Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2024 – 06:08 PM JST

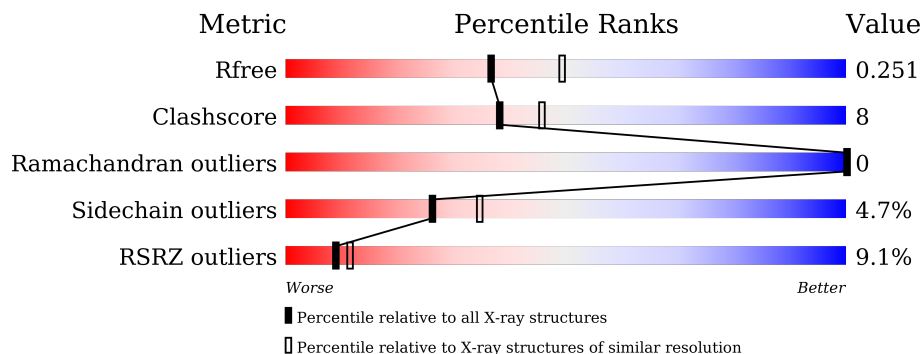|		
PDB ID	:	8IJG
Title	:	Crystal structure of alcohol dehydrogenase M5 from Burkholderia gladioli with NADP
Authors	:	Han, X.; Mei, Z.L.; Liu, W.D.; Sun, Z.T.; Ma, J.A.
Deposited on	:	2023-02-27
Resolution	:	2.27 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.27 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		4.7%
RSRZ outliers		9.1%

Worse　　　　　　　　　　　　　　　　　　　Better

▋Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	251	.%　　87%　　12%　••
1	B	251	12%　　82%　　16%　••
1	C	251	10%　　82%　　16%　•
1	D	251	14%　　79%　　19%　••

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7670 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 Putative short-chain dehydrogenases/reductase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1804	1119	326	357	2			
1	B	249	Total	C	N	O	S	0	0	0
			1801	1119	323	357	2			
1	C	250	Total	C	N	O	S	0	0	0
			1807	1122	324	359	2			
1	D	249	Total	C	N	O	S	0	0	0
			1791	1114	320	355	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ILE	VAL	engineered mutation	UNP F2LIG4
A	92	ALA	GLY	engineered mutation	UNP F2LIG4
A	138	ALA	SER	engineered mutation	UNP F2LIG4
A	140	LYS	ALA	engineered mutation	UNP F2LIG4
A	203	THR	LEU	engineered mutation	UNP F2LIG4
B	84	ILE	VAL	engineered mutation	UNP F2LIG4
B	92	ALA	GLY	engineered mutation	UNP F2LIG4
B	138	ALA	SER	engineered mutation	UNP F2LIG4
B	140	LYS	ALA	engineered mutation	UNP F2LIG4
B	203	THR	LEU	engineered mutation	UNP F2LIG4
C	84	ILE	VAL	engineered mutation	UNP F2LIG4
C	92	ALA	GLY	engineered mutation	UNP F2LIG4
C	138	ALA	SER	engineered mutation	UNP F2LIG4
C	140	LYS	ALA	engineered mutation	UNP F2LIG4
C	203	THR	LEU	engineered mutation	UNP F2LIG4
D	84	ILE	VAL	engineered mutation	UNP F2LIG4
D	92	ALA	GLY	engineered mutation	UNP F2LIG4
D	138	ALA	SER	engineered mutation	UNP F2LIG4
D	140	LYS	ALA	engineered mutation	UNP F2LIG4
D	203	THR	LEU	engineered mutation	UNP F2LIG4

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
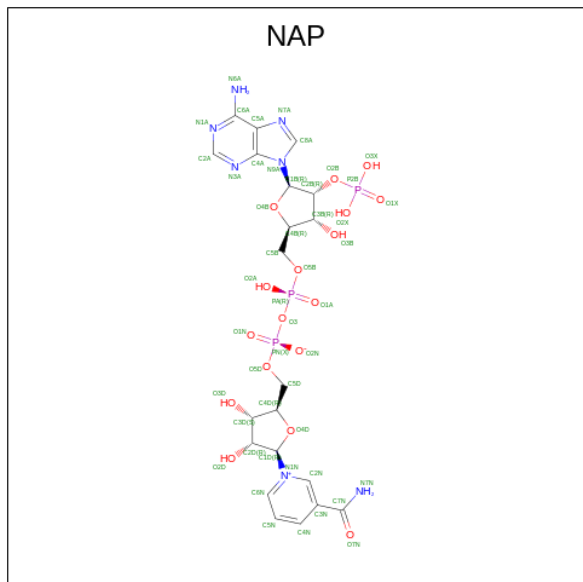
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	42	Total	O	0	0
			42	42		
3	C	69	Total	O	0	0
			69	69		
3	D	55	Total	O	0	0
			55	55		

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.

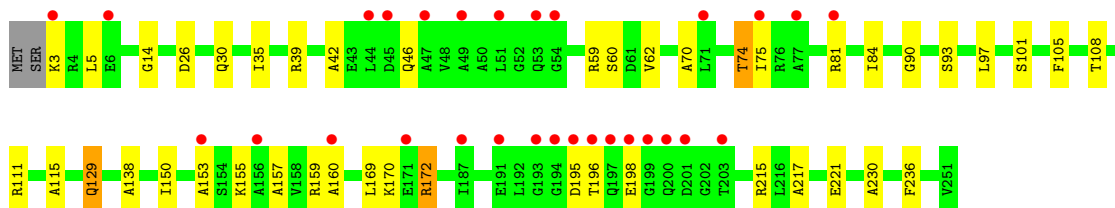- Molecule 1: Putative short-chain dehydrogenases/reductase family protein
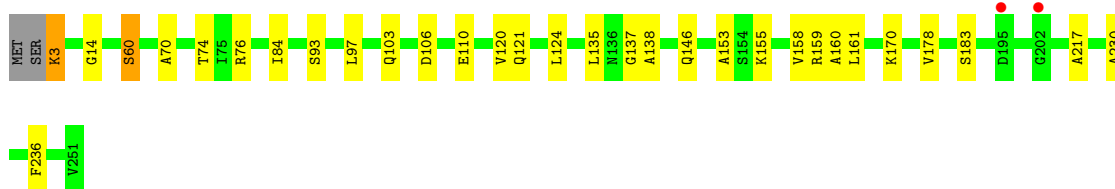
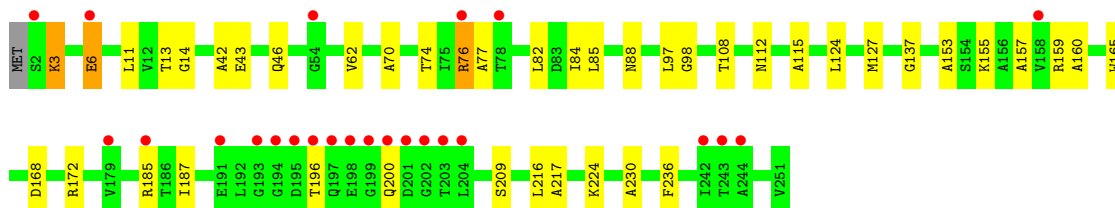- Molecule 1: Putative short-chain dehydrogenases/reductase family protein

