



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 AM UTC

PDB ID : 4I5E / pdb_00004i5e
Title : Crystal structure of Ralstonia sp. alcohol dehydrogenase in complex with NADP+
Authors : Jarasch, A.; Lerchner, A.; Meining, W.; Schiefner, A.; Skerra, A.
Deposited on : 2012-11-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

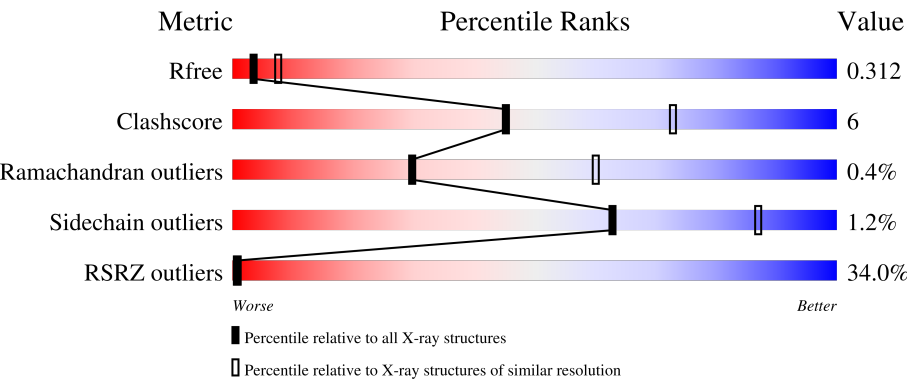
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	31% 83%11%• 5%
1	B	262	37% 83%11%• 5%
1	C	262	34% 83%12%5%
1	D	262	36% 84%11%• 5%
1	E	262	27% 84%11%• 5%

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Mol	Chain	Length	Quality of chain
1	F	262	26% 83% 12% 5%
1	G	262	42% 83% 12% 5%
1	H	262	26% 83% 11% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15560 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 Alcohol dehydrogenase/short-chain dehydrogenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	B	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	C	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	D	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	E	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	F	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	G	249	Total	C	N	O	0	0	0
			1882	1181	336	365			
1	H	249	Total	C	N	O	0	0	0
			1882	1181	336	365			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP C0IR58
A	-11	ALA	-	expression tag	UNP C0IR58
A	-10	SER	-	expression tag	UNP C0IR58
A	-9	ARG	-	expression tag	UNP C0IR58
A	-8	GLY	-	expression tag	UNP C0IR58
A	-7	SER	-	expression tag	UNP C0IR58
A	-6	HIS	-	expression tag	UNP C0IR58
A	-5	HIS	-	expression tag	UNP C0IR58
A	-4	HIS	-	expression tag	UNP C0IR58
A	-3	HIS	-	expression tag	UNP C0IR58
A	-2	HIS	-	expression tag	UNP C0IR58
A	-1	HIS	-	expression tag	UNP C0IR58
A	0	GLY	-	expression tag	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP C0IR58
B	-12	MET	-	expression tag	UNP C0IR58
B	-11	ALA	-	expression tag	UNP C0IR58
B	-10	SER	-	expression tag	UNP C0IR58
B	-9	ARG	-	expression tag	UNP C0IR58
B	-8	GLY	-	expression tag	UNP C0IR58
B	-7	SER	-	expression tag	UNP C0IR58
B	-6	HIS	-	expression tag	UNP C0IR58
B	-5	HIS	-	expression tag	UNP C0IR58
B	-4	HIS	-	expression tag	UNP C0IR58
B	-3	HIS	-	expression tag	UNP C0IR58
B	-2	HIS	-	expression tag	UNP C0IR58
B	-1	HIS	-	expression tag	UNP C0IR58
B	0	GLY	-	expression tag	UNP C0IR58
B	1	ALA	-	expression tag	UNP C0IR58
C	-12	MET	-	expression tag	UNP C0IR58
C	-11	ALA	-	expression tag	UNP C0IR58
C	-10	SER	-	expression tag	UNP C0IR58
C	-9	ARG	-	expression tag	UNP C0IR58
C	-8	GLY	-	expression tag	UNP C0IR58
C	-7	SER	-	expression tag	UNP C0IR58
C	-6	HIS	-	expression tag	UNP C0IR58
C	-5	HIS	-	expression tag	UNP C0IR58
C	-4	HIS	-	expression tag	UNP C0IR58
C	-3	HIS	-	expression tag	UNP C0IR58
C	-2	HIS	-	expression tag	UNP C0IR58
C	-1	HIS	-	expression tag	UNP C0IR58
C	0	GLY	-	expression tag	UNP C0IR58
C	1	ALA	-	expression tag	UNP C0IR58
D	-12	MET	-	expression tag	UNP C0IR58
D	-11	ALA	-	expression tag	UNP C0IR58
D	-10	SER	-	expression tag	UNP C0IR58
D	-9	ARG	-	expression tag	UNP C0IR58
D	-8	GLY	-	expression tag	UNP C0IR58
D	-7	SER	-	expression tag	UNP C0IR58
D	-6	HIS	-	expression tag	UNP C0IR58
D	-5	HIS	-	expression tag	UNP C0IR58
D	-4	HIS	-	expression tag	UNP C0IR58
D	-3	HIS	-	expression tag	UNP C0IR58
D	-2	HIS	-	expression tag	UNP C0IR58
D	-1	HIS	-	expression tag	UNP C0IR58
D	0	GLY	-	expression tag	UNP C0IR58

