Full wwPDB X-ray Structure Validation Report (i)

May 31, 2022 – 06:37 pm BST

PDB ID	:	7ZBO
Title	:	Amine Dehydrogenase MATOUAmDH2 in complex with NADP+
Authors	:	Bennett, M.; Ducrot, L.; Vergne-Vaxelaire, C.; Grogan, G.
Deposited on	:	2022-03-24
Resolution	:	2.32 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 (i) symbol.

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

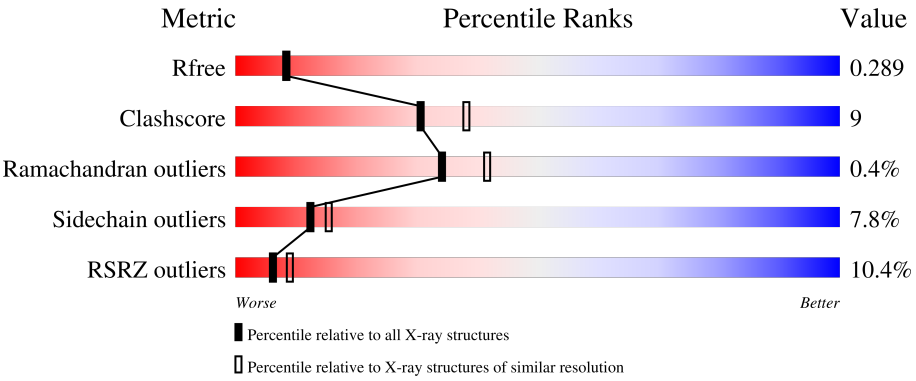
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	351	3% 80% 17%
1	B	351	15% 76% 20%
1	C	351	8% 77% 18%
1	D	351	15% 78% 17%

2 Entry composition

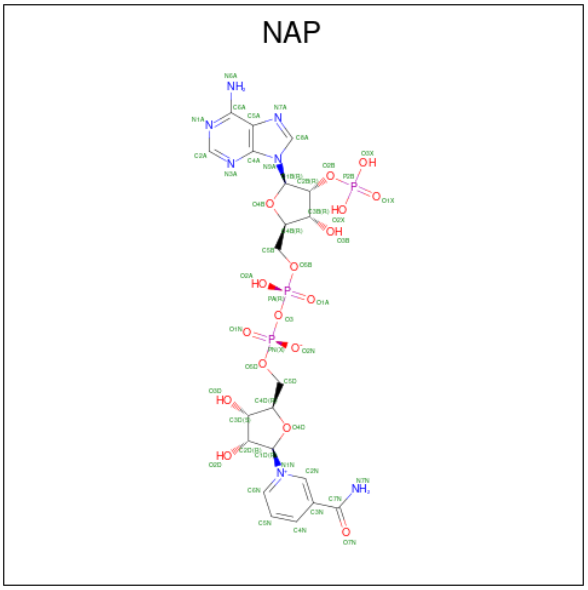
There are 3 unique types of molecules in this entry. The entry contains 10633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2623	1653	430	519	21			
1	B	343	Total	C	N	O	S	0	0	0
			2541	1602	413	505	21			
1	C	340	Total	C	N	O	S	0	0	0
			2553	1611	419	502	21			
1	D	340	Total	C	N	O	S	0	0	0
			2489	1562	413	494	20			

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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.

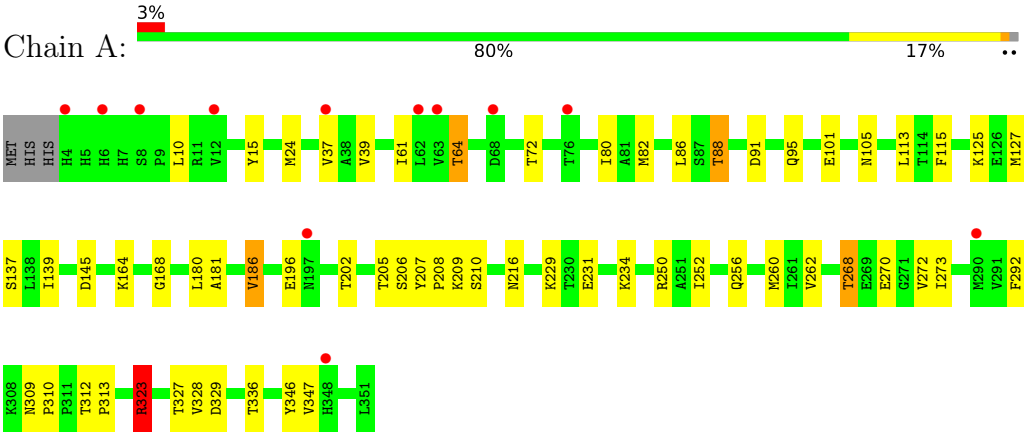
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	41	Total	O	0	0
			41	41		
3	C	71	Total	O	0	0
			71	71		
3	D	49	Total	O	0	0
			49	49		

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.

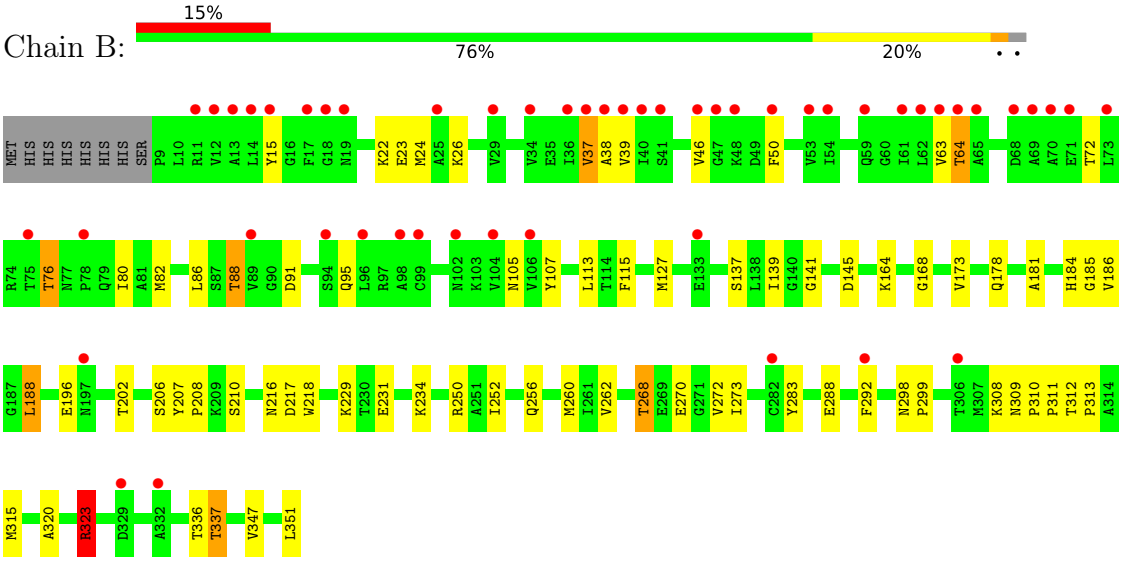
• Molecule 1: Amine Dehydrogenase

Chain A:



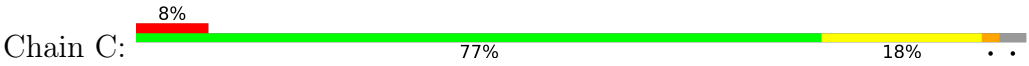
• Molecule 1: Amine Dehydrogenase

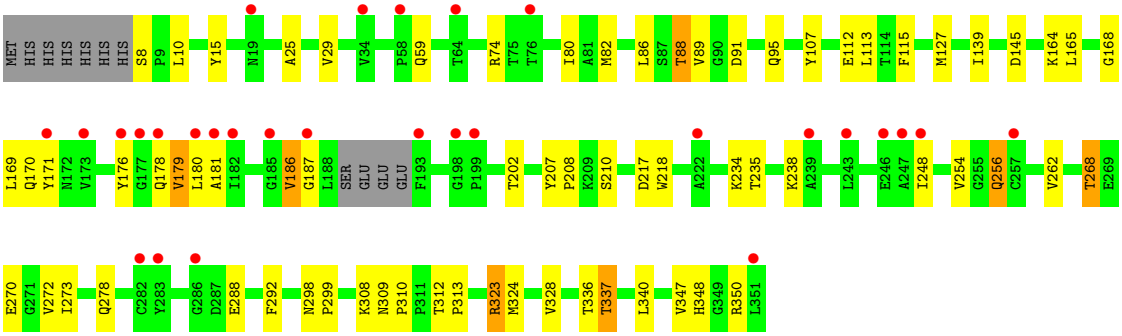
Chain B:



• Molecule 1: Amine Dehydrogenase

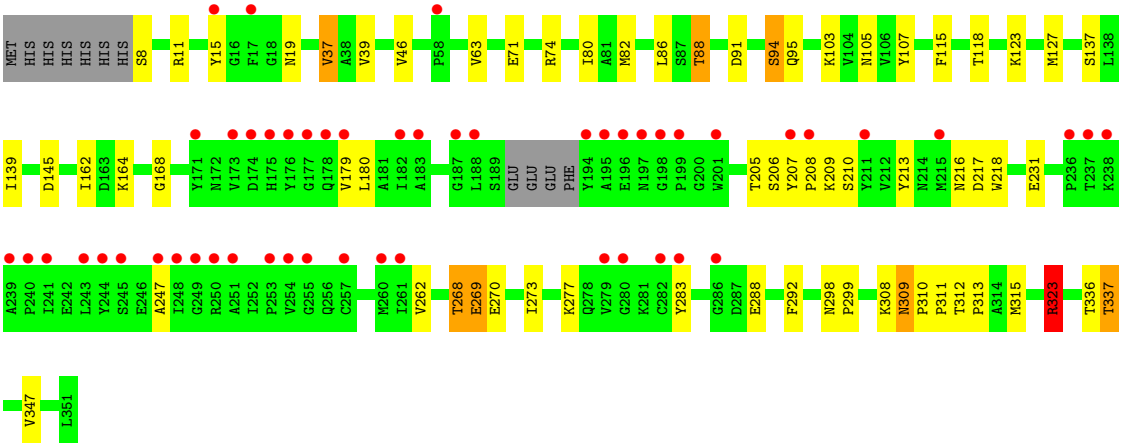
Chain C:





• Molecule 1: Amine Dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.10Å 112.19Å 153.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.21 – 2.32 64.21 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.21-2.32) 100.0 (64.21-2.32)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.237 , 0.288 0.241 , 0.289	Depositor DCC
R_{free} test set	3432 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10633	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0379e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.73	0/2676	0.88	3/3638 (0.1%)
1	B	0.73	0/2589	0.89	2/3520 (0.1%)
1	C	0.73	0/2601	0.89	4/3530 (0.1%)
1	D	0.72	0/2533	0.90	3/3444 (0.1%)
All	All	0.73	0/10399	0.89	12/14132 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	323	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	D	323	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	C	323	ARG	CG-CD-NE	7.99	128.57	111.80
1	D	323	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	323	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	323	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	323	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	323	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	269	GLU	CB-CA-C	5.65	121.69	110.40
1	B	323	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	350	ARG	CG-CD-NE	5.13	122.58	111.80
1	A	323	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2623	0	2544	41	0
1	B	2541	0	2440	60	0
1	C	2553	0	2504	46	0
1	D	2489	0	2388	45	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	74	0	0	1	0
3	B	41	0	0	0	0
3	C	71	0	0	2	0
3	D	49	0	0	3	0
All	All	10633	0	9976	188	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 9.