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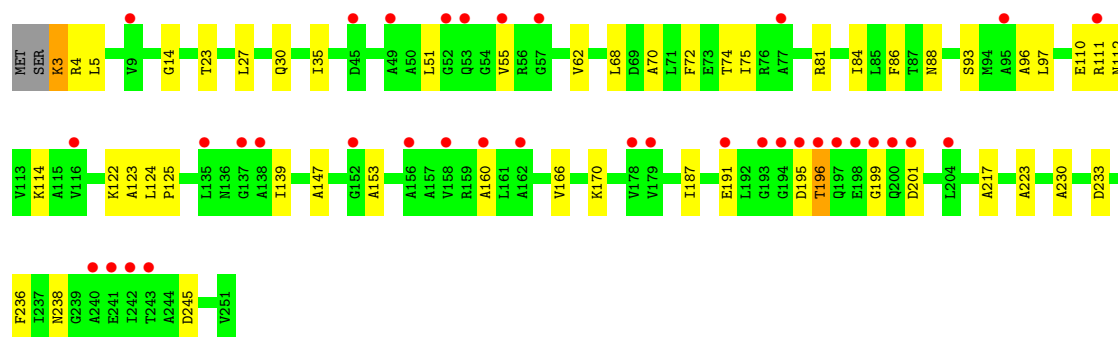# 4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.13Å 111.05Å 229.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.55 – 2.27 48.55 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.55-2.27) 99.3 (48.55-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.220 , 0.254 0.224 , 0.251	Depositor DCC
R_{free} test set	3131 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.031 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7670	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.43	0/1821	0.65	0/2462
1	B	0.41	0/1818	0.62	0/2459
1	C	0.42	0/1824	0.65	0/2467
1	D	0.40	0/1808	0.63	0/2447
All	All	0.41	0/7271	0.64	0/9835

There are no bond length outliers.

There are no bond angle outliers.