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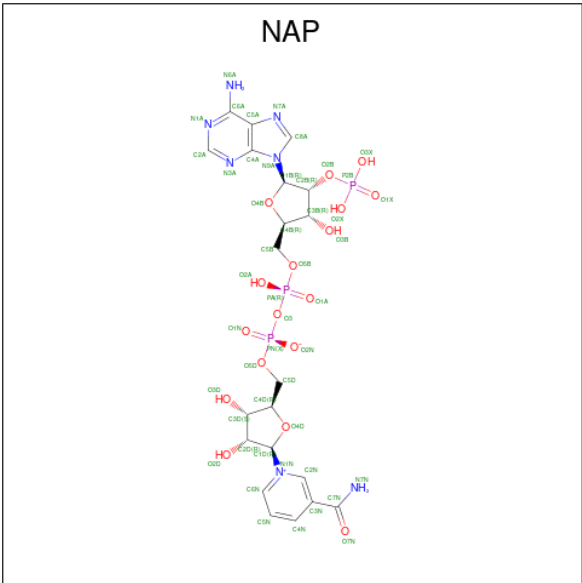
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	expression tag	UNP C0IR58
E	-12	MET	-	expression tag	UNP C0IR58
E	-11	ALA	-	expression tag	UNP C0IR58
E	-10	SER	-	expression tag	UNP C0IR58
E	-9	ARG	-	expression tag	UNP C0IR58
E	-8	GLY	-	expression tag	UNP C0IR58
E	-7	SER	-	expression tag	UNP C0IR58
E	-6	HIS	-	expression tag	UNP C0IR58
E	-5	HIS	-	expression tag	UNP C0IR58
E	-4	HIS	-	expression tag	UNP C0IR58
E	-3	HIS	-	expression tag	UNP C0IR58
E	-2	HIS	-	expression tag	UNP C0IR58
E	-1	HIS	-	expression tag	UNP C0IR58
E	0	GLY	-	expression tag	UNP C0IR58
E	1	ALA	-	expression tag	UNP C0IR58
F	-12	MET	-	expression tag	UNP C0IR58
F	-11	ALA	-	expression tag	UNP C0IR58
F	-10	SER	-	expression tag	UNP C0IR58
F	-9	ARG	-	expression tag	UNP C0IR58
F	-8	GLY	-	expression tag	UNP C0IR58
F	-7	SER	-	expression tag	UNP C0IR58
F	-6	HIS	-	expression tag	UNP C0IR58
F	-5	HIS	-	expression tag	UNP C0IR58
F	-4	HIS	-	expression tag	UNP C0IR58
F	-3	HIS	-	expression tag	UNP C0IR58
F	-2	HIS	-	expression tag	UNP C0IR58
F	-1	HIS	-	expression tag	UNP C0IR58
F	0	GLY	-	expression tag	UNP C0IR58
F	1	ALA	-	expression tag	UNP C0IR58
G	-12	MET	-	expression tag	UNP C0IR58
G	-11	ALA	-	expression tag	UNP C0IR58
G	-10	SER	-	expression tag	UNP C0IR58
G	-9	ARG	-	expression tag	UNP C0IR58
G	-8	GLY	-	expression tag	UNP C0IR58
G	-7	SER	-	expression tag	UNP C0IR58
G	-6	HIS	-	expression tag	UNP C0IR58
G	-5	HIS	-	expression tag	UNP C0IR58
G	-4	HIS	-	expression tag	UNP C0IR58
G	-3	HIS	-	expression tag	UNP C0IR58
G	-2	HIS	-	expression tag	UNP C0IR58
G	-1	HIS	-	expression tag	UNP C0IR58
G	0	GLY	-	expression tag	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP C0IR58
H	-12	MET	-	expression tag	UNP C0IR58
H	-11	ALA	-	expression tag	UNP C0IR58
H	-10	SER	-	expression tag	UNP C0IR58
H	-9	ARG	-	expression tag	UNP C0IR58
H	-8	GLY	-	expression tag	UNP C0IR58
H	-7	SER	-	expression tag	UNP C0IR58
H	-6	HIS	-	expression tag	UNP C0IR58
H	-5	HIS	-	expression tag	UNP C0IR58
H	-4	HIS	-	expression tag	UNP C0IR58
H	-3	HIS	-	expression tag	UNP C0IR58
H	-2	HIS	-	expression tag	UNP C0IR58
H	-1	HIS	-	expression tag	UNP C0IR58
H	0	GLY	-	expression tag	UNP C0IR58
H	1	ALA	-	expression tag	UNP C0IR58

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



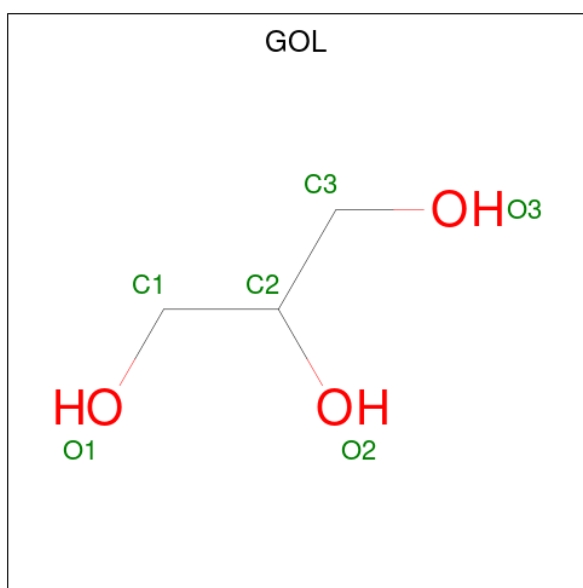
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

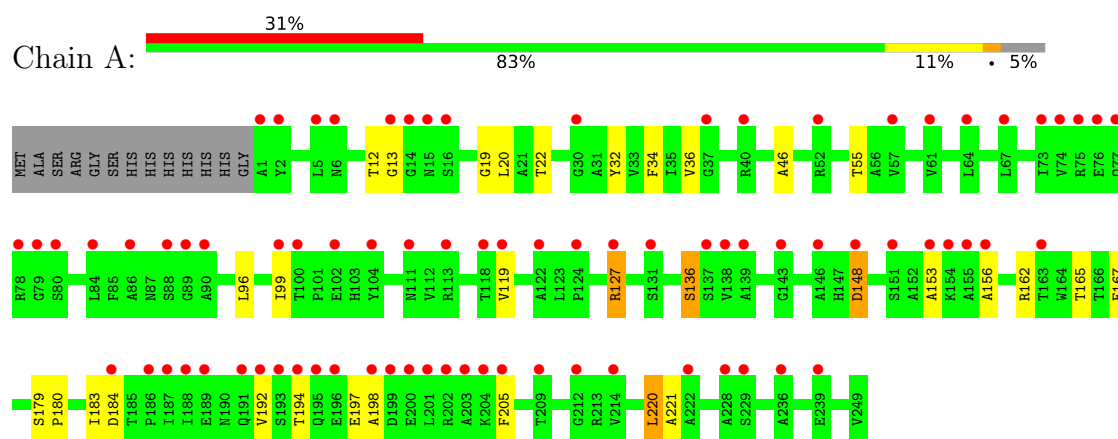
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	15	Total 15	O 15	0	0
4	C	10	Total 10	O 10	0	0
4	D	11	Total 11	O 11	0	0
4	E	12	Total 12	O 12	0	0
4	F	16	Total 16	O 16	0	0
4	G	8	Total 8	O 8	0	0
4	H	10	Total 10	O 10	0	0