All (188) 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:A:24:MET:HE2	1:A:82:MET:HG3	1.42	1.01
1:B:24:MET:HE2	1:B:82:MET:HG3	1.47	0.97
1:C:178:GLN:O	1:C:179:VAL:HG22	1.67	0.95
1:B:37:VAL:HG13	1:B:76:THR:HG23	1.48	0.93
1:B:168:GLY:HA3	1:B:292:PHE:CZ	2.04	0.93
1:B:145:ASP:OD1	1:B:337:THR:HG21	1.70	0.91
1:A:24:MET:CE	1:A:82:MET:HG3	2.03	0.88
1:C:145:ASP:OD1	1:C:337:THR:HG21	1.74	0.88
1:D:145:ASP:OD1	1:D:337:THR:HG21	1.75	0.86
1:C:80:ILE:HG12	1:C:82:MET:HE2	1.60	0.83
1:D:11:ARG:NH1	1:D:37:VAL:HG21	1.94	0.81
1:B:37:VAL:HG13	1:B:76:THR:CG2	2.13	0.79
1:B:38:ALA:HB2	1:B:76:THR:HG21	1.66	0.78
1:A:101:GLU:OE1	3:A:501:HOH:O	2.03	0.77
1:A:234:LYS:HD3	1:A:260:MET:HE1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PRO:HD2	1:B:315:MET:CE	2.18	0.73
1:D:46:VAL:O	1:D:63:VAL:O	2.06	0.73
1:A:24:MET:CE	1:A:82:MET:CG	2.68	0.72
1:D:218:TRP:HE1	1:D:337:THR:HG22	1.54	0.70
1:A:250:ARG:HH12	1:A:256:GLN:HE22	1.37	0.70
1:B:46:VAL:O	1:B:63:VAL:O	2.08	0.70
1:A:80:ILE:CD1	1:A:82:MET:HE1	2.21	0.70
1:A:307:MET:HE2	1:A:310:PRO:HB3	1.73	0.69
1:C:186:VAL:HG21	1:C:248:ILE:HG21	1.74	0.69
1:D:80:ILE:HD13	1:D:82:MET:HE1	1.75	0.69
1:B:250:ARG:HH12	1:B:256:GLN:HE22	1.41	0.67
1:D:80:ILE:CD1	1:D:82:MET:HE1	2.25	0.67
1:A:24:MET:HE1	1:A:82:MET:SD	2.34	0.66
1:D:218:TRP:NE1	1:D:337:THR:HG22	2.11	0.66
1:C:168:GLY:HA3	1:C:292:PHE:CE1	2.31	0.66
1:B:37:VAL:CG1	1:B:76:THR:HG23	2.25	0.66
1:B:105:ASN:HD22	1:B:137:SER:H	1.43	0.66
1:A:80:ILE:HD13	1:A:82:MET:HE1	1.77	0.65
1:A:105:ASN:HD22	1:A:137:SER:H	1.42	0.65
1:D:105:ASN:HD22	1:D:137:SER:H	1.44	0.65
1:A:88:THR:HG22	1:A:91:ASP:H	1.63	0.64
1:B:311:PRO:CD	1:B:315:MET:CE	2.75	0.64
1:B:88:THR:HG22	1:B:91:ASP:H	1.63	0.64
1:B:218:TRP:HE1	1:B:337:THR:HG22	1.62	0.64
1:C:89:VAL:HG23	1:C:112:GLU:OE1	1.99	0.63
1:C:169:LEU:HD22	1:C:171:TYR:HD1	1.64	0.62
1:B:80:ILE:HD13	1:B:82:MET:HE1	1.81	0.62
1:B:311:PRO:HG2	1:B:315:MET:HE2	1.81	0.62
1:C:88:THR:HG22	1:C:91:ASP:H	1.65	0.62
1:C:262:VAL:HB	1:C:278:GLN:HG2	1.81	0.62
1:D:88:THR:HG22	1:D:91:ASP:H	1.64	0.61
1:C:218:TRP:HE1	1:C:337:THR:HG22	1.65	0.61
1:A:24:MET:HE1	1:A:82:MET:CG	2.31	0.61
1:B:80:ILE:CD1	1:B:82:MET:HE1	2.30	0.61
1:A:24:MET:HE2	1:A:82:MET:CG	2.22	0.61
1:B:311:PRO:CD	1:B:315:MET:HE2	2.31	0.60
1:B:311:PRO:HD2	1:B:315:MET:HE1	1.83	0.59
1:B:24:MET:HE2	1:B:82:MET:CG	2.27	0.58
1:B:218:TRP:NE1	1:B:337:THR:HG22	2.17	0.58
1:C:181:ALA:HB1	1:C:186:VAL:HG11	1.84	0.58
1:C:218:TRP:NE1	1:C:337:THR:HG22	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:PRO:HB2	1:D:315:MET:HE3	1.86	0.57
1:D:168:GLY:HA3	1:D:292:PHE:CE2	2.38	0.57
1:A:168:GLY:HA3	1:A:292:PHE:CE2	2.39	0.57
1:B:168:GLY:HA3	1:B:292:PHE:CE2	2.37	0.57
1:C:82:MET:HE1	1:C:324:MET:HG2	1.85	0.57
1:D:310:PRO:HB2	1:D:315:MET:CE	2.35	0.56
1:D:310:PRO:CB	1:D:315:MET:HE1	2.36	0.56
1:C:254:VAL:O	3:C:501:HOH:O	2.18	0.54
1:C:115:PHE:CD1	1:C:336:THR:HG21	2.43	0.54
1:D:247:ALA:HA	3:D:547:HOH:O	2.06	0.54
1:B:311:PRO:CG	1:B:315:MET:HE2	2.39	0.53
1:C:178:GLN:O	1:C:179:VAL:CG2	2.48	0.53
1:D:145:ASP:OD2	1:D:323:ARG:HD2	2.09	0.53
1:A:181:ALA:O	1:A:186:VAL:HG13	2.09	0.52
1:A:80:ILE:HG12	1:A:82:MET:CE	2.39	0.52
1:D:311:PRO:CD	1:D:315:MET:HE2	2.39	0.52
1:B:181:ALA:O	1:B:186:VAL:HG13	2.09	0.52
1:C:80:ILE:HD13	1:C:82:MET:HE1	1.90	0.52
1:C:169:LEU:HD23	1:C:170:GLN:N	2.25	0.52
1:D:80:ILE:HG12	1:D:82:MET:CE	2.40	0.52
1:A:64:THR:HG21	1:A:72:THR:OG1	2.10	0.52
1:D:210:SER:HB3	1:D:262:VAL:HG11	1.92	0.51
1:B:168:GLY:HA3	1:B:292:PHE:CE1	2.44	0.51
1:B:64:THR:HG21	1:B:72:THR:OG1	2.11	0.50
1:A:210:SER:HB3	1:A:262:VAL:HG11	1.93	0.50
1:A:125:LYS:NZ	1:A:129:GLU:OE2	2.42	0.50
1:D:115:PHE:CD1	1:D:336:THR:HG21	2.46	0.50
1:B:115:PHE:CD1	1:B:336:THR:HG21	2.46	0.50
1:A:268:THR:HG21	1:A:272:VAL:HB	1.94	0.50
1:D:207:TYR:CD1	1:D:208:PRO:HA	2.47	0.50
1:B:311:PRO:HD2	1:B:315:MET:HE2	1.88	0.50
1:D:80:ILE:HG12	1:D:82:MET:HE2	1.94	0.49
1:C:80:ILE:CG1	1:C:82:MET:HE2	2.39	0.49
1:C:348:HIS:ND1	3:C:503:HOH:O	2.34	0.49
1:D:207:TYR:CG	1:D:208:PRO:HA	2.46	0.49
1:A:91:ASP:OD2	1:B:196:GLU:OE2	2.30	0.49
1:C:207:TYR:CG	1:C:208:PRO:HA	2.48	0.49
1:B:288:GLU:HB3	1:B:309:ASN:OD1	2.13	0.49
1:C:127:MET:HA	1:C:127:MET:CE	2.42	0.49
1:D:311:PRO:HD2	1:D:315:MET:HE1	1.95	0.48
1:B:210:SER:HB3	1:B:262:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:TYR:CG	1:B:208:PRO:HA	2.48	0.48
1:D:311:PRO:HD2	1:D:315:MET:CE	2.44	0.48
1:B:185:GLY:HA2	1:B:188:LEU:HD22	1.95	0.48
1:A:196:GLU:OE2	1:B:91:ASP:OD2	2.32	0.47
1:A:252:ILE:HG23	1:A:256:GLN:HE21	1.79	0.47
1:B:80:ILE:HG12	1:B:82:MET:HE2	1.96	0.47
1:C:207:TYR:CD1	1:C:208:PRO:HA	2.48	0.47
1:D:127:MET:HA	1:D:127:MET:CE	2.44	0.47
1:A:207:TYR:CG	1:A:208:PRO:HA	2.49	0.47
1:C:115:PHE:CD2	1:C:217:ASP:HB3	2.50	0.47
1:C:210:SER:HB3	1:C:262:VAL:HG11	1.96	0.47
1:B:80:ILE:HG12	1:B:82:MET:CE	2.44	0.47
1:C:186:VAL:HG21	1:C:248:ILE:CG2	2.45	0.47
1:B:115:PHE:CD2	1:B:217:ASP:HB3	2.49	0.47
1:A:268:THR:HG23	1:A:270:GLU:H	1.79	0.46
1:D:311:PRO:CD	1:D:315:MET:CE	2.93	0.46
1:D:311:PRO:N	1:D:315:MET:HE2	2.30	0.46
1:A:10:LEU:HD11	1:A:328:VAL:HG21	1.96	0.46
1:B:268:THR:HG21	1:B:272:VAL:HB	1.97	0.46
1:B:298:ASN:HA	1:B:299:PRO:C	2.35	0.46
1:B:252:ILE:HG23	1:B:256:GLN:HE21	1.80	0.46
1:B:268:THR:HG23	1:B:270:GLU:H	1.79	0.46
1:D:94:SER:HB2	3:D:545:HOH:O	2.15	0.46
1:B:86:LEU:HD13	1:B:91:ASP:HB3	1.97	0.46
1:B:145:ASP:OD2	1:B:323:ARG:HD3	2.15	0.46
1:B:310:PRO:HB2	1:B:315:MET:HE3	1.98	0.45
1:C:268:THR:HG23	1:C:270:GLU:H	1.81	0.45
1:D:115:PHE:CD2	1:D:217:ASP:HB3	2.51	0.45
1:C:268:THR:HG21	1:C:272:VAL:HB	1.97	0.45
1:D:268:THR:HG23	1:D:270:GLU:H	1.79	0.45
1:B:234:LYS:HB3	1:B:260:MET:CE	2.47	0.45
1:D:86:LEU:HD13	1:D:91:ASP:HB3	1.99	0.45
1:D:309:ASN:N	1:D:310:PRO:CD	2.80	0.45
1:D:310:PRO:CA	1:D:315:MET:HE1	2.47	0.45
1:A:115:PHE:CD2	1:A:336:THR:HG21	2.52	0.44
1:D:298:ASN:HA	1:D:299:PRO:C	2.38	0.44
1:D:311:PRO:N	1:D:315:MET:CE	2.80	0.44
1:A:164:LYS:HA	1:A:273:ILE:O	2.17	0.44
1:B:23:GLU:OE1	1:B:26:LYS:HD2	2.18	0.44
1:A:145:ASP:OD2	1:A:323:ARG:HD3	2.18	0.44
1:C:298:ASN:HA	1:C:299:PRO:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LYS:HA	1:D:273:ILE:O	2.17	0.44
1:A:298:ASN:HA	1:A:299:PRO:C	2.37	0.44
1:D:310:PRO:CB	1:D:315:MET:CE	2.95	0.44
1:C:10:LEU:HD11	1:C:328:VAL:HG21	1.99	0.44
1:B:234:LYS:HD3	1:B:260:MET:HE1	2.00	0.44
1:C:202:THR:CG2	1:C:234:LYS:HG3	2.48	0.44
1:A:86:LEU:HD13	1:A:91:ASP:HB3	2.00	0.43
1:B:127:MET:HA	1:B:127:MET:CE	2.47	0.43
1:C:179:VAL:HG23	1:C:180:LEU:N	2.33	0.43
1:A:346:TYR:CD2	1:D:162:ILE:HD12	2.53	0.43
1:C:164:LYS:HA	1:C:273:ILE:O	2.18	0.43
1:D:312:THR:N	1:D:313:PRO:CD	2.82	0.43
1:A:80:ILE:CG1	1:A:82:MET:HE1	2.48	0.43
1:C:187:GLY:HA2	1:C:256:GLN:NE2	2.34	0.43
1:B:173:VAL:HG11	1:B:184:HIS:CG	2.54	0.43
1:D:123:LYS:CG	3:D:526:HOH:O	2.67	0.43
1:C:127:MET:HA	1:C:127:MET:HE2	2.00	0.43
1:B:312:THR:N	1:B:313:PRO:CD	2.82	0.43
1:B:311:PRO:N	1:B:315:MET:CE	2.82	0.43
1:C:86:LEU:HD13	1:C:91:ASP:HB3	2.00	0.43
1:C:218:TRP:CZ2	1:C:337:THR:HG22	2.53	0.42
1:A:312:THR:N	1:A:313:PRO:CD	2.82	0.42
1:B:164:LYS:HA	1:B:273:ILE:O	2.18	0.42
1:B:309:ASN:N	1:B:310:PRO:CD	2.82	0.42
1:C:218:TRP:CE2	1:C:337:THR:HG22	2.54	0.42
1:D:71:GLU:OE2	1:D:74:ARG:NH2	2.39	0.42
1:A:80:ILE:HG12	1:A:82:MET:HE2	2.01	0.42
1:A:80:ILE:HG12	1:A:82:MET:HE1	2.00	0.42
1:B:107:TYR:CE2	1:B:320:ALA:HA	2.55	0.42
1:A:127:MET:HA	1:A:127:MET:CE	2.49	0.42
1:A:309:ASN:N	1:A:310:PRO:CD	2.83	0.42
1:C:169:LEU:HD22	1:C:171:TYR:CD1	2.50	0.42
1:D:218:TRP:CE2	1:D:337:THR:HG22	2.54	0.41
1:B:107:TYR:OH	1:B:141:GLY:O	2.23	0.41
1:C:176:TYR:HB3	1:C:180:LEU:HD23	2.02	0.41
1:C:312:THR:N	1:C:313:PRO:CD	2.82	0.41
1:B:234:LYS:HB3	1:B:260:MET:HE1	2.02	0.41
1:C:181:ALA:O	1:C:186:VAL:HG13	2.20	0.41
1:A:250:ARG:HH21	1:B:178:GLN:NE2	2.17	0.41
1:C:25:ALA:O	1:C:29:VAL:HG23	2.20	0.41
1:D:180:LEU:HD13	1:D:180:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:HA	1:B:139:ILE:O	2.21	0.41
1:C:309:ASN:N	1:C:310:PRO:CD	2.83	0.41
1:C:165:LEU:C	1:C:165:LEU:HD23	2.41	0.40
1:C:107:TYR:HA	1:C:139:ILE:O	2.21	0.40
1:B:24:MET:HE1	1:B:82:MET:SD	2.61	0.40
1:A:139:ILE:HD12	1:A:327:THR:HA	2.02	0.40
1:B:24:MET:CE	1:B:82:MET:CG	2.99	0.40
1:D:209:LYS:HG2	1:D:213:TYR:CD2	2.57	0.40
1:D:107:TYR:HA	1:D:139:ILE:O	2.21	0.40