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	1804	0	1832	25	0
1	B	1801	0	1830	36	0
1	C	1807	0	1835	40	0
1	D	1791	0	1815	34	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	4	0
3	A	109	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	0	1	0
3	C	69	0	0	0	0
3	D	55	0	0	0	0
All	All	7670	0	7412	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (112) 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:B:172:ARG:CG	1:B:172:ARG:HH11	1.67	1.08
1:B:172:ARG:HH11	1:B:172:ARG:HG3	1.12	1.07
1:C:124:LEU:HB3	1:C:172:ARG:NH1	1.80	0.96
1:D:111:ARG:NH2	2:D:301:NAP:N7A	2.21	0.87
1:C:124:LEU:HD13	1:C:172:ARG:NH1	1.93	0.83
1:B:172:ARG:HG3	1:B:172:ARG:NH1	1.90	0.78
1:C:124:LEU:HB3	1:C:172:ARG:HH12	1.58	0.67
1:D:35:ILE:HD13	1:D:75:ILE:HG12	1.79	0.65
1:B:172:ARG:CG	1:B:172:ARG:NH1	2.39	0.60
1:B:26:ASP:O	1:B:30:GLN:HG2	2.03	0.58
1:B:84:ILE:HG12	1:B:230:ALA:HB1	1.86	0.58
1:C:124:LEU:CD1	1:C:172:ARG:NH1	2.64	0.58
1:D:187:ILE:O	1:D:191:GLU:HG2	2.02	0.58
1:C:43:GLU:N	1:C:43:GLU:OE1	2.35	0.58
1:B:35:ILE:HD13	1:B:75:ILE:HG12	1.85	0.58
1:B:172:ARG:HH11	1:B:172:ARG:HG2	1.66	0.57
1:D:51:LEU:HD12	1:D:55:VAL:HG11	1.86	0.57
1:D:5:LEU:HD13	1:D:27:LEU:HD23	1.85	0.57
1:B:42:ALA:O	1:B:46:GLN:HG3	2.06	0.56
1:C:224:LYS:HB3	1:D:233:ASP:HB3	1.87	0.55
1:B:30:GLN:NE2	3:B:402:HOH:O	2.40	0.53
1:C:42:ALA:O	1:C:46:GLN:HG3	2.08	0.53
1:C:124:LEU:CB	1:C:172:ARG:HH12	2.21	0.53
1:C:124:LEU:CB	1:C:172:ARG:NH1	2.64	0.52
1:C:236:PHE:CE2	1:D:217:ALA:HB2	2.44	0.52
1:B:70:ALA:O	1:B:74:THR:HG23	2.10	0.52
1:C:124:LEU:HB3	1:C:172:ARG:HH11	1.69	0.52
1:D:84:ILE:HG12	1:D:230:ALA:HB1	1.91	0.51
1:B:97:LEU:HG	1:D:124:LEU:HD11	1.91	0.50
1:B:160:ALA:HB3	1:D:153:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HB2	1:C:6:GLU:HG2	1.94	0.50
1:C:62:VAL:HB	1:C:115:ALA:HB1	1.94	0.50
1:B:129:GLN:HG3	1:B:172:ARG:O	2.11	0.49
1:D:5:LEU:HD12	1:D:30:GLN:HG3	1.94	0.49
1:D:166:VAL:HG22	1:D:238:ASN:OD1	2.12	0.49
1:A:70:ALA:O	1:A:74:THR:HG23	2.12	0.49
1:A:97:LEU:HD22	1:C:165:TRP:CD1	2.48	0.49
1:B:39:ARG:NE	2:B:301:NAP:O2X	2.40	0.49
1:B:169:LEU:HD21	1:D:97:LEU:HD23	1.95	0.49
1:C:84:ILE:HG12	1:C:230:ALA:HB1	1.94	0.49
1:C:124:LEU:CD1	1:C:172:ARG:HH12	2.24	0.49
1:B:90:GLY:HA2	1:B:111:ARG:HG2	1.94	0.49
1:A:217:ALA:HB2	1:B:236:PHE:CE2	2.47	0.48
1:A:84:ILE:HG12	1:A:230:ALA:HB1	1.95	0.48
1:A:137:GLY:O	1:A:155:LYS:HE3	2.13	0.48
1:A:217:ALA:HB2	1:B:236:PHE:CD2	2.48	0.48
1:A:236:PHE:CE2	1:B:217:ALA:HB2	2.48	0.48
1:A:121:GLN:HG3	1:C:98:GLY:HA2	1.96	0.48
1:B:62:VAL:HB	1:B:115:ALA:HB1	1.96	0.47
1:D:51:LEU:HB3	1:D:55:VAL:HG21	1.95	0.47
1:C:70:ALA:O	1:C:74:THR:HG23	2.15	0.47
1:A:146:GLN:HG3	1:C:168:ASP:OD1	2.15	0.47
1:C:14:GLY:HA2	2:C:301:NAP:H1B	1.96	0.47
1:B:62:VAL:HG22	2:B:301:NAP:N1A	2.29	0.47
1:C:76:ARG:HG2	1:C:77:ALA:N	2.30	0.47
1:C:155:LYS:HA	1:C:155:LYS:HD2	1.70	0.47
1:C:185:ARG:HG3	1:C:216:LEU:HB3	1.97	0.47
1:A:124:LEU:HD11	1:C:97:LEU:HG	1.97	0.46
1:C:185:ARG:HG2	1:C:216:LEU:HD12	1.97	0.46
1:B:105:PHE:CD1	1:D:114:LYS:HD2	2.50	0.46
1:A:138:ALA:HB1	3:A:476:HOH:O	2.14	0.46
1:B:108:THR:HG21	1:B:150:ILE:HG22	1.97	0.46
1:C:217:ALA:HB2	1:D:236:PHE:CE2	2.51	0.46
1:C:185:ARG:HG3	1:C:216:LEU:CB	2.45	0.46
1:D:3:LYS:HB3	1:D:4:ARG:H	1.55	0.46
1:D:111:ARG:HG3	1:D:112:ASN:OD1	2.16	0.46
1:D:5:LEU:HB2	1:D:30:GLN:HB2	1.97	0.46
