2D	-3.04	102.49	106.93
2	A	801	NAP	C1B-N9A-C4A	-3.01	121.35	126.64
2	B	801	NAP	C1B-N9A-C4A	-3.01	121.36	126.64
2	F	801	NAP	C1B-N9A-C4A	-2.90	121.54	126.64
3	A	802	ZWP	C15-C16-N17	2.86	121.08	116.61
2	C	801	NAP	C1B-N9A-C4A	-2.79	121.74	126.64
2	D	801	NAP	C1B-N9A-C4A	-2.71	121.88	126.64
3	A	802	ZWP	C15-C16-C21	-2.69	117.92	121.39
2	F	801	NAP	C5B-C4B-C3B	-2.61	105.40	115.18
2	C	801	NAP	C6N-N1N-C2N	-2.58	119.62	121.97
2	D	801	NAP	C6N-N1N-C2N	-2.56	119.64	121.97
3	A	802	ZWP	C1-C2-C7	-2.52	129.82	134.17
2	E	801	NAP	C5B-C4B-C3B	-2.52	105.75	115.18
3	A	802	ZWP	C1-C2-C3	2.50	121.48	118.17
3	A	802	ZWP	C15-C7-C8	2.40	128.53	126.41
2	E	801	NAP	C3D-C2D-C1D	2.32	104.48	100.98
2	A	801	NAP	C5D-C4D-C3D	-2.30	106.58	115.18
2	C	801	NAP	O7N-C7N-N7N	-2.23	119.41	122.58
2	B	801	NAP	O4D-C1D-C2D	-2.22	103.68	106.93
2	F	801	NAP	C3N-C7N-N7N	2.17	120.36	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAP	C2N-C3N-C4N	2.15	120.70	118.26
2	B	801	NAP	O7N-C7N-C3N	-2.15	117.06	119.63
2	F	801	NAP	PN-O3-PA	-2.09	125.66	132.83
2	C	801	NAP	C3N-C7N-N7N	2.08	120.25	117.75
2	B	801	NAP	PN-O3-PA	-2.06	125.76	132.83
2	F	801	NAP	C6N-N1N-C2N	-2.05	120.10	121.97
3	A	802	ZWP	C10-C8-N9	-2.04	113.31	121.49
2	A	801	NAP	C5B-C4B-C3B	-2.01	107.66	115.18

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAP	O4D-C1D-N1N-C2N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	D	801	NAP	O4D-C1D-N1N-C2N
3	A	802	ZWP	C11-C10-C13-C14
3	A	802	ZWP	C11-C10-C8-C7
3	A	802	ZWP	C12-C10-C8-C7
2	C	801	NAP	PA-O3-PN-O2N
2	E	801	NAP	PA-O3-PN-O2N
2	B	801	NAP	PA-O3-PN-O2N
2	A	801	NAP	PA-O3-PN-O2N
2	D	801	NAP	PA-O3-PN-O2N
3	A	802	ZWP	C8-C10-C13-C14
2	F	801	NAP	PA-O3-PN-O2N
3	A	802	ZWP	C7-C15-C16-N17
2	E	801	NAP	O4B-C4B-C5B-O5B
2	F	801	NAP	O4B-C4B-C5B-O5B
2	C	801	NAP	O4B-C4B-C5B-O5B
2	B	801	NAP	O4B-C4B-C5B-O5B
2	F	801	NAP	PA-O3-PN-O1N
2	C	801	NAP	PA-O3-PN-O1N
2	B	801	NAP	PA-O3-PN-O1N
2	D	801	NAP	PA-O3-PN-O1N
2	F	801	NAP	C5B-O5B-PA-O1A
2	C	801	NAP	C5B-O5B-PA-O1A
2	C	801	NAP	C5D-O5D-PN-O1N
2	E	801	NAP	C5B-O5B-PA-O1A
2	E	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	C5B-O5B-PA-O1A

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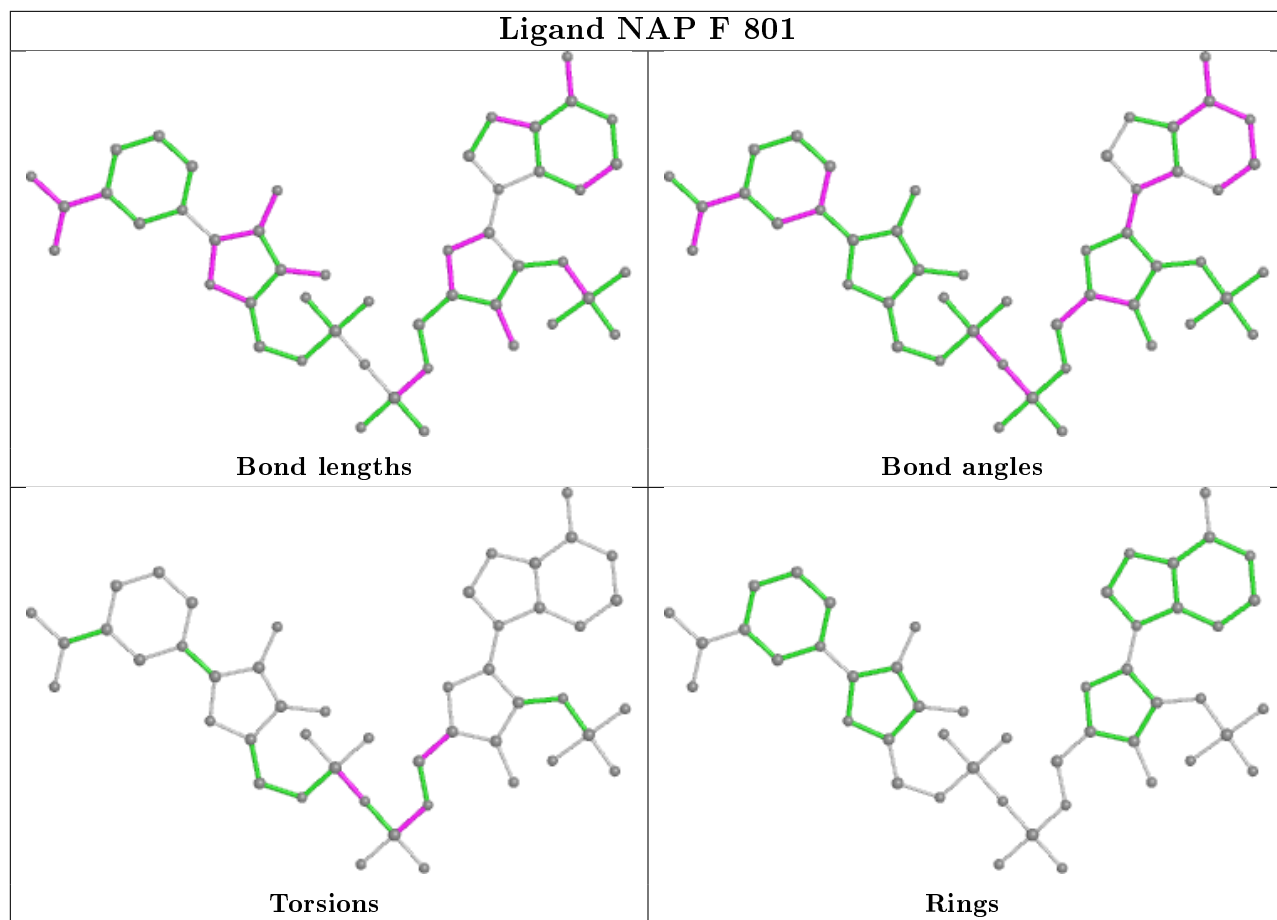
Mol	Chain	Res	Type	Atoms
2	D	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	O4B-C4B-C5B-O5B
2	D	801	NAP	O4B-C4B-C5B-O5B