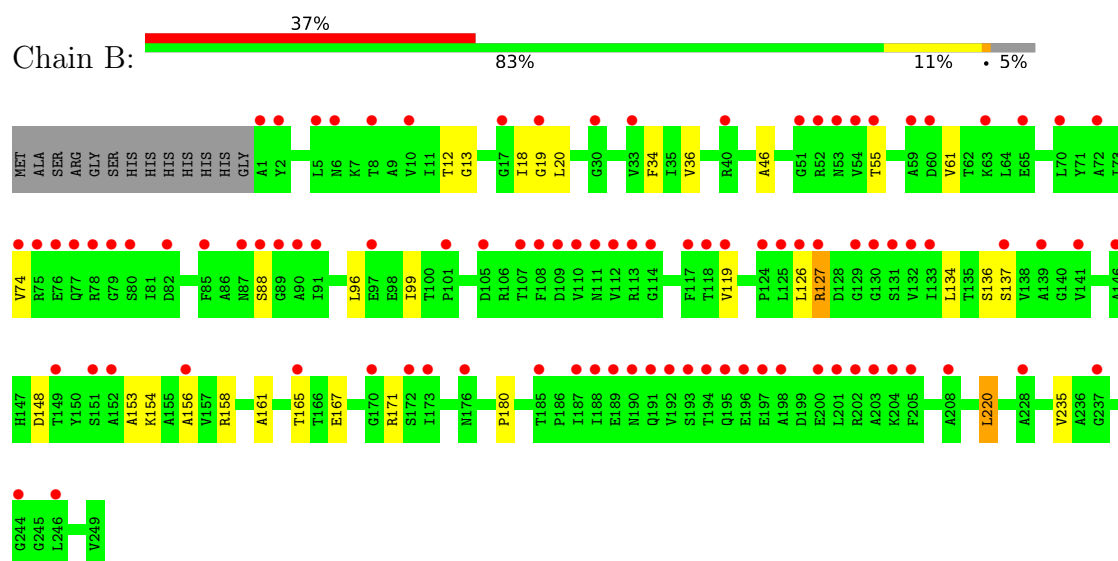
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

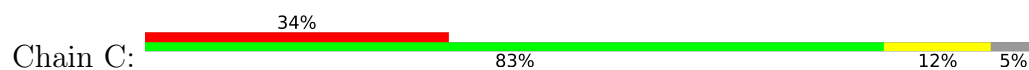
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

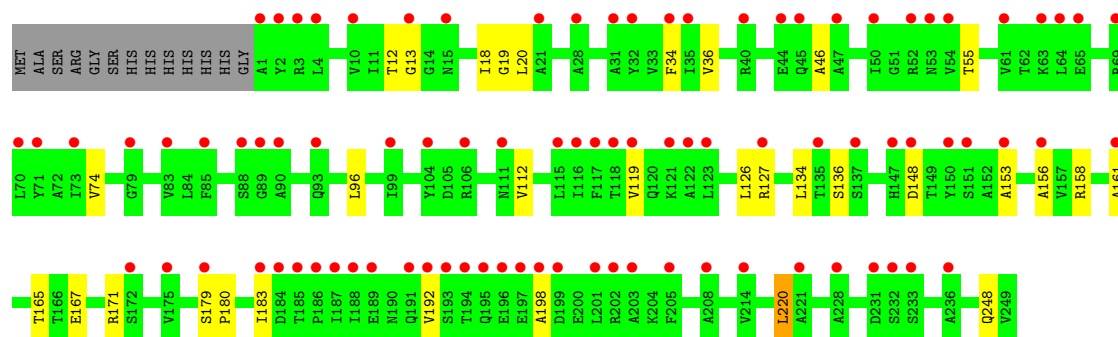


- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

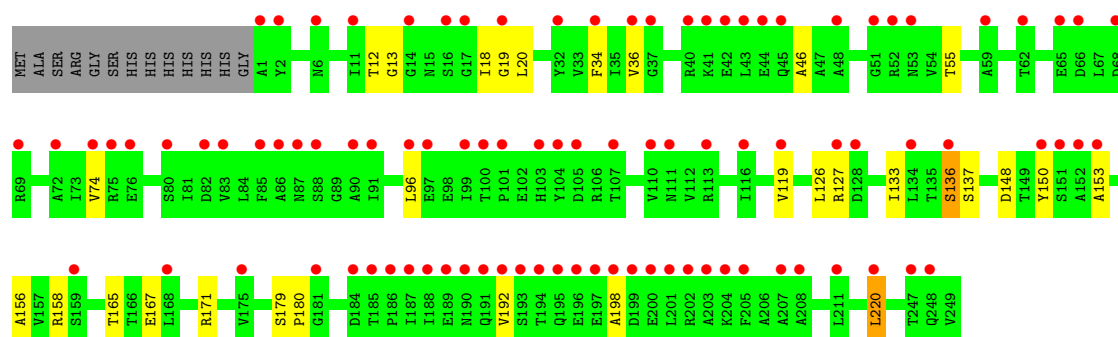
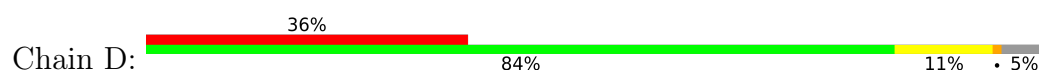


- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

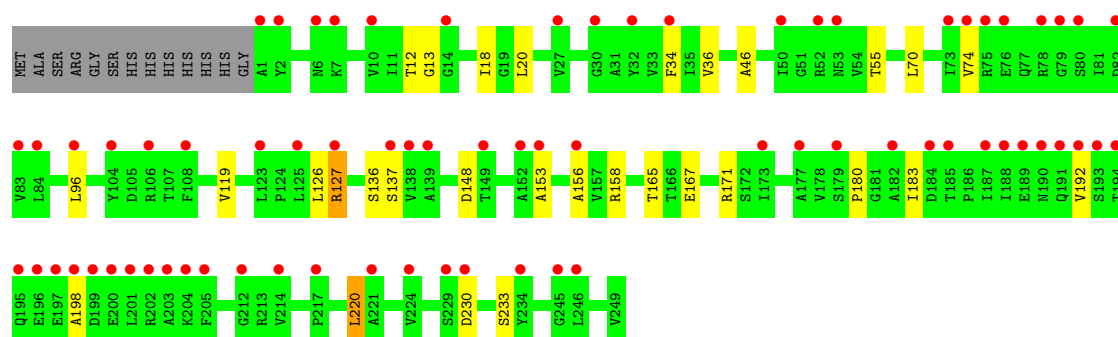
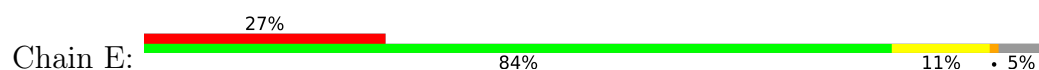