1:A:153:ALA:HB1	1:C:157:ALA:HB1	1.98	0.45
1:B:14:GLY:HA2	2:B:301:NAP:H1B	1.99	0.45
1:C:11:LEU:HD23	1:C:85:LEU:HD13	1.99	0.45
1:A:14:GLY:HA2	2:A:301:NAP:H1B	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HA	1:A:161:LEU:HD12	1.98	0.45
1:A:160:ALA:HB3	1:C:153:ALA:HA	1.99	0.45
1:D:23:THR:HA	1:D:223:ALA:HB1	1.98	0.45
1:D:111:ARG:NH2	2:D:301:NAP:C8A	2.80	0.45
1:B:172:ARG:NH1	1:B:172:ARG:HG2	2.28	0.44
1:D:86:PHE:CE2	1:D:88:ASN:HB2	2.52	0.44
1:B:5:LEU:HB2	1:B:30:GLN:HB2	1.99	0.44
1:C:108:THR:O	1:C:112:ASN:HB2	2.17	0.44
1:A:3:LYS:HD3	1:A:3:LYS:HA	1.64	0.44
1:A:76:ARG:NH2	3:A:404:HOH:O	2.42	0.44
1:B:5:LEU:HD12	1:B:30:GLN:HG3	1.99	0.43
1:A:97:LEU:HD22	1:C:165:TRP:CG	2.54	0.43
1:A:106:ASP:O	1:A:110:GLU:HB2	2.18	0.43
1:C:185:ARG:HE	1:C:216:LEU:HB2	1.84	0.43
1:C:196:THR:O	1:C:200:GLN:HG3	2.18	0.43
1:C:217:ALA:HB2	1:D:236:PHE:CD2	2.54	0.43
1:D:139:ILE:HG21	1:D:245:ASP:HB3	2.00	0.43
1:B:157:ALA:HB1	1:D:153:ALA:HB1	2.01	0.43
1:D:70:ALA:O	1:D:74:THR:HG23	2.19	0.43
1:A:236:PHE:CD2	1:B:217:ALA:HB2	2.54	0.43
1:B:138:ALA:HB3	1:B:155:LYS:HG3	2.00	0.42
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.73	0.42
1:D:62:VAL:HG22	2:D:301:NAP:N1A	2.32	0.42
1:B:62:VAL:HG22	2:B:301:NAP:C6A	2.49	0.42
1:B:215:ARG:NH1	1:B:221:GLU:OE2	2.37	0.42
1:C:137:GLY:O	2:C:301:NAP:H6N	2.20	0.42
1:D:72:PHE:CZ	1:D:123:ALA:HB2	2.54	0.42
1:D:196:THR:HG23	1:D:199:GLY:HA3	1.99	0.42
1:A:60:SER:HB2	3:A:483:HOH:O	2.19	0.42
1:D:14:GLY:HA2	2:D:301:NAP:H1B	2.01	0.42
1:A:135:LEU:HB2	1:A:178:VAL:HG22	2.02	0.42
1:D:96:ALA:HA	1:D:147:ALA:HA	2.02	0.42
1:D:122:LYS:O	1:D:125:PRO:HD2	2.19	0.42
1:A:153:ALA:HA	1:C:160:ALA:HB3	2.01	0.41
1:C:82:LEU:O	1:C:127:MET:HA	2.20	0.41
1:B:153:ALA:HA	1:D:160:ALA:HB3	2.03	0.41
1:C:13:THR:O	1:C:88:ASN:HB3	2.21	0.41
1:D:68:LEU:HB3	1:D:122:LYS:HD3	2.03	0.41
1:A:120:VAL:CG1	1:C:97:LEU:HD21	2.51	0.40
1:B:39:ARG:HE	1:B:39:ARG:HB2	1.72	0.40
1:B:59:ARG:NH1	1:B:59:ARG:HB3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/251 (98%)	244 (99%)	3 (1%)	0	100	100
1	B	247/251 (98%)	245 (99%)	2 (1%)	0	100	100
1	C	248/251 (99%)	247 (100%)	1 (0%)	0	100	100
1	D	247/251 (98%)	245 (99%)	2 (1%)	0	100	100
All	All	989/1004 (98%)	981 (99%)	8 (1%)	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	182/185 (98%)	175 (96%)	7 (4%)	33	44
1	B	182/185 (98%)	169 (93%)	13 (7%)	14	17
1	C	183/185 (99%)	177 (97%)	6 (3%)	38	51
1	D	180/185 (97%)	172 (96%)	8 (4%)	28	37
All	All	727/740 (98%)	693 (95%)	34 (5%)	26	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	60	SER
1	A	93	SER
1	A	103	GLN
1	A	159	ARG
1	A	170	LYS
1	A	183	SER
1	B	3	LYS
1	B	60	SER
1	B	74	THR
1	B	81	ARG
1	B	93	SER
1	B	101	SER
1	B	129	GLN
1	B	159	ARG
1	B	170	LYS
1	B	172	ARG
1	B	195	ASP
1	B	196	THR
1	B	198	GLU
1	C	3	LYS
1	C	6	GLU
1	C	76	ARG
1	C	159	ARG
1	C	187	ILE
1	C	209	SER
1	D	3	LYS
1	D	81	ARG
1	D	93	SER
1	D	110	GLU
1	D	170	LYS
1	D	195	ASP
1	D	196	THR
1	D	201	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	129	GLN
1	B	200	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	D	301	-	45,52,52	0.68	1 (2%)	56,80,80	0.82	1 (1%)
2	NAP	B	301	-	45,52,52	0.73	1 (2%)	56,80,80	0.86	2 (3%)
2	NAP	C	301	-	45,52,52	0.73	1 (2%)	56,80,80	0.87	2 (3%)
2	NAP	A	301	-	45,52,52	0.74	1 (2%)	56,80,80	0.86	3 (5%)