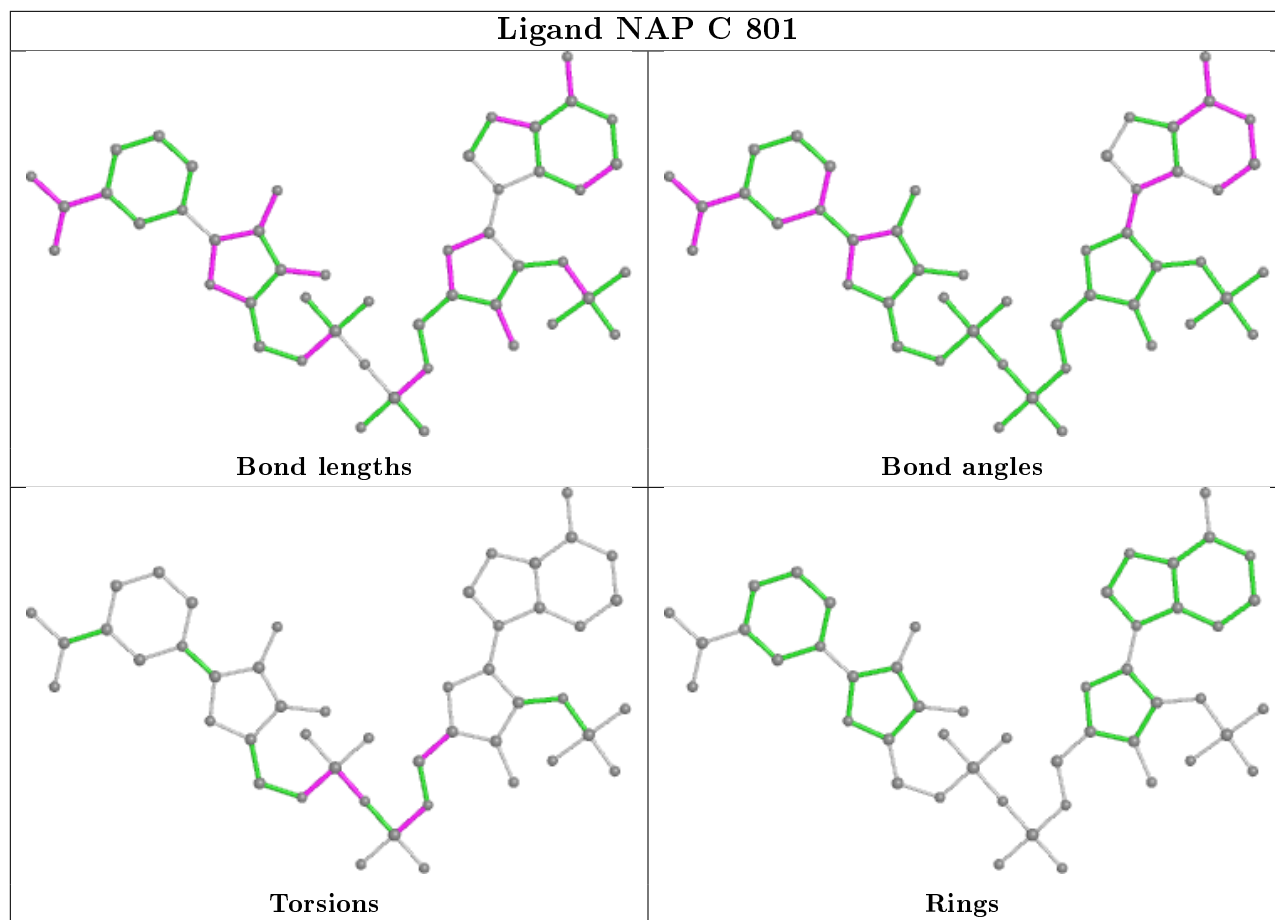
There are no ring outliers.

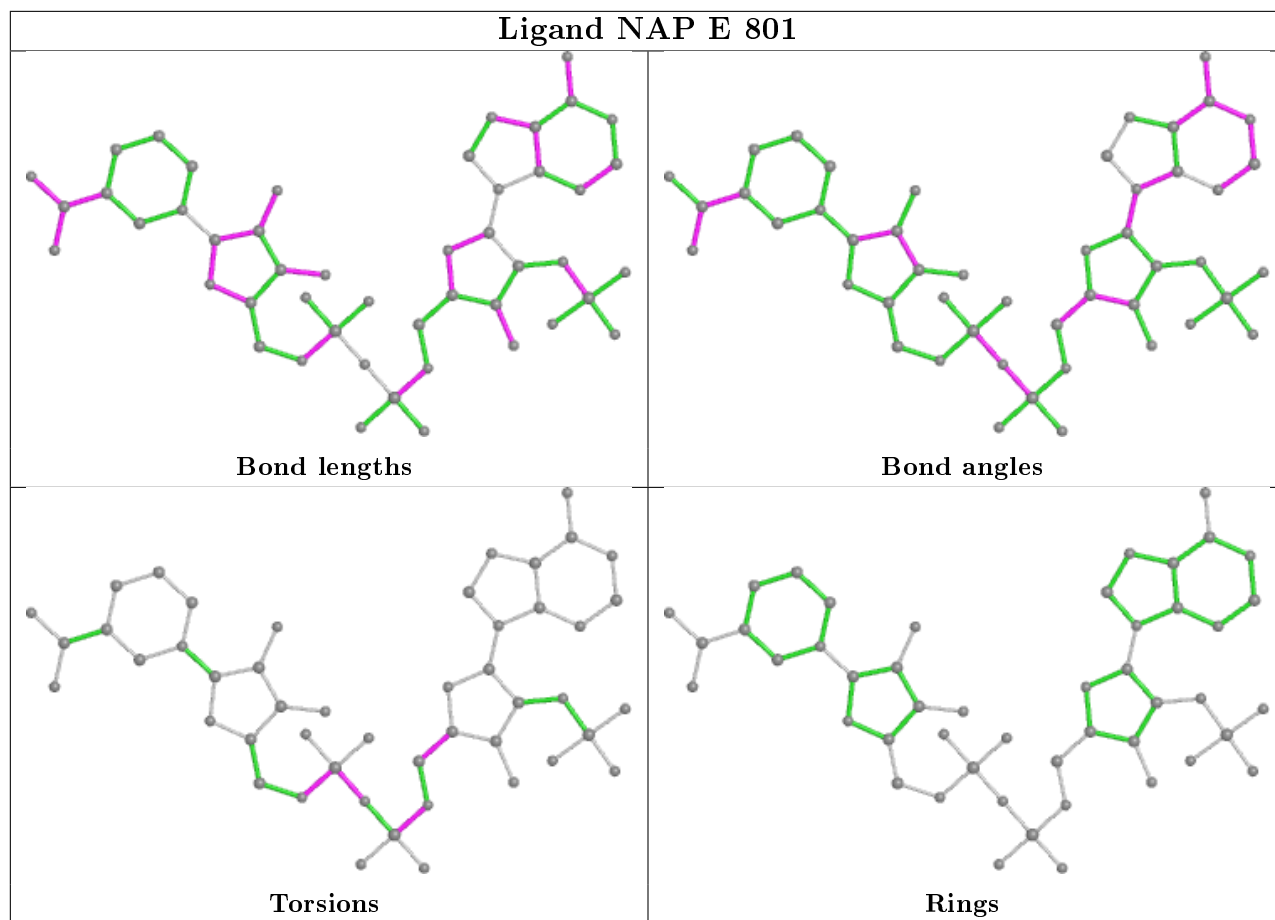
6 monomers are involved in 9 short contacts:

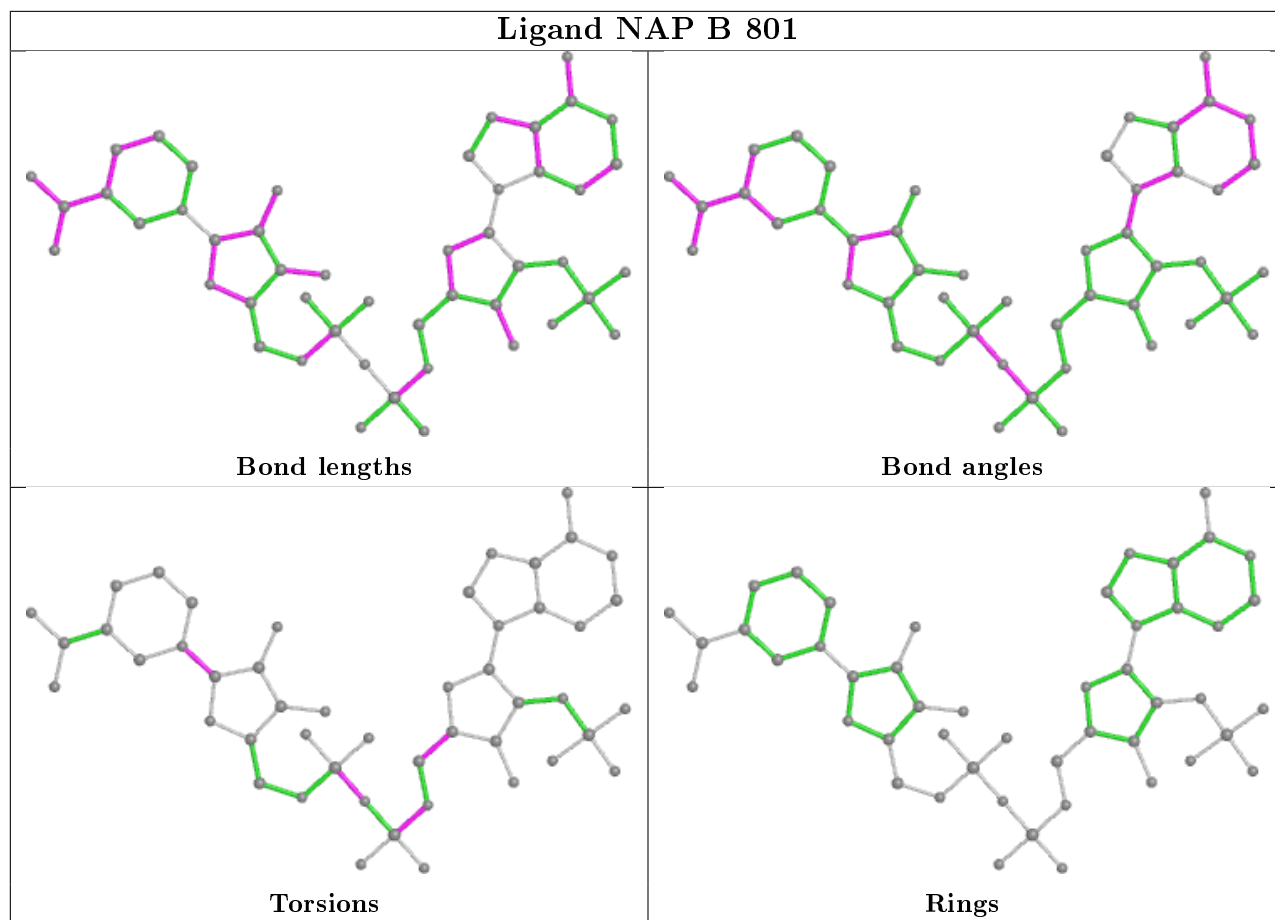
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	NAP	1	0
2	C	801	NAP	3	0
2	E	801	NAP	1	0
2	B	801	NAP	2	0
2	A	801	NAP	1	0
2	D	801	NAP	1	0

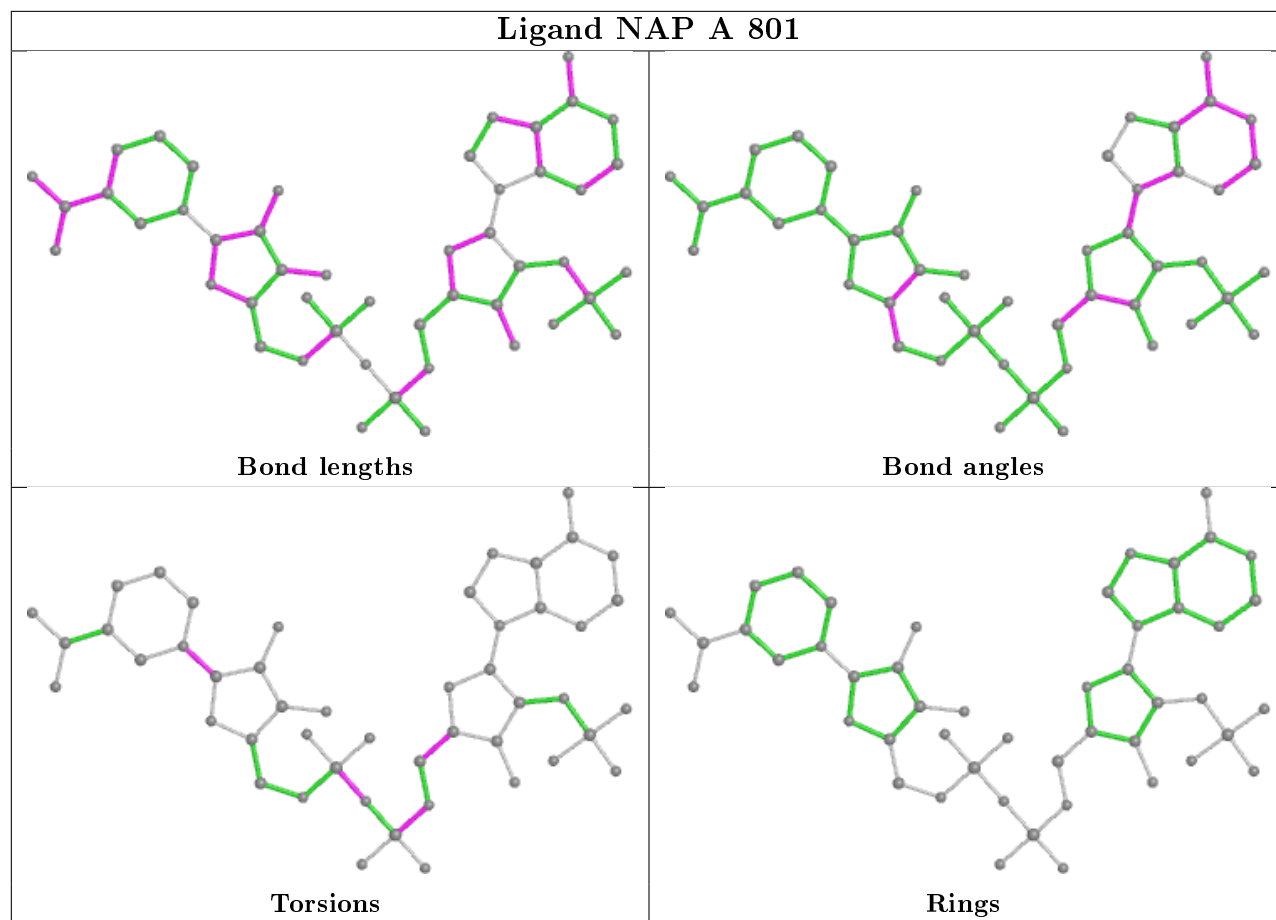
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