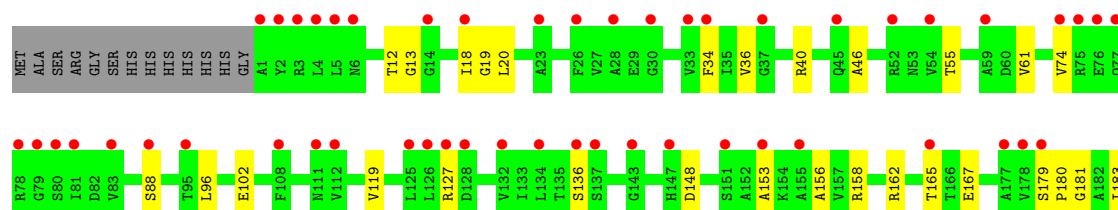
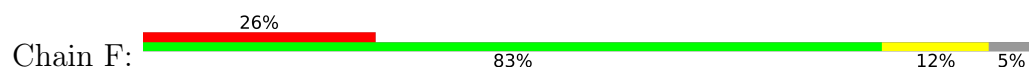
• Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

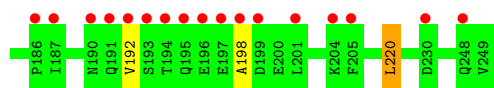


• Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



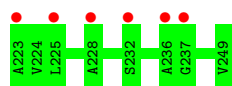
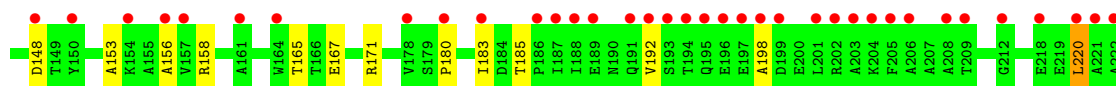
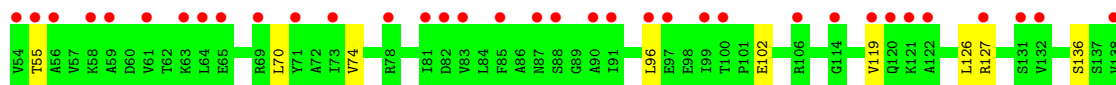
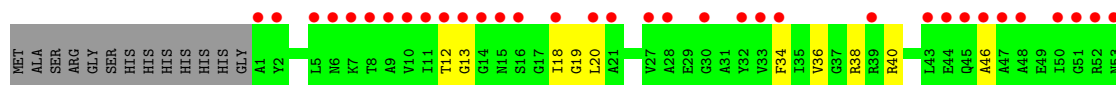
• Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase





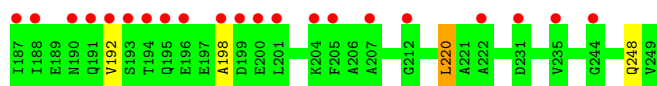
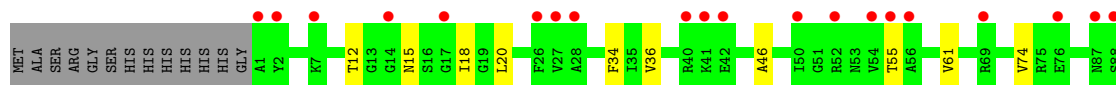
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain G: 42% 83% 12% 5%



- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

Chain H: 26% 83% 11% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.34Å 74.55Å 132.69Å 80.98° 85.99° 64.60°	Depositor
Resolution (Å)	29.60 – 2.80 29.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.60-2.80) 93.7 (29.60-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.261 , 0.305 0.268 , 0.312	Depositor DCC
R_{free} test set	2942 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	15560	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.28 % 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 4.8141e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.90	4/1905 (0.2%)	1.06	6/2581 (0.2%)
1	B	0.72	1/1905 (0.1%)	0.92	2/2581 (0.1%)
1	C	0.65	1/1905 (0.1%)	0.88	0/2581
1	D	0.68	1/1905 (0.1%)	0.87	0/2581
1	E	0.76	2/1905 (0.1%)	1.01	4/2581 (0.2%)
1	F	0.73	1/1905 (0.1%)	0.90	0/2581
1	G	0.67	1/1905 (0.1%)	0.87	0/2581
1	H	0.69	1/1905 (0.1%)	0.87	0/2581
All	All	0.73	12/15240 (0.1%)	0.92	12/20648 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ARG	CZ-NH1	-12.44	1.15	1.32
1	A	148	ASP	CG-OD1	-8.60	1.09	1.25
1	E	127	ARG	CD-NE	-7.59	1.35	1.46
1	G	127	ARG	CZ-NH1	-7.27	1.22	1.32
1	A	148	ASP	CG-OD2	-7.01	1.12	1.25
1	H	127	ARG	CZ-NH1	-6.83	1.23	1.32
1	E	127	ARG	CZ-NH1	-6.82	1.23	1.32
1	F	127	ARG	CZ-NH1	-6.56	1.23	1.32
1	A	127	ARG	CZ-NH2	-6.55	1.25	1.33
1	B	127	ARG	CD-NE	6.15	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	ARG	CZ-NH1	-6.00	1.24	1.32
1	D	127	ARG	CZ-NH1	-5.94	1.24	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	ARG	NE-CZ-NH2	14.14	131.93	119.20
1	A	127	ARG	NE-CZ-NH2	13.84	131.66	119.20
1	E	127	ARG	NE-CZ-NH1	-12.79	108.71	121.50
1	E	127	ARG	CD-NE-CZ	11.96	141.14	124.40
1	A	148	ASP	OD1-CG-OD2	-9.45	100.21	122.90
1	A	127	ARG	NH1-CZ-NH2	-8.63	108.08	119.30
1	A	127	ARG	CG-CD-NE	6.47	126.22	112.00
1	A	148	ASP	CB-CG-OD2	6.08	132.37	118.40
1	B	127	ARG	NH1-CZ-NH2	-5.83	111.71	119.30
1	B	127	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	E	127	ARG	NH1-CZ-NH2	-5.22	112.52	119.30
1	A	148	ASP	N-CA-C	5.18	119.86	111.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	127	ARG	Sidechain

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	1882	0	1922	22	0
1	B	1882	0	1922	26	0
1	C	1882	0	1922	23	0
1	D	1882	0	1922	23	0
1	E	1882	0	1922	23	0
1	F	1882	0	1922	27	2
1	G	1882	0	1922	24	2
1	H	1882	0	1922	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	1	0
2	B	48	0	25	5	0
2	C	48	0	25	1	0
2	D	48	0	25	4	0
2	E	48	0	25	4	0
2	F	48	0	25	7	0
2	G	48	0	25	6	0
2	H	48	0	25	6	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	E	6	0	8	0	0
4	A	14	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	11	0	0	2	0
4	E	12	0	0	1	0
4	F	16	0	0	0	0
4	G	8	0	0	0	0
4	H	10	0	0	1	0
All	All	15560	0	15608	179	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 6.