There are no symmetry-related clashes.

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	346/351 (99%)	330 (95%)	16 (5%)	0	100	100
1	B	341/351 (97%)	323 (95%)	17 (5%)	1 (0%)	41	50
1	C	336/351 (96%)	320 (95%)	14 (4%)	2 (1%)	25	30
1	D	336/351 (96%)	317 (94%)	17 (5%)	2 (1%)	25	30
All	All	1359/1404 (97%)	1290 (95%)	64 (5%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	179	VAL
1	D	179	VAL
1	C	186	VAL
1	D	283	TYR
1	B	283	TYR

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	280/289 (97%)	258 (92%)	22 (8%)	12 15
1	B	264/289 (91%)	242 (92%)	22 (8%)	11 13
1	C	272/289 (94%)	255 (94%)	17 (6%)	18 24
1	D	256/289 (89%)	233 (91%)	23 (9%)	9 11
All	All	1072/1156 (93%)	988 (92%)	84 (8%)	12 15

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	37	VAL
1	A	39	VAL
1	A	61	ILE
1	A	64	THR
1	A	88	THR
1	A	95	GLN
1	A	113	LEU
1	A	132	LYS
1	A	180	LEU
1	A	186	VAL
1	A	202	THR
1	A	205	THR
1	A	206	SER
1	A	209	LYS
1	A	216	ASN
1	A	229	LYS
1	A	231	GLU
1	A	268	THR
1	A	323	ARG
1	A	329	ASP
1	A	347	VAL
1	B	15	TYR
1	B	22	LYS

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Mol	Chain	Res	Type
1	B	37	VAL
1	B	39	VAL
1	B	50	PHE
1	B	64	THR
1	B	76	THR
1	B	88	THR
1	B	95	GLN
1	B	113	LEU
1	B	188	LEU
1	B	202	THR
1	B	206	SER
1	B	216	ASN
1	B	229	LYS
1	B	231	GLU
1	B	268	THR
1	B	308	LYS
1	B	323	ARG
1	B	337	THR
1	B	347	VAL
1	B	351	LEU
1	C	8	SER
1	C	15	TYR
1	C	59	GLN
1	C	74	ARG
1	C	88	THR
1	C	95	GLN
1	C	113	LEU
1	C	235	THR
1	C	238	LYS
1	C	256	GLN
1	C	268	THR
1	C	288	GLU
1	C	308	LYS
1	C	323	ARG
1	C	337	THR
1	C	340	LEU
1	C	347	VAL
1	D	8	SER
1	D	15	TYR
1	D	19	ASN
1	D	37	VAL
1	D	39	VAL

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Mol	Chain	Res	Type
1	D	88	THR
1	D	94	SER
1	D	95	GLN
1	D	103	LYS
1	D	118	THR
1	D	205	THR
1	D	206	SER
1	D	216	ASN
1	D	231	GLU
1	D	268	THR
1	D	269	GLU
1	D	277	LYS
1	D	288	GLU
1	D	308	LYS
1	D	309	ASN
1	D	323	ARG
1	D	337	THR
1	D	347	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	95	GLN
1	A	105	ASN
1	A	214	ASN
1	A	256	GLN
1	A	348	HIS
1	B	20	GLN
1	B	95	GLN
1	B	105	ASN
1	B	178	GLN
1	B	214	ASN
1	B	216	ASN
1	B	256	GLN
1	B	348	HIS
1	C	95	GLN
1	C	294	ASN
1	C	348	HIS
1	D	20	GLN
1	D	95	GLN
1	D	105	ASN

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Mol	Chain	Res	Type
1	D	214	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 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	A	401	-	45,52,52	0.95	3 (6%)	56,80,80	1.03	5 (8%)
2	NAP	C	401	-	45,52,52	0.81	2 (4%)	56,80,80	1.07	4 (7%)
2	NAP	D	401	-	45,52,52	0.84	1 (2%)	56,80,80	0.95	5 (8%)
2	NAP	B	401	-	45,52,52	0.94	2 (4%)	56,80,80	0.97	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	A	401	-	-	7/31/67/67	0/5/5/5
2	NAP	C	401	-	-	10/31/67/67	0/5/5/5
2	NAP	D	401	-	-	6/31/67/67	0/5/5/5
2	NAP	B	401	-	-	7/31/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	P2B-O2B	3.54	1.66	1.59
2	D	401	NAP	P2B-O2B	3.47	1.65	1.59
2	B	401	NAP	C2N-N1N	3.22	1.38	1.35
2	A	401	NAP	C2N-N1N	3.08	1.38	1.35
2	B	401	NAP	P2B-O2B	2.82	1.64	1.59
2	C	401	NAP	P2B-O2B	2.59	1.64	1.59
2	C	401	NAP	C2N-N1N	2.44	1.37	1.35
2	A	401	NAP	C8A-N7A	-2.00	1.31	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAP	C6N-N1N-C2N	-3.35	118.92	121.97
2	B	401	NAP	C6N-N1N-C2N	-3.21	119.05	121.97
2	A	401	NAP	C6N-N1N-C2N	-3.07	119.17	121.97
2	D	401	NAP	C6N-N1N-C2N	-2.80	119.42	121.97
2	C	401	NAP	C5A-C6A-N6A	2.67	124.41	120.35
2	D	401	NAP	C3B-C2B-C1B	-2.62	97.96	102.89
2	A	401	NAP	O4D-C1D-C2D	-2.48	103.31	106.93
2	B	401	NAP	O2X-P2B-O2B	2.41	116.79	105.99
2	C	401	NAP	C3B-C2B-C1B	-2.28	98.61	102.89
2	A	401	NAP	C3B-C2B-C1B	-2.27	98.62	102.89
2	D	401	NAP	C5A-C6A-N6A	2.22	123.73	120.35
2	C	401	NAP	O2B-C2B-C1B	2.19	118.00	110.10
2	B	401	NAP	O2B-P2B-O1X	-2.14	101.15	109.39
2	A	401	NAP	C5A-C6A-N6A	2.07	123.50	120.35
2	A	401	NAP	O3B-C3B-C2B	-2.07	105.29	111.17
2	D	401	NAP	C1B-N9A-C4A	-2.04	123.05	126.64
2	D	401	NAP	O2A-PA-O1A	2.03	122.28	112.24