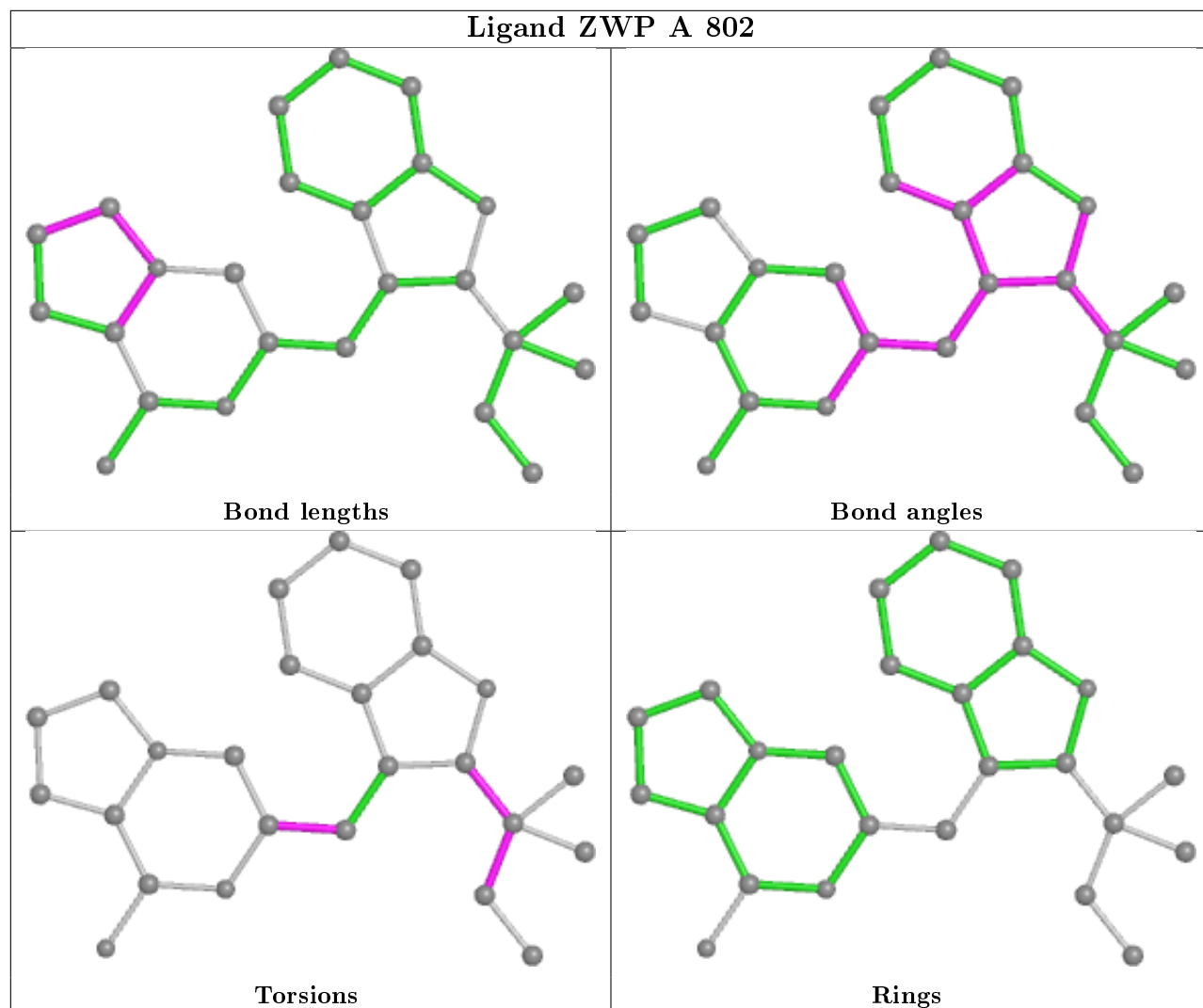


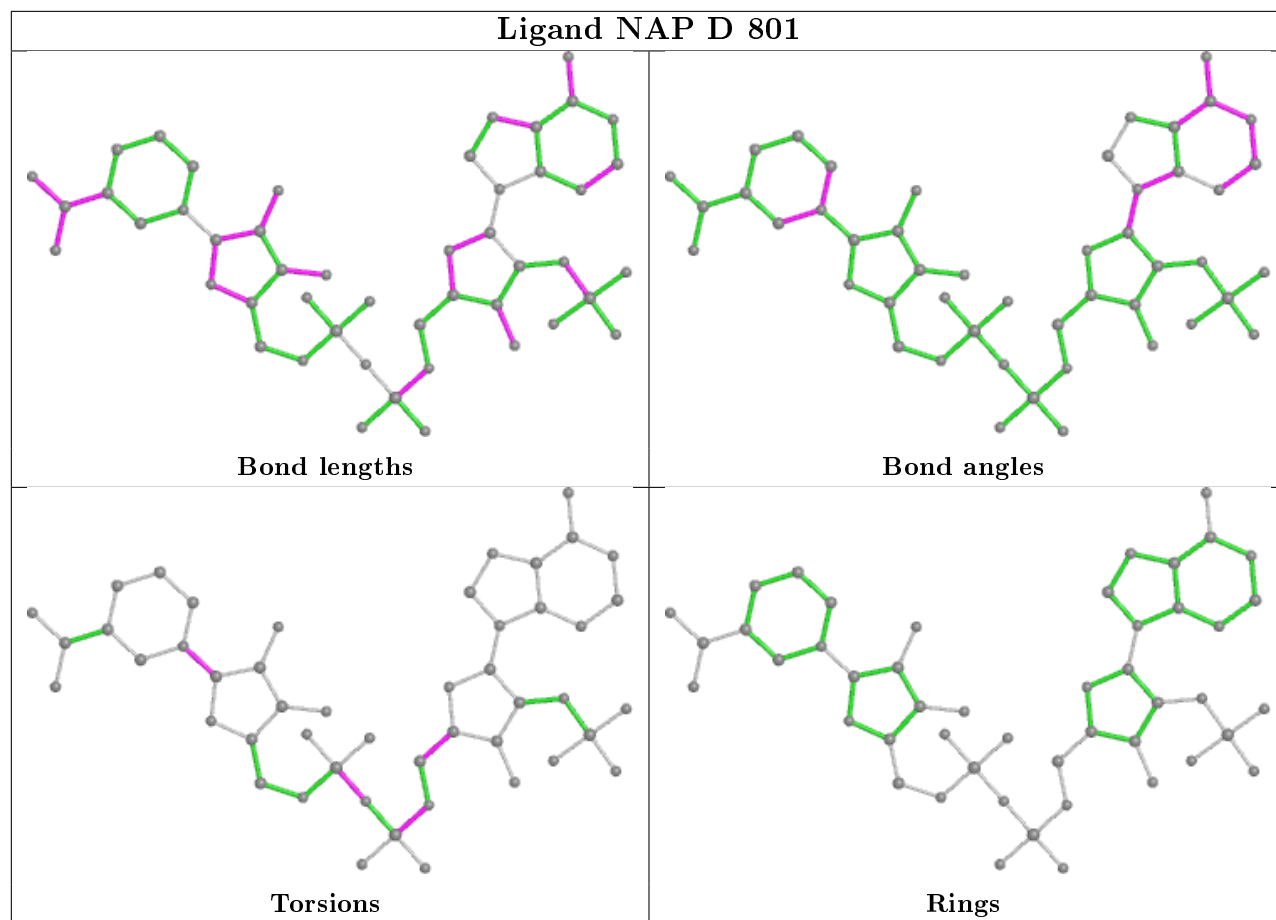












5.7 Other polymers [\(i\)](#)

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%)	0.62	15 (5%) 23 25	34, 49, 73, 132	0
1	B	257/265 (96%)	0.64	21 (8%) 11 13	33, 50, 79, 122	0
1	C	257/265 (96%)	0.91	34 (13%) 3 3	33, 57, 109, 194	0
1	D	257/265 (96%)	0.88	34 (13%) 3 3	34, 55, 100, 133	0
1	E	257/265 (96%)	2.07	111 (43%) 0 0	52, 83, 131, 177	0
1	F	257/265 (96%)	2.93	162 (63%) 0 0	57, 84, 145, 173	0
All	All	1542/1590 (96%)	1.34	377 (24%) 0 0	33, 63, 118, 194	0