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	D	301	-	-	4/31/67/67	0/5/5/5
2	NAP	B	301	-	-	5/31/67/67	0/5/5/5
2	NAP	C	301	-	-	4/31/67/67	0/5/5/5
2	NAP	A	301	-	-	4/31/67/67	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2N-N1N	2.85	1.38	1.35
2	A	301	NAP	C2N-N1N	2.75	1.38	1.35
2	C	301	NAP	C2N-N1N	2.62	1.38	1.35
2	D	301	NAP	C2N-N1N	2.55	1.38	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	C5A-C6A-N6A	2.75	124.53	120.35
2	A	301	NAP	C5A-C6A-N6A	2.49	124.14	120.35
2	C	301	NAP	C6N-N1N-C2N	-2.31	119.87	121.97
2	D	301	NAP	C5A-C6A-N6A	2.21	123.70	120.35
2	B	301	NAP	C5A-C6A-N6A	2.16	123.63	120.35
2	B	301	NAP	O2B-P2B-O1X	-2.14	101.11	109.39
2	A	301	NAP	C3B-C2B-C1B	-2.11	98.92	102.89
2	A	301	NAP	C6N-N1N-C2N	-2.08	120.08	121.97

There are no chirality outliers.

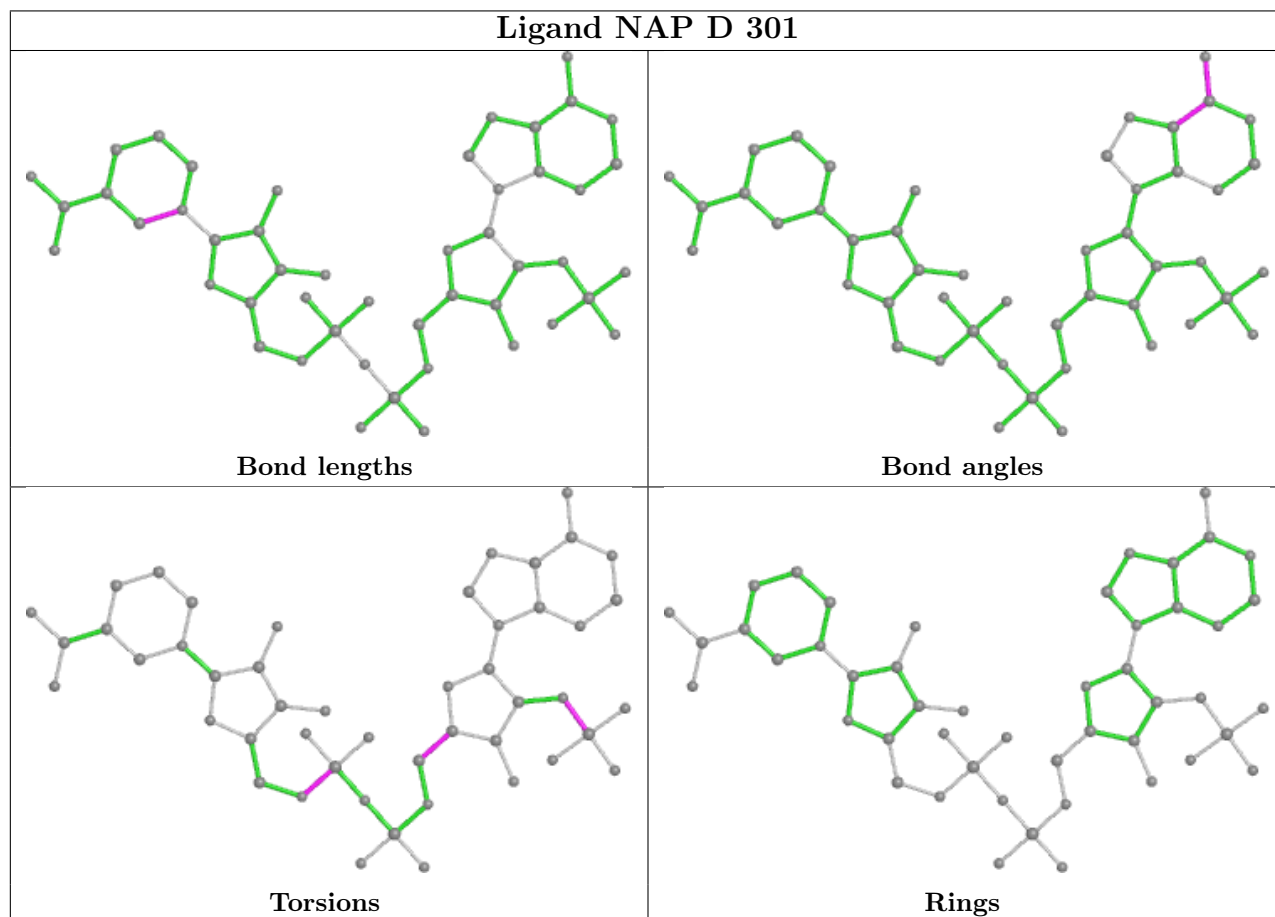All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.
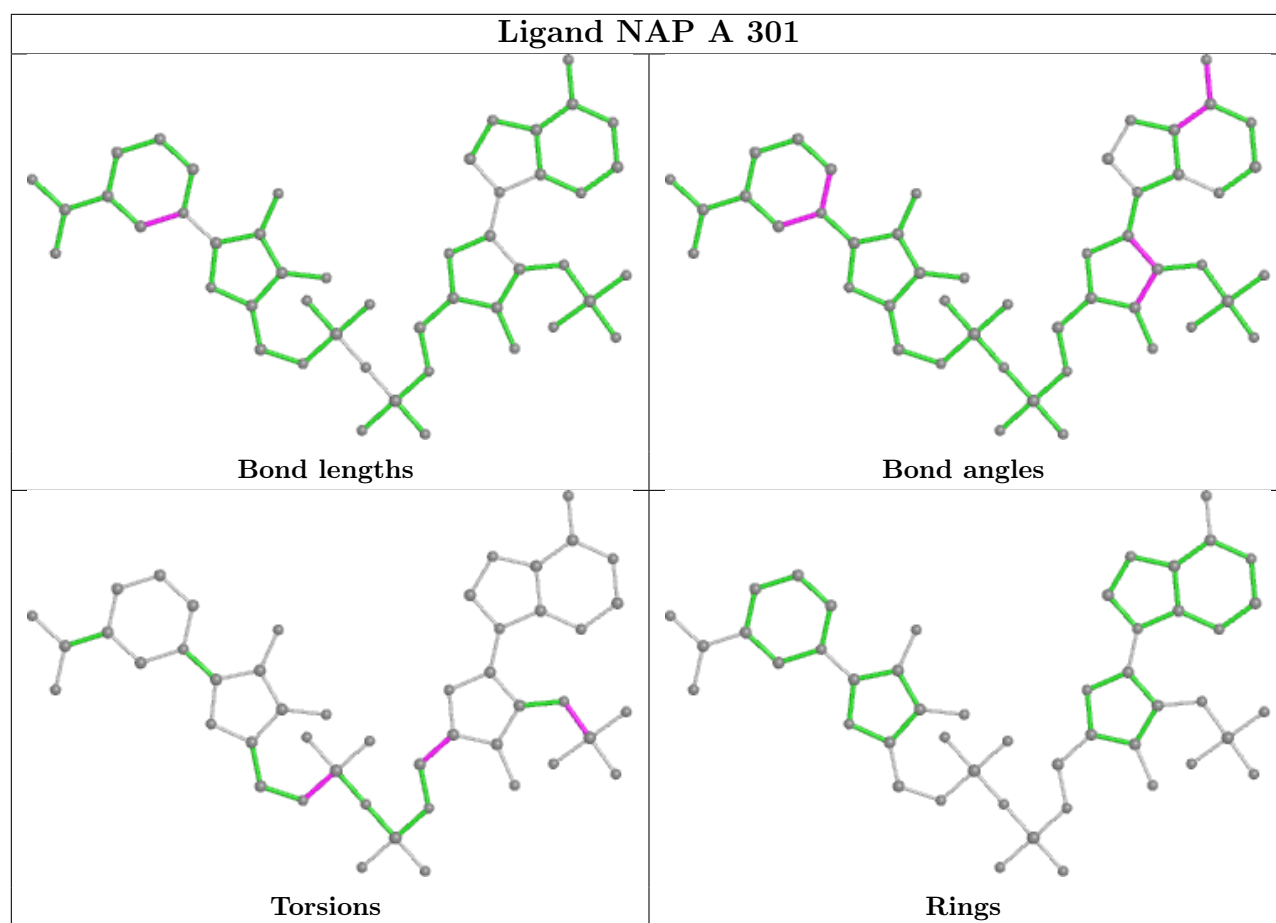
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	NAP	4	0
2	B	301	NAP	4	0
2	C	301	NAP	2	0
2	A	301	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 then 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.