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	C2D-C1D-N1N-C2N
2	B	401	NAP	C2D-C1D-N1N-C6N
2	C	401	NAP	C5B-O5B-PA-O2A
2	C	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	C3B-C4B-C5B-O5B
2	B	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	C1B-C2B-O2B-P2B
2	C	401	NAP	C5B-O5B-PA-O3
2	D	401	NAP	C2B-O2B-P2B-O2X
2	C	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	C	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	O4B-C4B-C5B-O5B

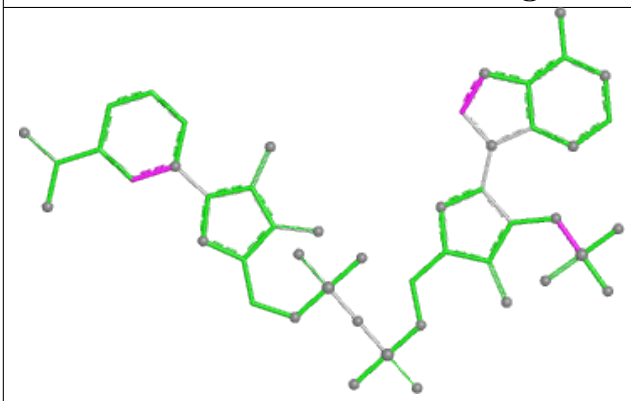
There are no ring outliers.

No monomer is involved in short contacts.

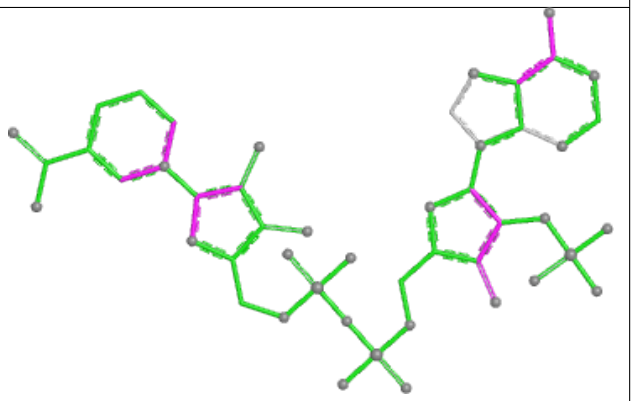
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