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	9	THR	11.3
1	E	67	PRO	10.3
1	F	223	ALA	9.8
1	B	263	LEU	9.7
1	F	121	VAL	9.0
1	C	9	THR	8.8
1	F	118	ASP	8.4
1	F	182	MET	8.2
1	F	197	VAL	8.1
1	F	130	ILE	8.1
1	E	263	LEU	7.8
1	F	263	LEU	7.8
1	E	14	GLY	7.7
1	F	169	TRP	7.7
1	F	255	VAL	7.6
1	F	201	GLY	7.5
1	E	11	GLN	7.5
1	F	116	LEU	7.4
1	F	14	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	F	120	THR	6.9
1	C	67	PRO	6.9
1	E	40	ILE	6.4
1	F	131	ARG	6.4
1	F	48	ALA	6.3
1	A	9	THR	6.3
1	F	119	LEU	6.2
1	F	163	LEU	6.2
1	E	242	TYR	6.1
1	E	9	THR	6.1
1	F	190	LEU	5.9
1	F	262	MET	5.8
1	E	10	ASP	5.8
1	F	129	ILE	5.8
1	E	255	VAL	5.8
1	E	71	VAL	5.8
1	F	106	THR	5.7
1	E	161	HIS	5.7
1	E	216	TYR	5.6
1	F	216	TYR	5.6
1	F	133	VAL	5.5
1	E	201	GLY	5.4
1	F	122	ASP	5.4
1	F	217	ASP	5.3
1	E	197	VAL	5.3
1	F	161	HIS	5.3
1	F	62	PHE	5.3
1	F	68	ASP	5.2
1	F	77	LEU	5.2
1	C	216	TYR	5.2
1	F	63	PRO	5.2
1	F	186	LEU	5.1
1	F	19	VAL	5.1
1	E	64	SER	5.1
1	E	17	VAL	5.0
1	D	68	ASP	5.0
1	F	207	ALA	5.0
1	F	64	SER	4.9
1	F	176	CYS	4.9
1	F	65	THR	4.8
1	F	49	GLN	4.8
1	F	236	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	264	LEU	4.8
1	E	62	PHE	4.8
1	F	205	THR	4.7
1	F	94	ALA	4.7
1	C	211	ILE	4.6
1	E	55	VAL	4.6
1	F	203	VAL	4.6
1	F	104	VAL	4.6
1	F	96	GLY	4.5
1	E	198	VAL	4.5
1	F	209	LYS	4.5
1	F	221	GLU	4.5
1	F	112	ALA	4.4
1	F	198	VAL	4.4
1	F	10	ASP	4.4
1	F	45	GLY	4.4
1	E	39	ALA	4.2
1	F	108	ALA	4.2
1	E	265	VAL	4.2
1	F	44	VAL	4.2
1	F	164	ARG	4.2
1	F	23	THR	4.2
1	D	214	ASP	4.1
1	A	181	ALA	4.1
1	F	134	ALA	4.1
1	E	190	LEU	4.1
1	D	216	TYR	4.1
1	F	204	LEU	4.1
1	E	245	LEU	4.0
1	E	256	VAL	4.0
1	F	265	VAL	4.0
1	F	219	ALA	4.0
1	E	92	GLN	4.0
1	F	43	ILE	4.0
1	F	229	VAL	4.0
1	E	235	PRO	4.0
1	F	135	PRO	3.9
1	F	110	MET	3.9
1	E	223	ALA	3.9
1	F	220	VAL	3.9
1	F	166	ASN	3.9
1	F	256	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	250	TYR	3.9
1	E	104	VAL	3.8
1	F	162	CYS	3.8
1	F	56	ALA	3.8
1	C	163	LEU	3.8
1	F	12	LEU	3.8
1	B	9	THR	3.8
1	E	152	SER	3.8
1	B	67	PRO	3.8
1	F	114	PRO	3.8
1	E	207	ALA	3.7
1	E	257	SER	3.7
1	E	53	ASP	3.7
1	F	74	ARG	3.7
1	E	232	THR	3.7
1	E	41	VAL	3.7
1	A	162	CYS	3.7
1	F	72	ALA	3.6
1	F	51	LEU	3.6
1	F	264	LEU	3.6
1	F	188	ILE	3.6
1	D	63	PRO	3.6
1	F	136	LEU	3.6
1	E	70	ILE	3.6
1	E	51	LEU	3.6
1	E	19	VAL	3.6
1	F	97	ASN	3.6
1	C	10	ASP	3.6
1	F	244	TYR	3.6
1	C	221	GLU	3.6
1	D	67	PRO	3.6
1	E	31	CYS	3.5
1	F	158	SER	3.5
1	E	34	ALA	3.5
1	F	52	LYS	3.5
1	F	213	GLY	3.5
1	C	116	LEU	3.4
1	F	230	GLY	3.4
1	A	163	LEU	3.4
1	E	18	LEU	3.4
1	E	238	VAL	3.4
1	F	113	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	167	PRO	3.4
1	E	192	PRO	3.4
1	C	215	ALA	3.4
1	E	164	ARG	3.4
1	E	163	LEU	3.4
1	F	137	MET	3.4
1	F	53	ASP	3.4
1	D	94	ALA	3.4
1	B	162	CYS	3.4
1	F	234	SER	3.3
1	F	200	PRO	3.3
1	D	9	THR	3.3
1	E	260	GLY	3.3
1	F	226	LYS	3.3
1	F	245	LEU	3.3
1	F	124	VAL	3.3
1	F	147	ASN	3.3
1	F	165	PRO	3.3
1	F	138	VAL	3.3
1	E	175	TYR	3.3
1	F	235	PRO	3.3
1	F	179	VAL	3.3
1	E	225	ALA	3.3
1	F	107	ALA	3.2
1	C	199	ALA	3.2
1	E	204	LEU	3.2
1	F	28	PHE	3.2
1	F	20	ILE	3.2
1	E	65	THR	3.2
1	E	94	ALA	3.2
1	F	142	LEU	3.1
1	F	181	ALA	3.1
1	B	14	GLY	3.1
1	E	43	ILE	3.1
1	F	61	SER	3.1
1	D	255	VAL	3.1
1	F	100	ILE	3.1
1	F	157	THR	3.1
1	E	32	ALA	3.1
1	F	227	SER	3.0
1	D	57	ARG	3.0
1	E	148	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	37	HIS	3.0