Ligand NAP D 301

Ligand NAP B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 301

Bond lengths

Bond angles

Torsions

Rings
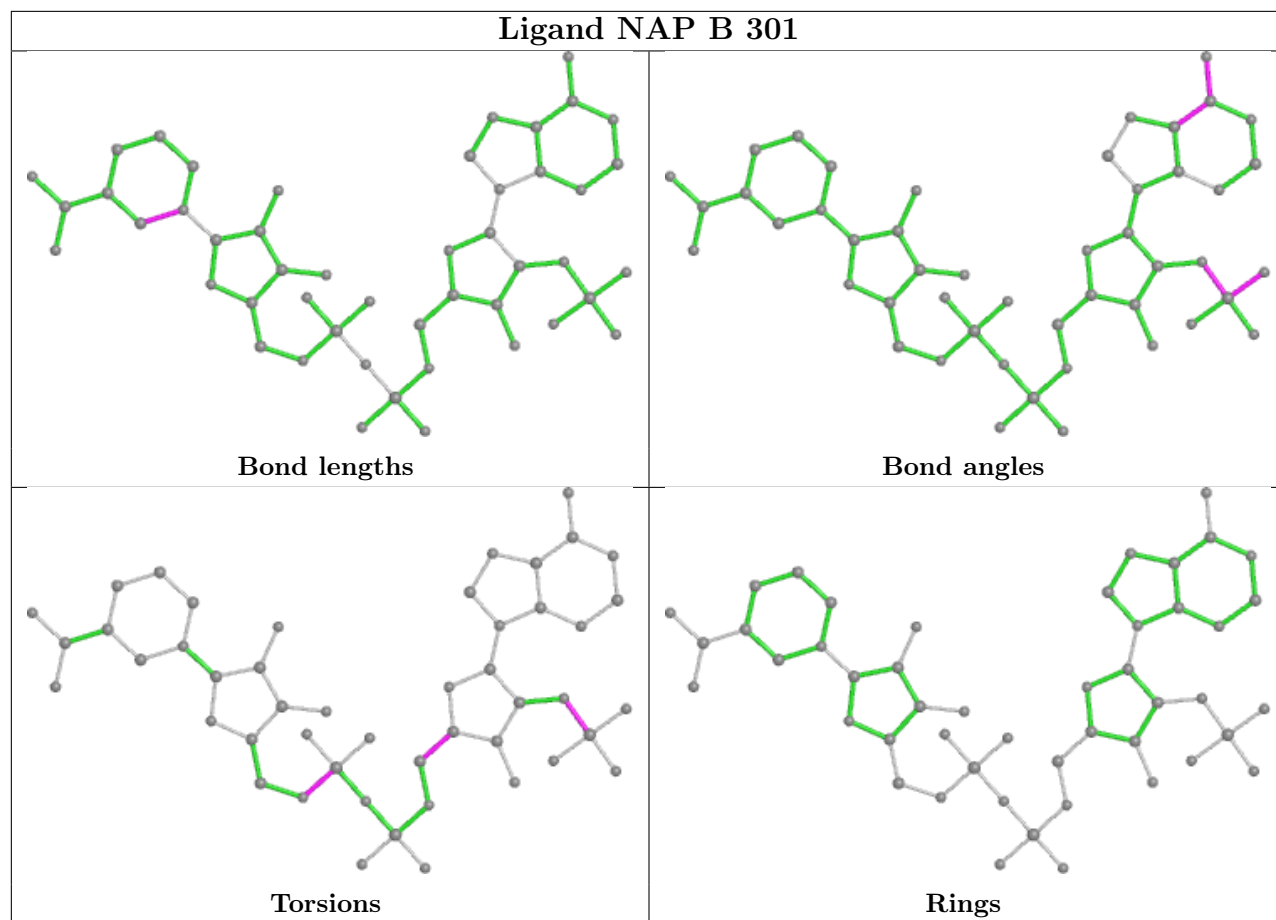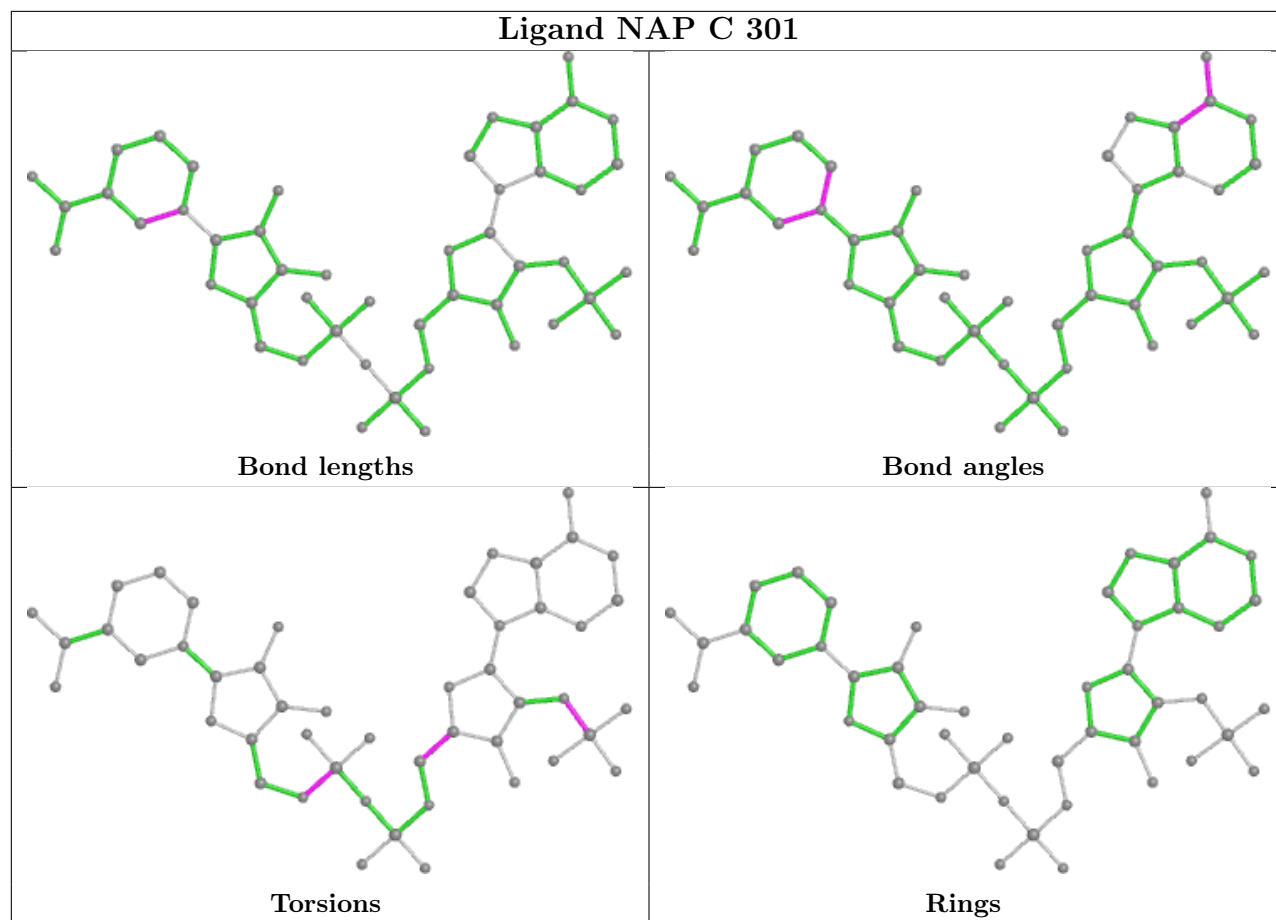
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	249/251 (99%)	0.14	2 (0%)	86	89	29, 39, 54, 77	0
1	B	249/251 (99%)	0.69	29 (11%)	4	6	37, 52, 75, 91	0
1	C	250/251 (99%)	0.67	24 (9%)	8	10	32, 45, 73, 87	0
1	D	249/251 (99%)	0.84	36 (14%)	2	3	38, 51, 76, 101	0
All	All	997/1004 (99%)	0.59	91 (9%)	9	11	29, 47, 71, 101	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	ASP	5.7
1	C	195	ASP	5.4
1	C	2	SER	5.2
1	C	196	THR	5.1
1	D	53	GLN	4.9
1	B	196	THR	4.6
1	C	185	ARG	4.5
1	B	195	ASP	4.3
1	D	196	THR	4.3
1	C	194	GLY	4.3
1	D	178	VAL	4.0
1	B	54	GLY	3.8
1	C	198	GLU	3.8
1	D	49	ALA	3.7
1	B	193	GLY	3.5
1	B	53	GLN	3.5
1	D	198	GLU	3.5
1	B	187	ILE	3.5
1	A	195	ASP	3.4
1	C	54	GLY	3.2
1	B	6	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	197	GLN	3.1
1	D	95	ALA	3.1
1	B	197	GLN	3.0
1	C	200	GLN	3.0
1	D	158	VAL	3.0
1	C	202	GLY	3.0
1	D	179	VAL	3.0
1	B	3	LYS	2.9
1	D	45	ASP	2.9
1	C	78	THR	2.8
1	C	244	ALA	2.8
1	C	242	ILE	2.8
1	B	156	ALA	2.8
1	C	76	ARG	2.8
1	D	199	GLY	2.8
1	A	202	GLY	2.7
1	B	198	GLU	2.7
1	D	9	VAL	2.7
1	C	243	THR	2.7
1	D	77	ALA	2.6