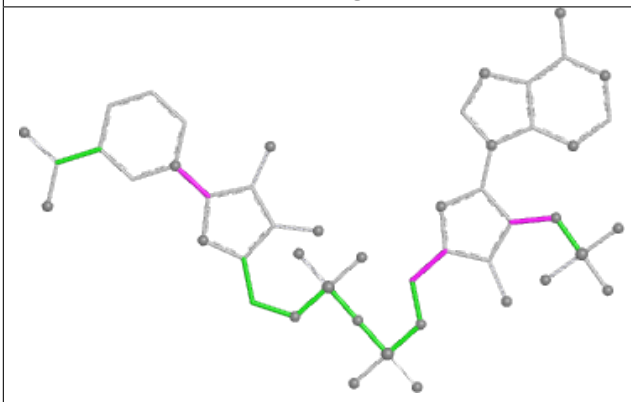
Ligand NAP A 401



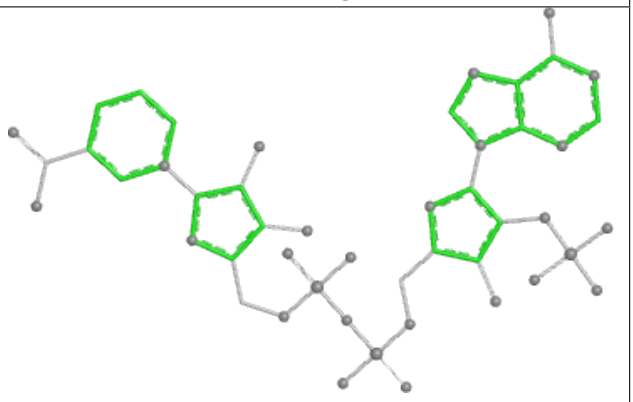
Bond lengths



Bond angles

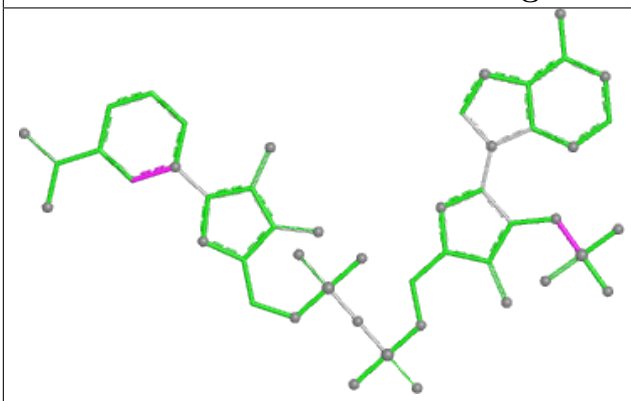


Torsions

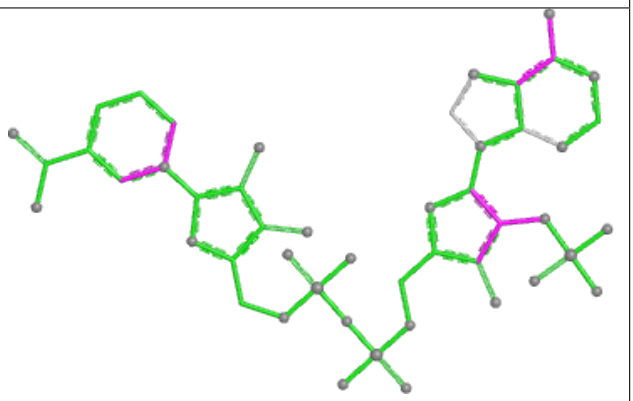


Rings

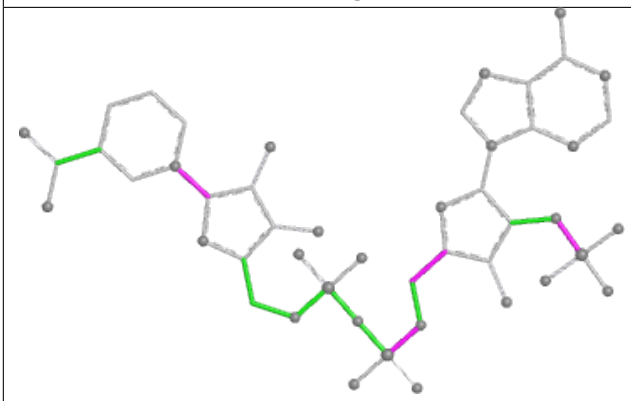
Ligand NAP C 401



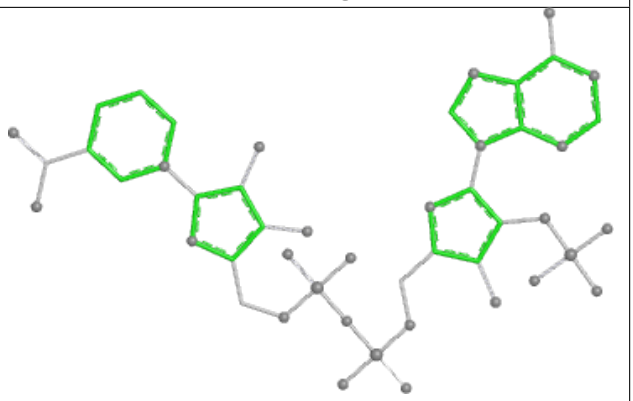
Bond lengths



Bond angles

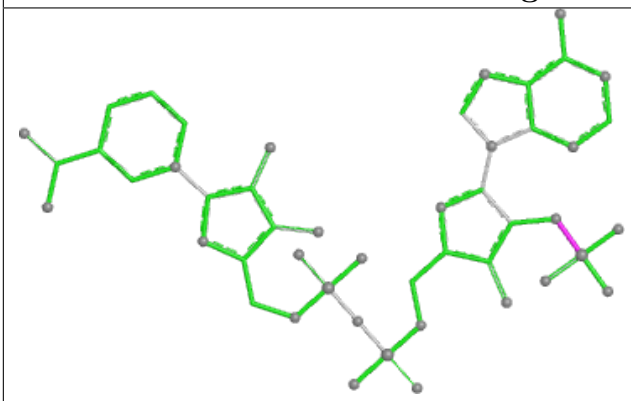


Torsions

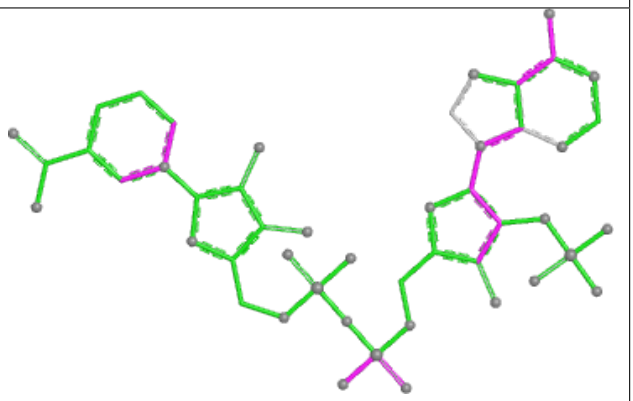


Rings

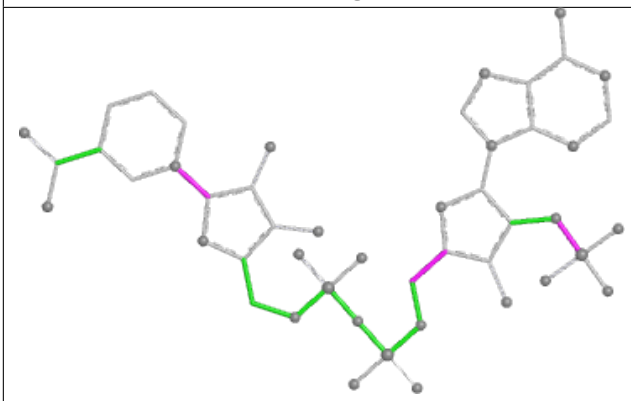
Ligand NAP D 401



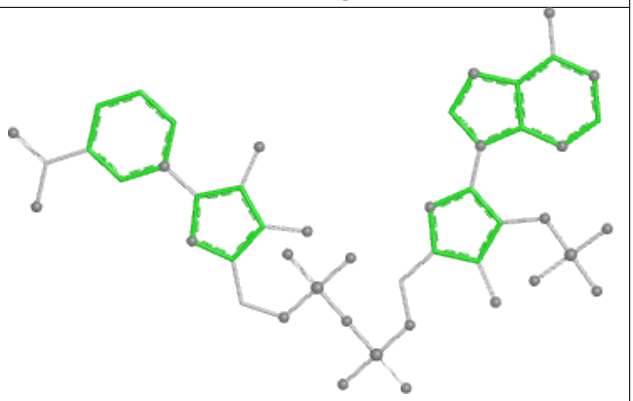
Bond lengths



Bond angles

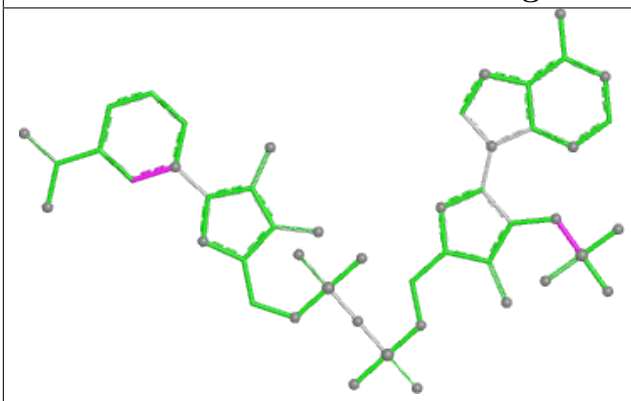


Torsions

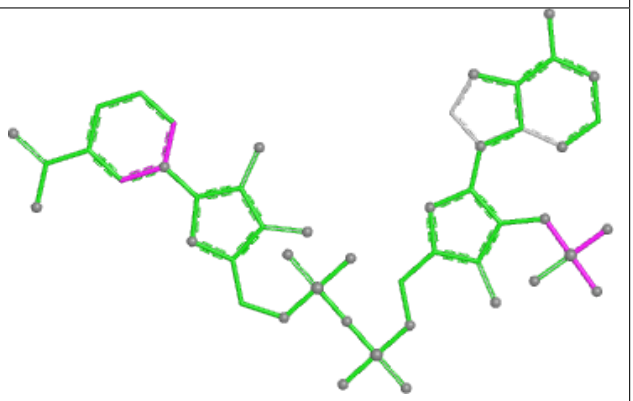


Rings

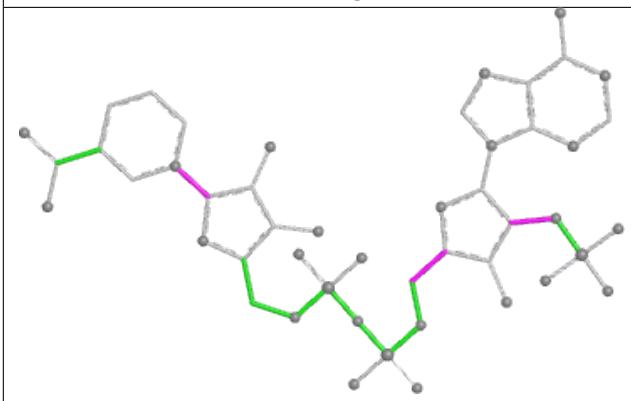
Ligand NAP B 401



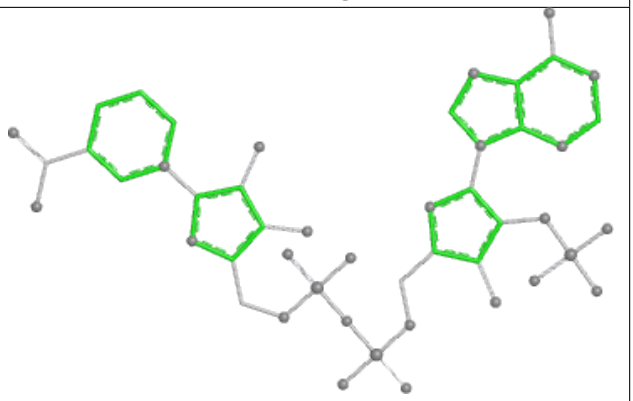
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	348/351 (99%)	0.58	12 (3%) 45 52	18, 29, 55, 82	0
1	B	343/351 (97%)	1.14	51 (14%) 2 3	20, 38, 86, 115	0
1	C	340/351 (96%)	0.78	29 (8%) 10 15	17, 31, 62, 81	0
1	D	340/351 (96%)	1.07	51 (15%) 2 3	17, 33, 115, 164	0
All	All	1371/1404 (97%)	0.89	143 (10%) 6 9	17, 32, 82, 164	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	GLY	9.7
1	D	199	PRO	9.1
1	C	198	GLY	9.1
1	B	38	ALA	8.8
1	D	255	GLY	8.6
1	D	248	ILE	8.3
1	D	198	GLY	8.3
1	D	254	VAL	7.9
1	D	286	GLY	7.8
1	B	65	ALA	7.8
1	C	176	TYR	7.8
1	B	39	VAL	7.4
1	D	197	ASN	7.1
1	D	251	ALA	6.9
1	D	240	PRO	6.9
1	C	199	PRO	6.5
1	B	47	GLY	6.3
1	D	176	TYR	6.2
1	D	182	ILE	6.1
1	B	75	THR	6.0
1	B	50	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	69	ALA	5.9
1	D	249	GLY	5.7
1	B	332	ALA	5.6
1	D	282	CYS	5.5
1	D	195	ALA	5.4
1	D	194	TYR	5.3
1	C	177	GLY	5.2
1	D	178	GLN	5.2
1	D	173	VAL	5.0
1	B	40	ILE	5.0
1	B	29	VAL	4.9
1	D	179	VAL	4.9
1	C	193	PHE	4.7
1	C	282	CYS	4.6
1	A	8	SER	4.6
1	B	64	THR	4.6
1	D	260	MET	4.5
1	D	236	PRO	4.4
1	B	14	LEU	4.3
1	D	280	GLY	4.2
1	D	253	PRO	4.1
1	D	188	LEU	4.1
1	D	244	TYR	4.0
1	B	78	PRO	4.0
1	D	196	GLU	3.9
1	A	4	HIS	3.9
1	B	46	VAL	3.8
1	B	25	ALA	3.8