All (179) 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:E:183:ILE:HB	2:E:301:NAP:N7N	1.90	0.86
1:E:183:ILE:HB	2:E:301:NAP:H72N	1.41	0.83
1:G:183:ILE:HB	2:G:301:NAP:N7N	2.01	0.75
1:B:34:PHE:CD1	1:B:55:THR:HB	2.26	0.71
1:E:34:PHE:CD1	1:E:55:THR:HB	2.29	0.67
1:A:194:THR:OG1	1:A:197:GLU:HG3	1.95	0.67
1:G:119:VAL:HG12	1:H:96:LEU:HD21	1.77	0.67
1:F:34:PHE:CD1	1:F:55:THR:HB	2.31	0.66
1:H:34:PHE:CD1	1:H:55:THR:HB	2.30	0.66
1:G:34:PHE:CD1	1:G:55:THR:HB	2.31	0.65
1:D:34:PHE:CD1	1:D:55:THR:HB	2.32	0.65
1:C:34:PHE:CD1	1:C:55:THR:HB	2.32	0.64
1:B:34:PHE:HD1	1:B:55:THR:HB	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:CZ	3:A:302:GOL:H11	2.35	0.61
1:E:34:PHE:HD1	1:E:55:THR:HB	1.66	0.61
1:A:119:VAL:HG12	1:B:96:LEU:HD21	1.83	0.60
1:D:133:ILE:HG13	4:D:411:HOH:O	2.02	0.60
1:G:34:PHE:HD1	1:G:55:THR:HB	1.67	0.59
1:F:34:PHE:HD1	1:F:55:THR:HB	1.67	0.59
1:A:34:PHE:CD1	1:A:55:THR:HB	2.39	0.58
1:H:15:ASN:OD1	2:H:301:NAP:O3B	2.21	0.58
1:A:180:PRO:HB3	1:A:220:LEU:CD1	2.33	0.58
1:C:183:ILE:HB	2:C:301:NAP:N7N	2.19	0.58
1:C:34:PHE:HD1	1:C:55:THR:HB	1.69	0.58
1:E:180:PRO:HB3	1:E:220:LEU:HD13	1.85	0.58
1:H:34:PHE:HD1	1:H:55:THR:HB	1.68	0.58
1:B:153:ALA:O	1:B:156:ALA:HB3	2.03	0.57
1:H:18:ILE:HD12	2:H:301:NAP:H51N	1.87	0.57
1:A:96:LEU:HD21	1:B:119:VAL:HG12	1.85	0.57
1:G:153:ALA:O	1:G:156:ALA:HB3	2.05	0.57
1:D:137:SER:HB2	2:D:301:NAP:H6N	1.88	0.56
1:E:180:PRO:HB3	1:E:220:LEU:CD1	2.35	0.56
1:F:61:VAL:HG22	2:F:301:NAP:N1A	2.20	0.56
1:D:34:PHE:HD1	1:D:55:THR:HB	1.70	0.56
1:A:183:ILE:HB	2:A:301:NAP:N7N	2.21	0.55
1:F:18:ILE:HD13	1:F:220:LEU:HD22	1.86	0.55
1:A:180:PRO:HB3	1:A:220:LEU:HD13	1.87	0.55
1:H:18:ILE:HD13	1:H:220:LEU:HD22	1.88	0.55
1:F:183:ILE:HB	2:F:301:NAP:N7N	2.22	0.54
1:G:180:PRO:HB3	1:G:220:LEU:HD13	1.89	0.54
1:H:180:PRO:HB3	1:H:220:LEU:HD13	1.90	0.54
1:B:137:SER:HB2	2:B:301:NAP:H6N	1.90	0.54
1:C:18:ILE:HD13	1:C:220:LEU:HD22	1.90	0.54
1:H:137:SER:HB2	2:H:301:NAP:H6N	1.88	0.54
1:G:180:PRO:HB3	1:G:220:LEU:CD1	2.37	0.54
1:D:180:PRO:HB3	1:D:220:LEU:CD1	2.38	0.53
1:D:18:ILE:HD13	1:D:220:LEU:HD22	1.91	0.53
1:F:153:ALA:O	1:F:156:ALA:HB3	2.09	0.53
2:G:301:NAP:H52A	2:G:301:NAP:H52N	1.91	0.53
1:B:18:ILE:HD13	1:B:220:LEU:HD22	1.89	0.53
1:F:61:VAL:HG22	2:F:301:NAP:C6A	2.38	0.53
1:H:180:PRO:HB3	1:H:220:LEU:CD1	2.39	0.53
1:C:180:PRO:HB3	1:C:220:LEU:CD1	2.39	0.52
1:F:180:PRO:HB3	1:F:220:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:SER:OG	2:H:301:NAP:H5N	2.09	0.52
1:E:96:LEU:HD21	1:F:119:VAL:HG12	1.91	0.52
1:G:18:ILE:HD13	1:G:220:LEU:HD22	1.91	0.52
1:E:13:GLY:HA2	2:E:301:NAP:H1B	1.92	0.51
1:H:153:ALA:O	1:H:156:ALA:HB3	2.11	0.51
1:E:18:ILE:HD13	1:E:220:LEU:HD22	1.91	0.51
1:F:180:PRO:HB3	1:F:220:LEU:CD1	2.41	0.51
1:A:13:GLY:O	1:A:19:GLY:HA3	2.11	0.51
1:D:153:ALA:O	1:D:156:ALA:HB3	2.11	0.51
1:D:180:PRO:HB3	1:D:220:LEU:HD13	1.92	0.50
1:C:180:PRO:HB3	1:C:220:LEU:HD13	1.92	0.50
1:B:180:PRO:HB3	1:B:220:LEU:CD1	2.42	0.50
1:A:148:ASP:OD2	1:B:167:GLU:OE2	2.30	0.49
1:G:185:THR:OG1	2:G:301:NAP:O2N	2.22	0.49
1:C:153:ALA:O	1:C:156:ALA:HB3	2.12	0.49
1:G:18:ILE:HD11	2:G:301:NAP:H71N	1.78	0.49
1:B:34:PHE:CE2	1:B:74:VAL:HG13	2.47	0.48
1:E:20:LEU:HD13	1:E:46:ALA:HB1	1.96	0.48
1:E:119:VAL:HG12	1:F:96:LEU:HD21	1.95	0.48
1:D:137:SER:OG	2:D:301:NAP:H5N	2.13	0.48
1:B:154:LYS:HE3	2:B:301:NAP:O2D	2.13	0.48
1:C:12:THR:HA	1:C:36:VAL:HB	1.95	0.48
1:C:34:PHE:CE2	1:C:74:VAL:HG13	2.49	0.48
1:D:20:LEU:HD13	1:D:46:ALA:HB1	1.97	0.47
1:H:12:THR:HA	1:H:36:VAL:HB	1.97	0.47
2:D:301:NAP:O3X	2:D:301:NAP:H1B	2.15	0.47
1:E:34:PHE:CE2	1:E:74:VAL:HG13	2.49	0.47
1:H:34:PHE:CE2	1:H:74:VAL:HG13	2.50	0.47
1:E:153:ALA:O	1:E:156:ALA:HB3	2.15	0.47
1:G:12:THR:HA	1:G:36:VAL:HB	1.97	0.47
1:A:167:GLU:OE2	1:B:148:ASP:OD1	2.33	0.47
1:B:180:PRO:HB3	1:B:220:LEU:HD13	1.96	0.47
1:D:12:THR:HA	1:D:36:VAL:HB	1.97	0.46
1:F:12:THR:HA	1:F:36:VAL:HB	1.96	0.46
1:A:99:ILE:HD11	1:A:148:ASP:HB2	1.98	0.46
1:D:34:PHE:CE2	1:D:74:VAL:HG13	2.50	0.46