1	D	55	VAL	2.6
1	B	201	ASP	2.6
1	B	51	LEU	2.6
1	B	81	ARG	2.6
1	D	160	ALA	2.6
1	D	111	ARG	2.6
1	D	243	THR	2.6
1	B	77	ALA	2.6
1	D	135	LEU	2.5
1	C	193	GLY	2.5
1	B	203	THR	2.5
1	D	201	ASP	2.5
1	B	199	GLY	2.5
1	B	194	GLY	2.5
1	D	204	LEU	2.5
1	B	200	GLN	2.4
1	D	200	GLN	2.4
1	C	6	GLU	2.4
1	C	191	GLU	2.4
1	D	240	ALA	2.4
1	D	52	GLY	2.4
1	D	197	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	137	GLY	2.3
1	D	162	ALA	2.3
1	C	204	LEU	2.3
1	B	47	ALA	2.3
1	D	194	GLY	2.3
1	C	199	GLY	2.2
1	B	191	GLU	2.2
1	D	191	GLU	2.2
1	C	158	VAL	2.2
1	B	160	ALA	2.2
1	C	203	THR	2.2
1	D	116	VAL	2.2
1	C	201	ASP	2.2
1	B	71	LEU	2.2
1	C	179	VAL	2.2
1	D	241	GLU	2.2
1	B	153	ALA	2.1
1	D	156	ALA	2.1
1	D	193	GLY	2.1
1	B	44	LEU	2.1
1	B	171	GLU	2.1
1	D	138	ALA	2.1
1	B	45	ASP	2.1
1	D	242	ILE	2.1
1	D	57	GLY	2.1
1	D	152	GLY	2.0
1	B	75	ILE	2.0
1	B	49	ALA	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
2	NAP	B	301	48/48	0.90	0.13	43,50,55,62	0
2	NAP	D	301	48/48	0.94	0.14	41,49,55,57	0
2	NAP	C	301	48/48	0.95	0.12	38,48,57,59	0
2	NAP	A	301	48/48	0.97	0.12	22,34,38,44	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.
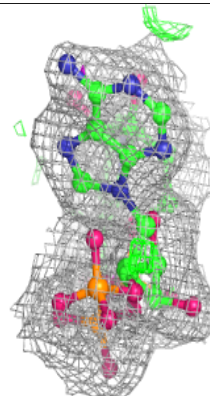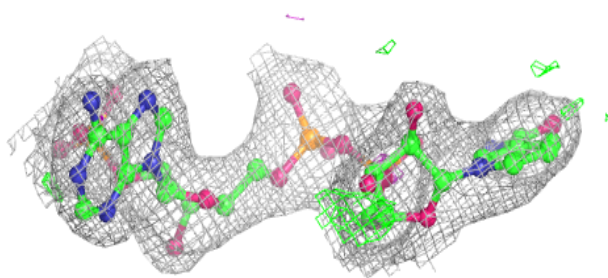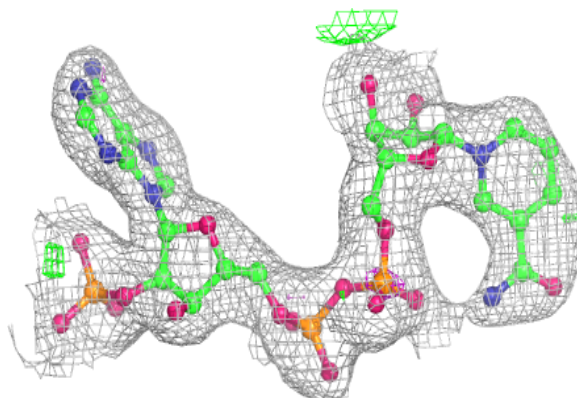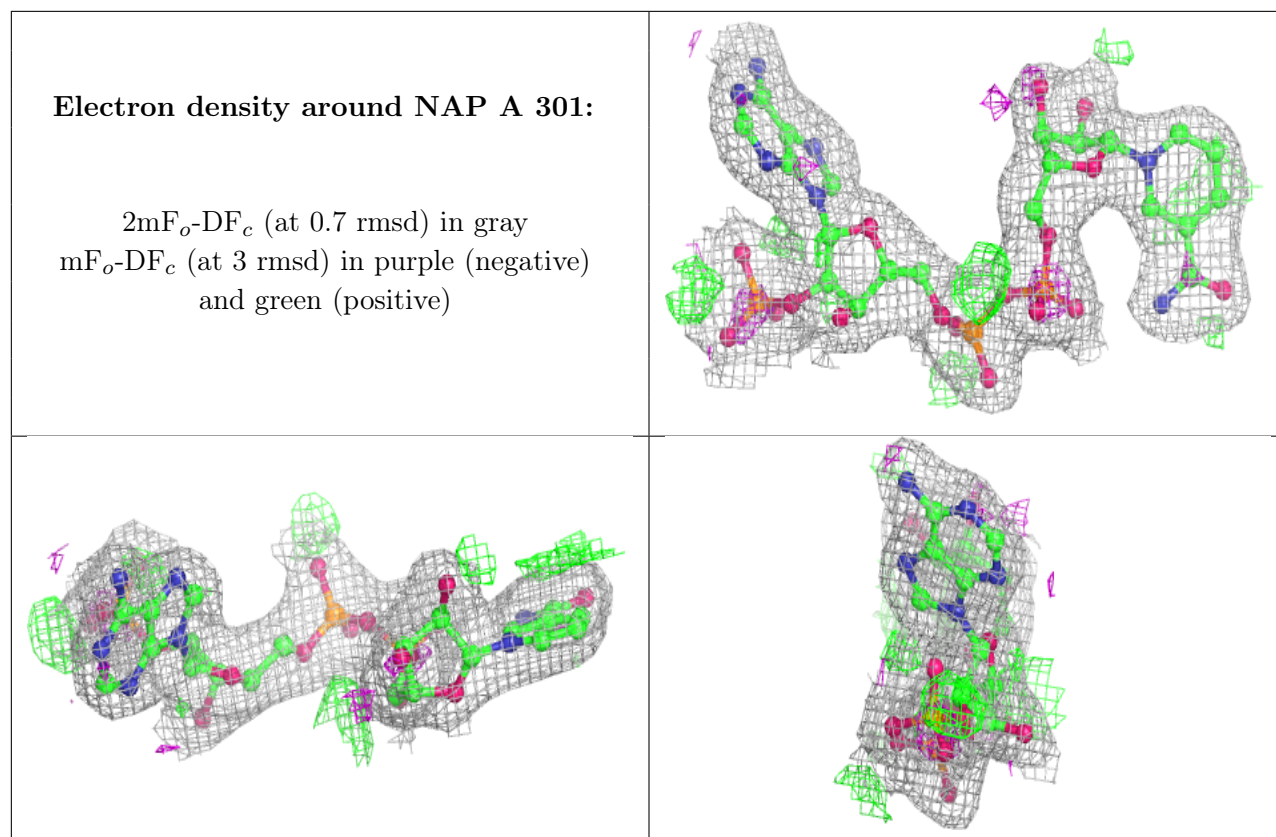