1	B	17	PHE	3.7
1	B	133	GLU	3.7
1	D	283	TYR	3.7
1	B	104	VAL	3.7
1	C	246	GLU	3.6
1	B	34	VAL	3.6
1	D	187	GLY	3.6
1	B	62	LEU	3.6
1	D	201	TRP	3.5
1	B	70	ALA	3.4
1	B	54	ILE	3.4
1	A	12	VAL	3.3
1	A	348	HIS	3.3
1	C	182	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	211	TYR	3.2
1	B	73	LEU	3.2
1	C	239	ALA	3.2
1	B	15	TYR	3.1
1	A	197	ASN	3.1
1	B	13	ALA	3.1
1	B	98	ALA	3.0
1	B	68	ASP	3.0
1	A	37	VAL	3.0
1	C	247	ALA	2.9
1	B	63	VAL	2.9
1	D	15	TYR	2.9
1	B	48	LYS	2.8
1	D	245	SER	2.7
1	C	187	GLY	2.7
1	D	183	ALA	2.7
1	D	238	LYS	2.7
1	B	282	CYS	2.7
1	B	306	THR	2.7
1	B	18	GLY	2.7
1	D	208	PRO	2.6
1	A	6	HIS	2.6
1	C	248	ILE	2.6
1	B	41	SER	2.6
1	B	329	ASP	2.6
1	B	197	ASN	2.6
1	D	241	ILE	2.6
1	D	257	CYS	2.6
1	C	171	TYR	2.6
1	D	243	LEU	2.6
1	B	292	PHE	2.6
1	B	36	ILE	2.6
1	B	59	GLN	2.5
1	D	250	ARG	2.5
1	C	286	GLY	2.5
1	D	279	VAL	2.5
1	D	174	ASP	2.5
1	B	106	VAL	2.5
1	C	283	TYR	2.5
1	B	99	CYS	2.5
1	D	239	ALA	2.4
1	C	34	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	76	THR	2.4
1	D	207	TYR	2.4
1	C	351	LEU	2.4
1	A	68	ASP	2.4
1	D	237	THR	2.4
1	C	185	GLY	2.3
1	D	175	HIS	2.3
1	B	12	VAL	2.3
1	D	58	PRO	2.3
1	C	173	VAL	2.3
1	B	94	SER	2.3
1	B	37	VAL	2.3
1	B	61	ILE	2.3
1	C	76	THR	2.3
1	A	63	VAL	2.3
1	C	58	PRO	2.3
1	B	11	ARG	2.2
1	B	96	LEU	2.2
1	B	19	ASN	2.2
1	B	71	GLU	2.2
1	C	178	GLN	2.2
1	D	215	MET	2.2
1	B	102	ASN	2.1
1	C	243	LEU	2.1
1	C	64	THR	2.1
1	C	19	ASN	2.1
1	D	247	ALA	2.1
1	B	53	VAL	2.1
1	A	290	MET	2.1
1	B	89	VAL	2.1
1	D	17	PHE	2.1
1	D	171	TYR	2.1
1	C	222	ALA	2.0
1	C	257	CYS	2.0
1	C	181	ALA	2.0
1	A	62	LEU	2.0
1	C	180	LEU	2.0
1	D	261	ILE	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)

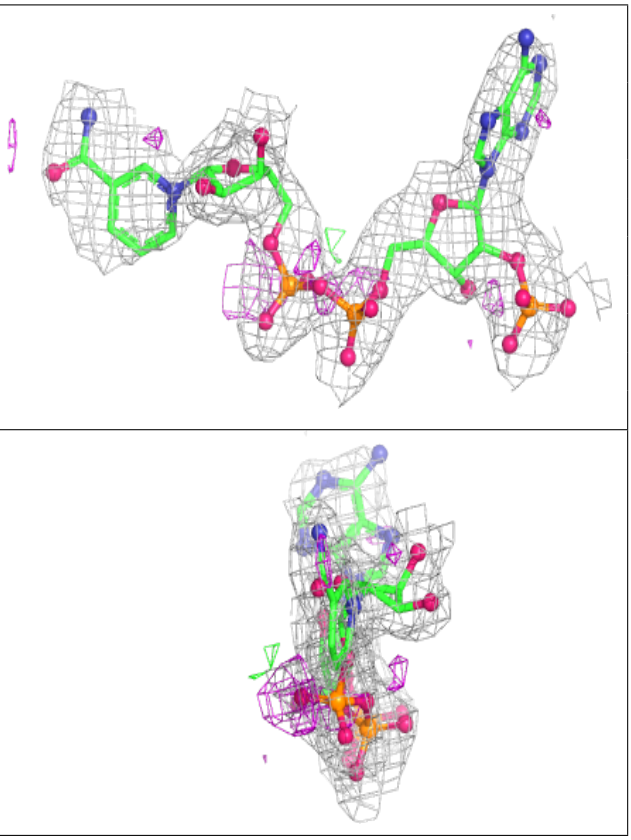
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	401	48/48	0.84	0.23	33,46,59,72	0
2	NAP	A	401	48/48	0.87	0.18	22,28,40,44	0
2	NAP	D	401	48/48	0.87	0.17	28,43,61,64	0
2	NAP	C	401	48/48	0.89	0.19	20,28,34,37	2

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.

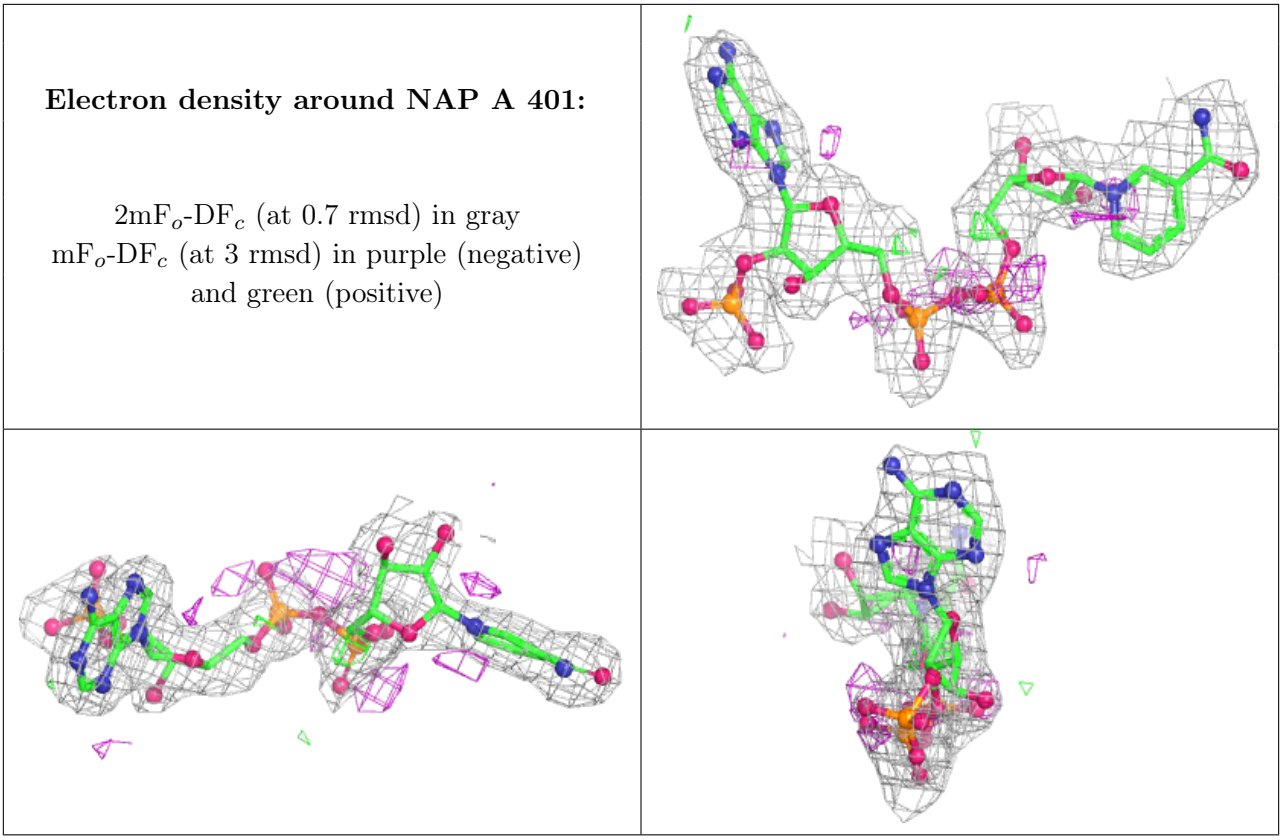
Electron density around NAP B 401:

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



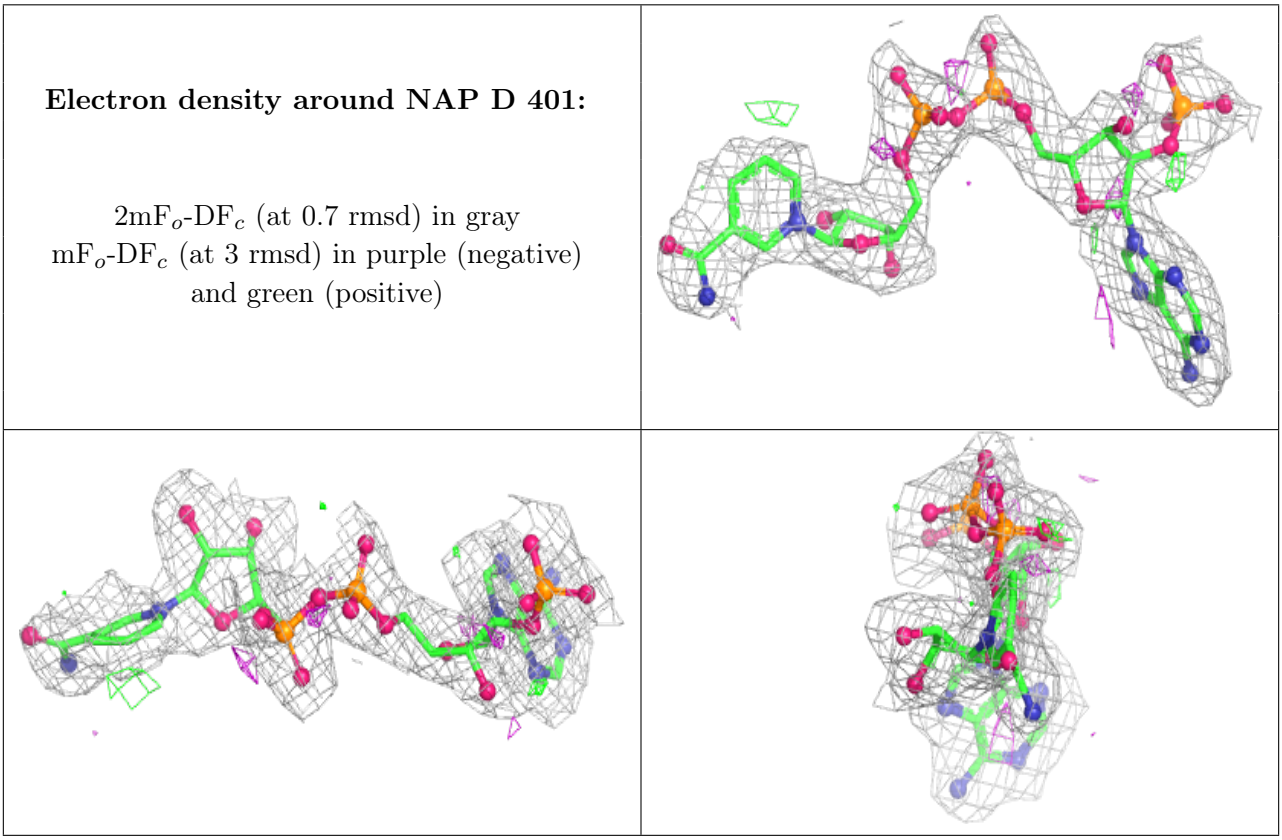
Electron density around NAP A 401:

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



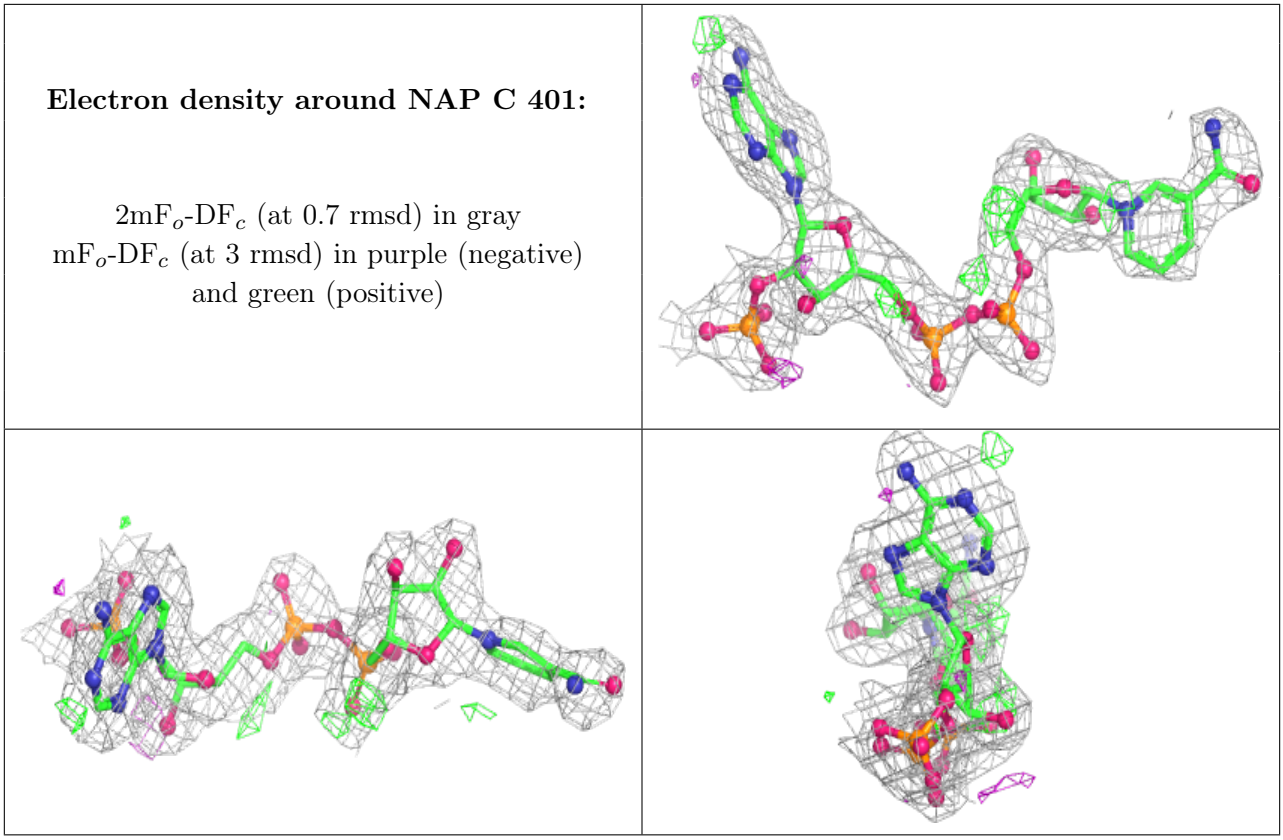
Electron density around NAP D 401:

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



Electron density around NAP C 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.