1:A:192:VAL:HG21	1:A:198:ALA:HB2	1.97	0.46
1:B:34:PHE:HE2	1:B:74:VAL:HG13	1.80	0.46
1:B:20:LEU:HD13	1:B:46:ALA:HB1	1.98	0.46
1:G:34:PHE:CE2	1:G:74:VAL:HG13	2.50	0.46
1:A:34:PHE:HD1	1:A:55:THR:HB	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:HD3	1:C:158:ARG:C	2.40	0.46
1:D:13:GLY:O	1:D:19:GLY:HA3	2.16	0.46
1:B:12:THR:HA	1:B:36:VAL:HB	1.98	0.46
1:C:34:PHE:HE2	1:C:74:VAL:HG13	1.80	0.46
1:H:34:PHE:HE2	1:H:74:VAL:HG13	1.81	0.46
1:H:61:VAL:HG22	2:H:301:NAP:N1A	2.31	0.46
1:B:134:LEU:HD12	1:B:161:ALA:HB2	1.98	0.46
1:D:150:TYR:OH	2:D:301:NAP:C6N	2.64	0.46
1:F:34:PHE:CE2	1:F:74:VAL:HG13	2.50	0.46
1:F:158:ARG:C	1:F:158:ARG:HD3	2.41	0.46
1:G:34:PHE:HE2	1:G:74:VAL:HG13	1.80	0.46
1:E:12:THR:HA	1:E:36:VAL:HB	1.98	0.45
1:C:126:LEU:O	1:C:171:ARG:NH2	2.49	0.45
1:E:192:VAL:HG21	1:E:198:ALA:HB2	1.99	0.45
1:F:88:SER:HB2	2:F:301:NAP:C4A	2.45	0.45
1:B:126:LEU:O	1:B:171:ARG:NH2	2.49	0.45
1:D:34:PHE:HE2	1:D:74:VAL:HG13	1.82	0.45
1:E:34:PHE:HE2	1:E:74:VAL:HG13	1.80	0.45
1:E:167:GLU:OE2	1:F:148:ASP:OD1	2.35	0.45
1:G:183:ILE:HB	2:G:301:NAP:H72N	1.76	0.45
1:H:135:THR:HG21	2:H:301:NAP:H4D	1.98	0.45
1:H:192:VAL:HG21	1:H:198:ALA:HB2	1.99	0.45
1:B:13:GLY:O	1:B:19:GLY:HA3	2.17	0.45
1:C:136:SER:HB3	1:C:179:SER:OG	2.16	0.45
1:G:192:VAL:HG21	1:G:198:ALA:HB2	1.99	0.45
1:E:230:ASP:O	1:E:233:SER:HB3	2.18	0.44
1:G:20:LEU:HD13	1:G:46:ALA:HB1	1.97	0.44
1:G:96:LEU:HD21	1:H:119:VAL:HG12	1.99	0.44
1:A:153:ALA:O	1:A:156:ALA:HB3	2.17	0.44
1:C:96:LEU:HD21	1:D:119:VAL:HG12	1.98	0.44
1:C:148:ASP:OD1	1:D:167:GLU:OE2	2.34	0.44
1:F:61:VAL:HG13	2:F:301:NAP:C2A	2.47	0.44
1:A:20:LEU:HD13	1:A:46:ALA:HB1	2.00	0.44
1:C:20:LEU:HD13	1:C:46:ALA:HB1	1.99	0.44
1:H:157:VAL:HG21	4:H:409:HOH:O	2.17	0.44
1:C:192:VAL:HG21	1:C:198:ALA:HB2	1.99	0.44
1:G:167:GLU:OE2	1:H:148:ASP:OD1	2.36	0.44
1:H:20:LEU:HD13	1:H:46:ALA:HB1	1.99	0.44
1:C:134:LEU:HD12	1:C:161:ALA:HB2	2.00	0.44
1:E:158:ARG:HD3	1:E:158:ARG:C	2.43	0.44
1:F:20:LEU:HD13	1:F:46:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:HG21	1:D:198:ALA:HB2	1.99	0.44
1:F:34:PHE:HE2	1:F:74:VAL:HG13	1.82	0.44
1:A:162:ARG:HD3	1:C:248:GLN:O	2.18	0.44
1:F:162:ARG:HD3	1:H:248:GLN:O	2.18	0.43
1:F:180:PRO:HG2	2:F:301:NAP:C6N	2.48	0.43
1:F:192:VAL:HG21	1:F:198:ALA:HB2	1.99	0.43
1:E:148:ASP:OD1	1:F:167:GLU:OE2	2.35	0.43
1:B:158:ARG:C	1:B:158:ARG:HD3	2.44	0.43
1:B:235:VAL:HA	4:D:403:HOH:O	2.19	0.43
1:G:158:ARG:HD3	1:G:158:ARG:C	2.43	0.43
1:E:70:LEU:O	1:E:74:VAL:HG23	2.18	0.43
1:A:180:PRO:HB3	1:A:220:LEU:HD11	2.01	0.43
1:B:61:VAL:HG22	2:B:301:NAP:C6A	2.49	0.43
1:E:126:LEU:O	1:E:171:ARG:NH2	2.51	0.43
1:G:38:ARG:H	2:G:301:NAP:P2B	2.42	0.43
1:D:136:SER:HB3	1:D:179:SER:OG	2.20	0.42
1:G:13:GLY:O	1:G:19:GLY:HA3	2.19	0.42
1:H:158:ARG:HD3	1:H:158:ARG:C	2.43	0.42
1:A:12:THR:HA	1:A:36:VAL:HB	2.01	0.42
1:D:158:ARG:HD3	1:D:158:ARG:C	2.44	0.42
1:H:126:LEU:O	1:H:171:ARG:NH2	2.52	0.42
1:A:22:THR:HA	1:A:221:ALA:HB1	2.01	0.42
1:H:136:SER:HB3	1:H:179:SER:OG	2.19	0.42
1:C:167:GLU:OE2	1:D:148:ASP:OD1	2.37	0.42
1:E:137:SER:OG	2:E:301:NAP:H5N	2.20	0.42
1:G:126:LEU:O	1:G:171:ARG:NH2	2.52	0.42
1:F:136:SER:HB3	1:F:179:SER:OG	2.19	0.42
1:F:13:GLY:O	1:F:19:GLY:HA3	2.20	0.42
1:C:119:VAL:HG12	1:D:96:LEU:HD21	2.01	0.42
1:F:181:GLY:O	2:F:301:NAP:H4N	2.19	0.41
1:C:112:VAL:HG23	1:C:153:ALA:HB1	2.02	0.41
1:G:148:ASP:OD1	1:H:167:GLU:OE2	2.39	0.41
1:B:18:ILE:CG2	1:B:220:LEU:HD23	2.51	0.41
1:B:34:PHE:CE1	1:B:55:THR:HB	2.54	0.41
2:B:301:NAP:O2N	2:B:301:NAP:H2N	2.21	0.41
4:E:411:HOH:O	1:F:162:ARG:HD2	2.20	0.41
1:C:13:GLY:O	1:C:19:GLY:HA3	2.21	0.41
1:A:136:SER:HB3	1:A:179:SER:OG	2.21	0.41
1:B:99:ILE:HD11	1:B:148:ASP:HB2	2.03	0.41
1:A:32:TYR:HH	1:A:55:THR:HG1	1.65	0.41
1:G:70:LEU:O	1:G:74:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:O	1:D:171:ARG:NH2	2.54	0.40
1:B:88:SER:HB2	2:B:301:NAP:C4A	2.52	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:40:ARG:NH2	1:G:102:GLU:OE2[1_655]	1.91	0.29
1:F:102:GLU:OE2	1:G:40:ARG:NH2[1_655]	2.13	0.07