Electron density around NAP B 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
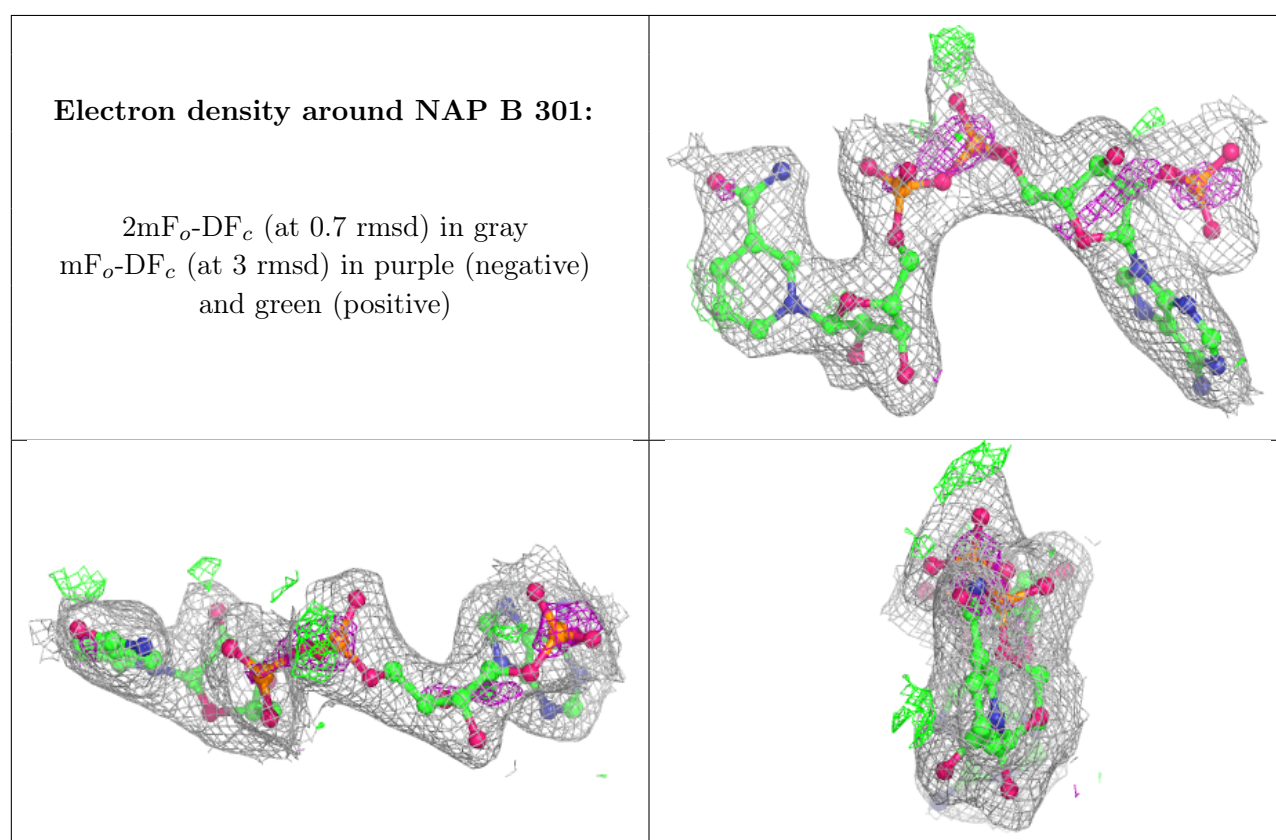
Electron density around NAP D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
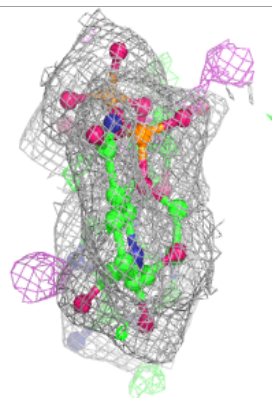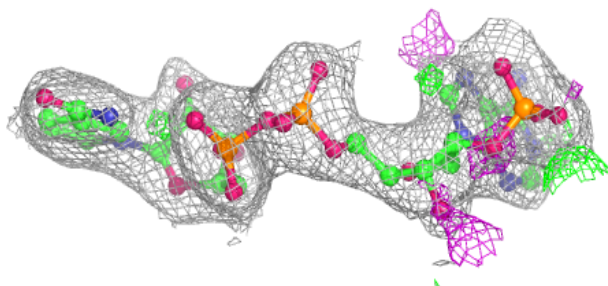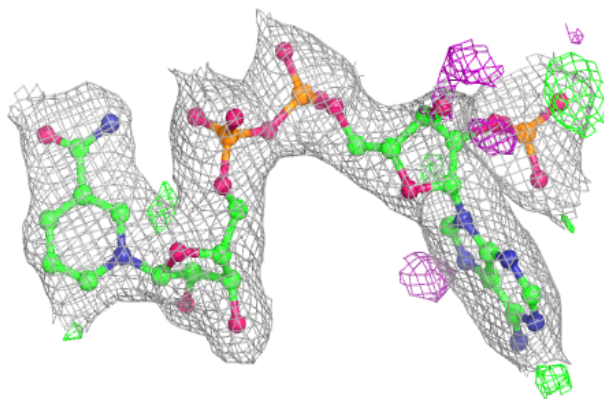
Electron density around NAP C 301:

$2mF_o$-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 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.