1	F	208	VAL	3.0
1	C	263	LEU	3.0
1	F	103	ILE	3.0
1	D	97	ASN	3.0
1	F	18	LEU	3.0
1	E	97	ASN	3.0
1	C	81	ASP	3.0
1	D	163	LEU	3.0
1	A	176	CYS	3.0
1	E	96	GLY	3.0
1	F	168	GLY	3.0
1	F	175	TYR	3.0
1	C	162	CYS	2.9
1	F	126	ARG	2.9
1	E	95	ALA	2.9
1	E	38	GLY	2.9
1	F	132	LEU	2.9
1	E	36	GLY	2.9
1	F	17	VAL	2.9
1	B	199	ALA	2.9
1	E	100	ILE	2.8
1	F	171	VAL	2.8
1	E	93	LEU	2.8
1	B	187	ALA	2.8
1	E	240	GLN	2.8
1	E	181	ALA	2.8
1	E	149	CYS	2.8
1	E	226	LYS	2.8
1	F	60	SER	2.8
1	F	184	ARG	2.8
1	E	147	ASN	2.8
1	E	196	ASN	2.8
1	E	83	VAL	2.8
1	E	22	GLY	2.7
1	D	263	LEU	2.7
1	D	176	CYS	2.7
1	E	229	VAL	2.7
1	F	34	ALA	2.7
1	F	66	ASP	2.7
1	F	81	ASP	2.7
1	E	193	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	110	MET	2.7
1	E	262	MET	2.7
1	D	113	PRO	2.7
1	F	187	ALA	2.7
1	C	265	VAL	2.7
1	F	71	VAL	2.7
1	F	123	SER	2.7
1	F	177	GLY	2.7
1	B	178	ALA	2.7
1	E	28	PHE	2.7
1	F	218	ALA	2.7
1	C	58	LEU	2.7
1	F	160	ALA	2.7
1	E	85	GLN	2.7
1	E	20	ILE	2.6
1	E	66	ASP	2.6
1	F	117	GLU	2.6
1	E	105	ILE	2.6
1	F	127	PRO	2.6
1	E	246	MET	2.6
1	B	255	VAL	2.6
1	F	193	LEU	2.6
1	A	177	GLY	2.6
1	E	107	ALA	2.6
1	E	251	ALA	2.6
1	F	80	SER	2.6
1	A	164	ARG	2.6
1	E	155	THR	2.6
1	E	35	LEU	2.6
1	A	64	SER	2.6
1	F	57	ARG	2.6
1	F	98	SER	2.6
1	F	143	PRO	2.6
1	F	26	ILE	2.6
1	F	210	ASP	2.6
1	E	180	GLU	2.6
1	C	264	LEU	2.5
1	F	178	ALA	2.5
1	D	64	SER	2.5
1	F	254	SER	2.5
1	E	61	SER	2.5
1	B	176	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	202	ALA	2.5
1	C	110	MET	2.5
1	B	97	ASN	2.5
1	B	158	SER	2.5
1	E	73	VAL	2.5
1	B	163	LEU	2.5
1	D	166	ASN	2.4
1	E	158	SER	2.4
1	A	263	LEU	2.4
1	D	162	CYS	2.4
1	A	199	ALA	2.4
1	B	65	THR	2.4
1	D	265	VAL	2.4
1	E	12	LEU	2.4
1	F	156	LEU	2.4
1	E	206	GLU	2.4
1	E	241	ALA	2.4
1	B	214	ASP	2.4
1	F	42	THR	2.4
1	F	172	ILE	2.4
1	E	44	VAL	2.4
1	B	181	ALA	2.4
1	C	166	ASN	2.4
1	E	26	ILE	2.4
1	E	60	SER	2.3
1	D	48	ALA	2.3
1	E	236	GLU	2.3
1	E	165	PRO	2.3
1	C	217	ASP	2.3
1	C	55	VAL	2.3
1	E	254	SER	2.3
1	D	51	LEU	2.3
1	E	176	CYS	2.3
1	D	207	ALA	2.3
1	F	29	ALA	2.3
1	D	65	THR	2.3
1	E	217	ASP	2.3
1	F	99	LYS	2.3
1	C	11	GLN	2.3
1	D	72	ALA	2.3
1	C	63	PRO	2.3
1	F	115	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	62	PHE	2.3
1	D	209	LYS	2.3
1	C	177	GLY	2.3
1	F	215	ALA	2.3
1	B	264	LEU	2.3
1	E	126	ARG	2.3
1	F	86	ASP	2.3
1	A	178	ALA	2.2
1	B	134	ALA	2.2
1	B	256	VAL	2.2
1	D	52	LYS	2.2
1	F	159	GLY	2.2
1	E	56	ALA	2.2
1	E	227	SER	2.2
1	E	252	SER	2.2
1	F	139	ALA	2.2
1	F	183	SER	2.2
1	E	30	VAL	2.2
1	C	69	ASP	2.2
1	E	15	SER	2.2
1	C	40	ILE	2.2
1	E	243	ILE	2.2
1	A	264	LEU	2.2
1	F	69	ASP	2.2
1	F	67	PRO	2.2
1	E	228	THR	2.2
1	D	210	ASP	2.2
1	D	211	ILE	2.2
1	E	52	LYS	2.2
1	F	91	LEU	2.2
1	B	82	THR	2.2
1	F	128	GLY	2.2
1	C	236	GLU	2.2
1	D	188	ILE	2.1
1	C	258	THR	2.1
1	F	214	ASP	2.1
1	B	197	VAL	2.1
1	D	75	CYS	2.1
1	C	120	THR	2.1
1	E	117	GLU	2.1
1	F	24	SER	2.1
1	A	255	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	79	ASN	2.1
1	E	162	CYS	2.1
1	F	251	ALA	2.1
1	A	38	GLY	2.1
1	C	213	GLY	2.1
1	F	199	ALA	2.1
1	F	21	GLY	2.1
1	D	217	ASP	2.1
1	E	48	ALA	2.1
1	D	116	LEU	2.1
1	C	198	VAL	2.0
1	A	226	LYS	2.0
1	E	200	PRO	2.0
1	F	243	ILE	2.0
1	F	180	GLU	2.0
1	D	46	SER	2.0
1	C	225	ALA	2.0
1	F	224	GLU	2.0
1	D	92	GLN	2.0
1	C	158	SER	2.0
1	E	37	HIS	2.0
1	C	117	GLU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