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	247/262 (94%)	235 (95%)	10 (4%)	2 (1%)	16	44
1	B	247/262 (94%)	240 (97%)	6 (2%)	1 (0%)	30	60
1	C	247/262 (94%)	238 (96%)	9 (4%)	0	100	100
1	D	247/262 (94%)	238 (96%)	8 (3%)	1 (0%)	30	60
1	E	247/262 (94%)	240 (97%)	6 (2%)	1 (0%)	30	60
1	F	247/262 (94%)	238 (96%)	9 (4%)	0	100	100
1	G	247/262 (94%)	239 (97%)	7 (3%)	1 (0%)	30	60
1	H	247/262 (94%)	240 (97%)	6 (2%)	1 (0%)	30	60
All	All	1976/2096 (94%)	1908 (97%)	61 (3%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	SER
1	A	136	SER

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Mol	Chain	Res	Type
1	G	136	SER
1	H	136	SER
1	A	184	ASP
1	D	136	SER
1	E	136	SER

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	194/204 (95%)	191 (98%)	3 (2%)	57	84
1	B	194/204 (95%)	191 (98%)	3 (2%)	57	84
1	C	194/204 (95%)	192 (99%)	2 (1%)	68	88
1	D	194/204 (95%)	192 (99%)	2 (1%)	68	88
1	E	194/204 (95%)	192 (99%)	2 (1%)	68	88
1	F	194/204 (95%)	192 (99%)	2 (1%)	68	88
1	G	194/204 (95%)	192 (99%)	2 (1%)	68	88
1	H	194/204 (95%)	192 (99%)	2 (1%)	68	88
All	All	1552/1632 (95%)	1534 (99%)	18 (1%)	63	87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	165	THR
1	A	220	LEU
1	B	127	ARG
1	B	165	THR
1	B	220	LEU
1	C	165	THR
1	C	220	LEU
1	D	165	THR
1	D	220	LEU

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Mol	Chain	Res	Type
1	E	165	THR
1	E	220	LEU
1	F	165	THR
1	F	220	LEU
1	G	165	THR
1	G	220	LEU
1	H	165	THR
1	H	220	LEU