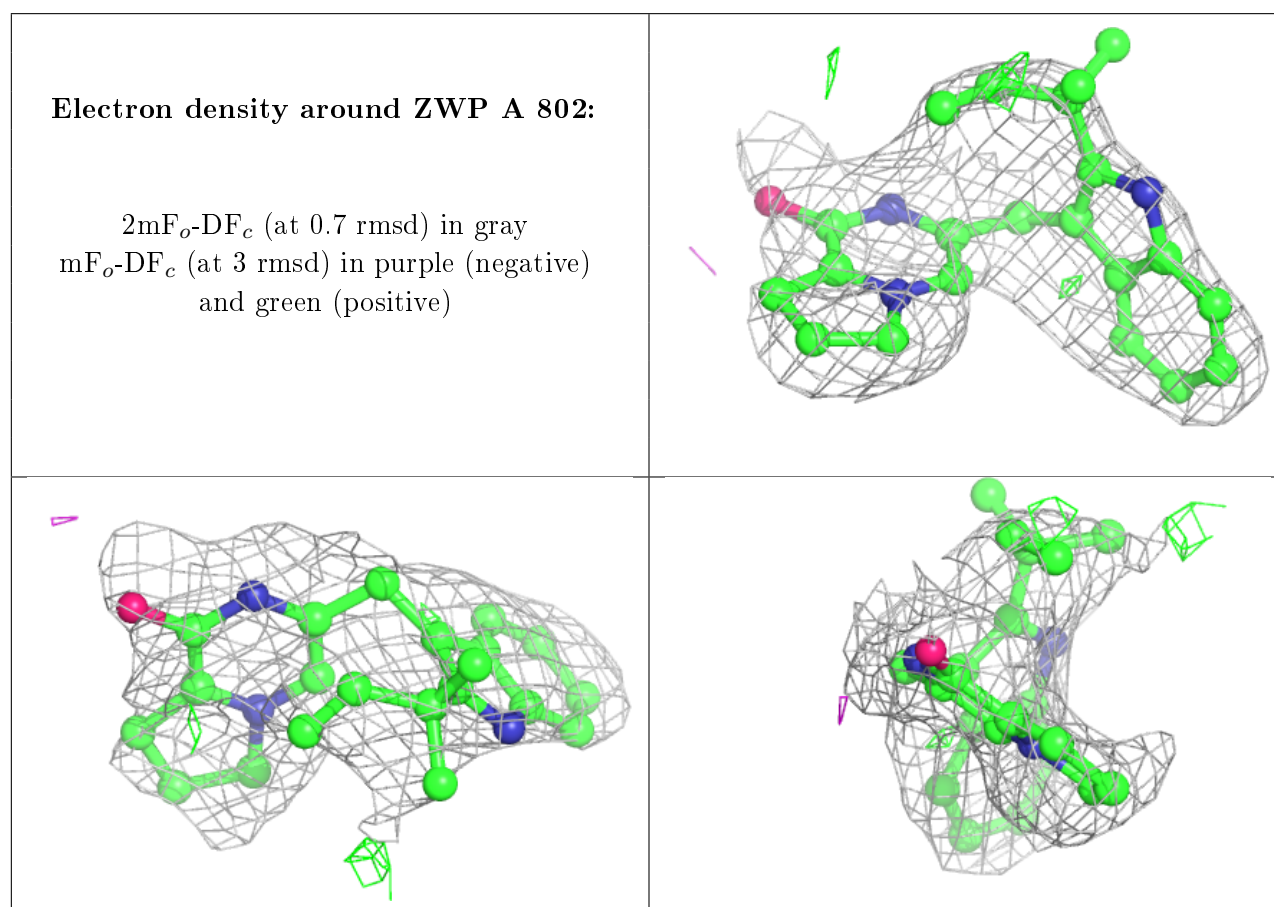
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZWP	A	802	25/25	0.74	0.21	65,76,80,82	0

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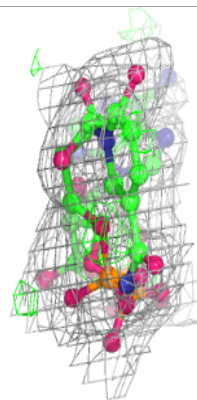
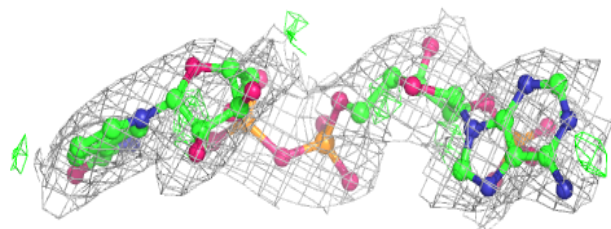
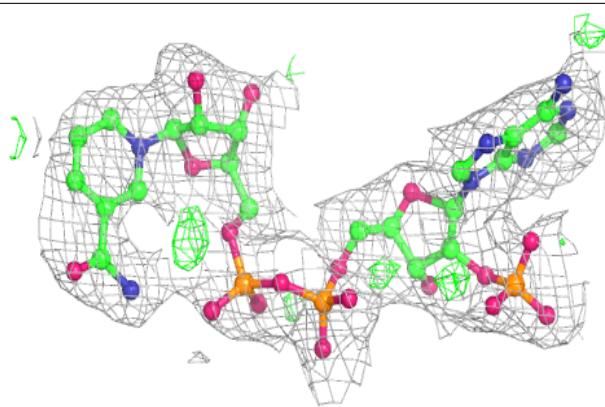
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	E	801	48/48	0.82	0.14	63,76,85,89	0
2	NAP	F	801	48/48	0.83	0.21	55,71,80,83	0
2	NAP	D	801	48/48	0.90	0.12	47,53,60,62	0
2	NAP	B	801	48/48	0.91	0.13	44,51,67,90	0
2	NAP	C	801	48/48	0.93	0.12	48,54,63,68	0
2	NAP	A	801	48/48	0.95	0.13	37,46,51,58	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.

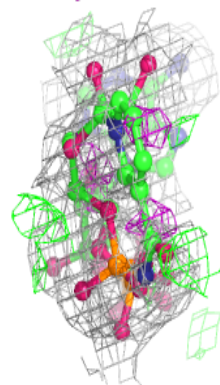
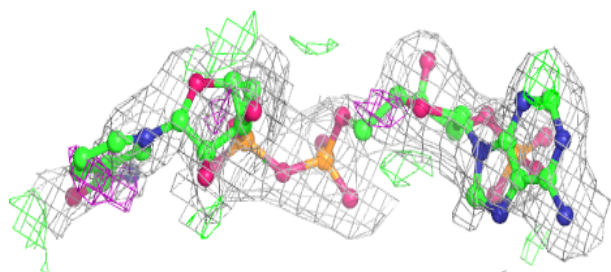
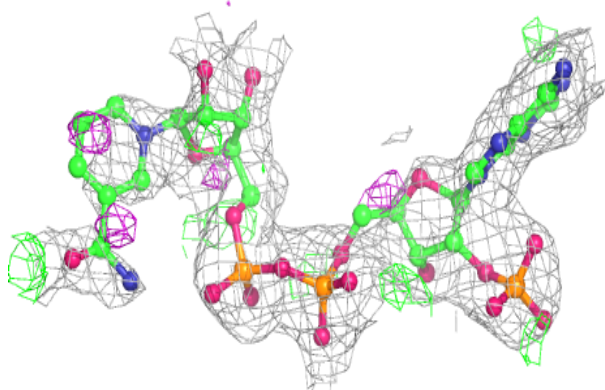


Electron density around NAP E 801:

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

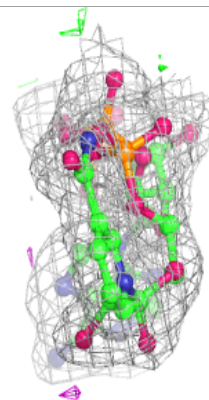
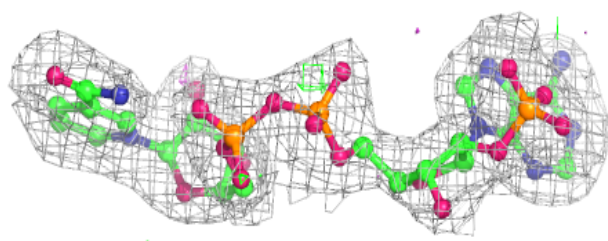
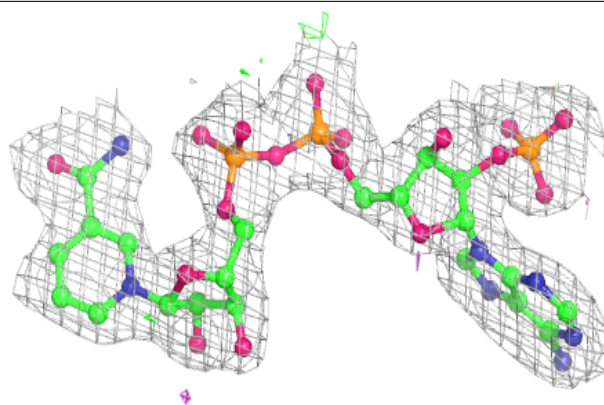
**Electron density around NAP F 801:**

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

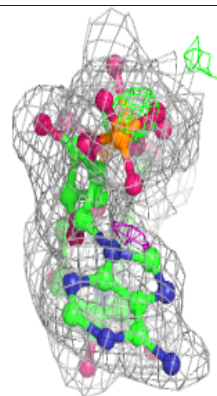
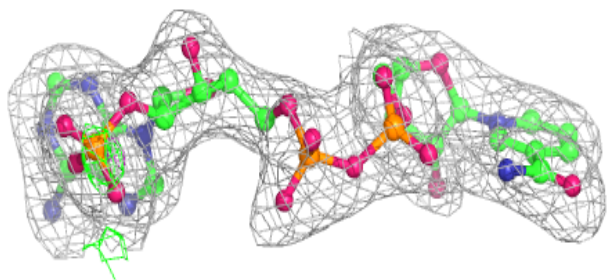
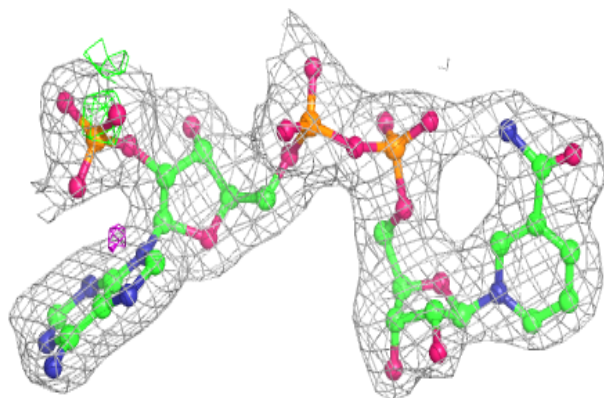


Electron density around NAP D 801:

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

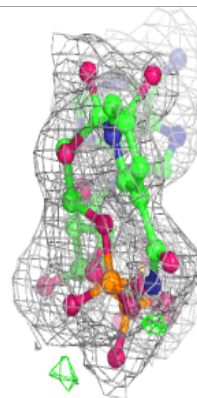
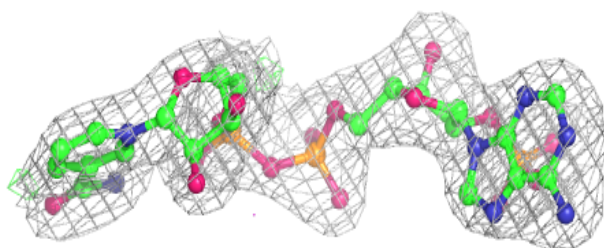
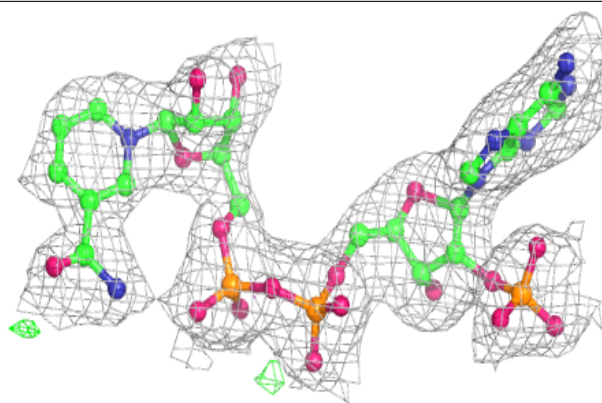
**Electron density around NAP B 801:**

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

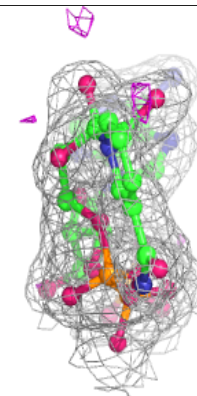
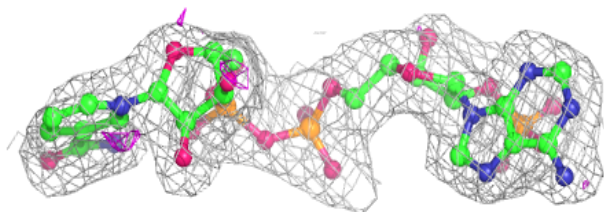
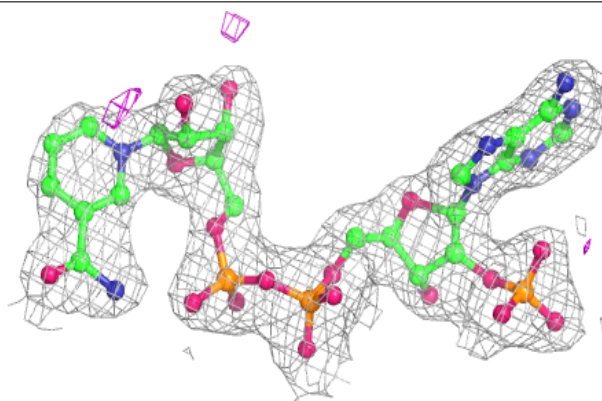


Electron density around NAP C 801:

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

**Electron density around NAP 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)



6.5 Other polymers

There are no such residues in this entry.