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

Mol	Chain	Res	Type
1	A	120	GLN
1	B	120	GLN
1	D	120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	301	-	50,52,52	1.47	6 (12%)	71,80,80	1.97	19 (26%)
2	NAP	G	301	-	50,52,52	1.30	6 (12%)	71,80,80	1.83	18 (25%)
2	NAP	B	301	-	50,52,52	1.52	5 (10%)	71,80,80	1.71	19 (26%)
2	NAP	C	301	-	50,52,52	1.31	6 (12%)	71,80,80	1.73	16 (22%)
3	GOL	B	302	-	5,5,5	0.37	0	5,5,5	0.41	0
3	GOL	E	302	-	5,5,5	0.64	0	5,5,5	0.61	0
2	NAP	A	301	-	50,52,52	1.47	7 (14%)	71,80,80	1.71	11 (15%)
2	NAP	H	301	-	50,52,52	1.36	6 (12%)	71,80,80	1.71	13 (18%)
3	GOL	A	302	-	5,5,5	0.41	0	5,5,5	0.31	0
3	GOL	C	302	-	5,5,5	0.29	0	5,5,5	0.39	0
2	NAP	D	301	-	50,52,52	1.56	7 (14%)	71,80,80	1.83	17 (23%)
2	NAP	E	301	-	50,52,52	1.34	7 (14%)	71,80,80	1.73	16 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	F	301	-	-	6/35/67/67	0/5/5/5
2	NAP	G	301	-	-	9/35/67/67	0/5/5/5
2	NAP	B	301	-	-	6/35/67/67	0/5/5/5
2	NAP	C	301	-	-	5/35/67/67	0/5/5/5
3	GOL	B	302	-	-	4/4/4/4	-
3	GOL	E	302	-	-	2/4/4/4	-
2	NAP	A	301	-	-	8/35/67/67	0/5/5/5
2	NAP	H	301	-	-	9/35/67/67	0/5/5/5
3	GOL	A	302	-	-	4/4/4/4	-
3	GOL	C	302	-	-	4/4/4/4	-
2	NAP	D	301	-	-	9/35/67/67	0/5/5/5
2	NAP	E	301	-	-	8/35/67/67	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C5A-C4A	6.34	1.50	1.39
2	F	301	NAP	C5A-C4A	5.36	1.48	1.39
2	D	301	NAP	C5A-C4A	5.28	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	PN-O3	5.23	1.65	1.59
2	E	301	NAP	C5A-C4A	5.15	1.48	1.39
2	G	301	NAP	C5A-C4A	4.93	1.47	1.39
2	A	301	NAP	C5A-C4A	4.88	1.47	1.39
2	C	301	NAP	C5A-C4A	4.79	1.47	1.39
2	H	301	NAP	C5A-C4A	4.56	1.47	1.39
2	A	301	NAP	PA-O3	4.30	1.64	1.59
2	H	301	NAP	PN-O3	3.95	1.63	1.59
2	F	301	NAP	C8A-N7A	3.95	1.39	1.31
2	B	301	NAP	C8A-N7A	3.84	1.39	1.31
2	A	301	NAP	PN-O3	3.71	1.63	1.59
2	F	301	NAP	O4D-C1D	3.56	1.45	1.40
2	C	301	NAP	C5A-C6A	3.47	1.50	1.41
2	G	301	NAP	C5A-C6A	3.17	1.49	1.41
2	A	301	NAP	C5A-C6A	3.15	1.49	1.41
2	H	301	NAP	C5A-C6A	3.09	1.49	1.41
2	D	301	NAP	O4D-C1D	3.05	1.44	1.40
2	B	301	NAP	C5A-N7A	-3.03	1.33	1.39
2	G	301	NAP	PN-O3	2.99	1.62	1.59
2	H	301	NAP	O4D-C1D	2.96	1.44	1.40
2	D	301	NAP	C5A-N7A	-2.84	1.33	1.39
2	C	301	NAP	C8A-N7A	2.79	1.37	1.31
2	C	301	NAP	PA-O3	2.77	1.62	1.59
2	D	301	NAP	PA-O3	2.76	1.62	1.59
2	G	301	NAP	PA-O3	2.76	1.62	1.59
2	F	301	NAP	C5A-C6A	2.76	1.48	1.41
2	D	301	NAP	C5A-C6A	2.72	1.48	1.41
2	B	301	NAP	C5A-C6A	2.65	1.48	1.41
2	D	301	NAP	C8A-N7A	2.63	1.36	1.31
2	B	301	NAP	PA-O3	2.60	1.62	1.59
2	E	301	NAP	C5A-C6A	2.59	1.48	1.41
2	H	301	NAP	PA-O3	2.56	1.62	1.59
2	A	301	NAP	C8A-N7A	2.55	1.36	1.31
2	G	301	NAP	O4D-C1D	2.49	1.44	1.40
2	E	301	NAP	PA-O3	2.45	1.62	1.59
2	F	301	NAP	C5A-N7A	-2.38	1.34	1.39
2	A	301	NAP	O4D-C1D	2.38	1.44	1.40
2	H	301	NAP	C8A-N7A	2.38	1.36	1.31
2	G	301	NAP	C8A-N7A	2.33	1.36	1.31
2	C	301	NAP	PN-O3	2.25	1.61	1.59
2	E	301	NAP	C5A-N7A	-2.23	1.35	1.39
2	E	301	NAP	C8A-N7A	2.17	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAP	C4A-N9A	-2.12	1.33	1.37
2	C	301	NAP	C4A-N9A	-2.10	1.33	1.37
2	A	301	NAP	C5A-N7A	-2.09	1.35	1.39
2	E	301	NAP	P2B-O2B	2.08	1.63	1.59
2	F	301	NAP	PA-O3	2.02	1.61	1.59

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	C5A-C4A-N3A	-6.06	118.37	126.72
2	G	301	NAP	C5A-C4A-N3A	-5.47	119.19	126.72
2	A	301	NAP	C5A-C4A-N3A	-5.45	119.21	126.72
2	H	301	NAP	C5A-C4A-N3A	-5.40	119.29	126.72
2	F	301	NAP	C5A-C4A-N3A	-5.34	119.37	126.72
2	C	301	NAP	C5A-C4A-N3A	-5.22	119.53	126.72
2	E	301	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
2	F	301	NAP	O4B-C1B-N9A	4.95	117.59	108.09
2	E	301	NAP	N3A-C4A-N9A	4.88	135.47	127.17
2	G	301	NAP	N3A-C4A-N9A	4.66	135.10	127.17
2	B	301	NAP	C5A-C4A-N3A	-4.60	120.39	126.72
2	H	301	NAP	N3A-C4A-N9A	4.55	134.90	127.17
2	A	301	NAP	N3A-C4A-N9A	4.46	134.75	127.17
2	D	301	NAP	N3A-C4A-N9A	4.46	134.75	127.17
2	F	301	NAP	C4A-C5A-N7A	-4.28	105.69	110.58
2	F	301	NAP	C4D-O4D-C1D	-4.21	106.07	109.92
2	B	301	NAP	O4B-C1B-N9A	4.12	116.00	108.09
2	G	301	NAP	N3A-C2A-N1A	-4.11	122.36	128.58
2	A	301	NAP	C4A-C5A-N7A	-4.09	105.90	110.58
2	H	301	NAP	N3A-C2A-N1A	-4.02	122.50	128.58
2	D	301	NAP	C4A-C5A-N7A	-3.98	106.03	110.58
2	G	301	NAP	C2A-N3A-C4A	3.98	121.55	111.83
2	A	301	NAP	C4A-N9A-C8A	3.96	109.89	105.74
2	E	301	NAP	C4A-N9A-C8A	3.95	109.89	105.74
2	D	301	NAP	C6N-N1N-C2N	-3.95	118.52	121.88
2	C	301	NAP	C2A-N3A-C4A	3.95	121.48	111.83
2	H	301	NAP	C2A-N3A-C4A	3.95	121.47	111.83
2	F	301	NAP	C2A-N3A-C4A	3.93	121.43	111.83
2	F	301	NAP	N3A-C2A-N1A	-3.92	122.64	128.58
2	C	301	NAP	C4A-C5A-N7A	-3.88	106.14	110.58
2	H	301	NAP	C4A-N9A-C8A	3.83	109.76	105.74
2	A	301	NAP	C2A-N3A-C4A	3.80	121.11	111.83
2	H	301	NAP	C4A-C5A-N7A	-3.80	106.24	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	N3A-C4A-N9A	3.77	133.57	127.17
2	B	301	NAP	N3A-C2A-N1A	-3.74	122.93	128.58
2	B	301	NAP	C4A-C5A-N7A	-3.72	106.33	110.58
2	F	301	NAP	O3-PA-O1A	-3.71	99.56	110.70
2	A	301	NAP	N3A-C2A-N1A	-3.70	122.98	128.58
2	E	301	NAP	C6N-N1N-C2N	-3.67	118.76	121.88
2	G	301	NAP	C4A-N9A-C8A	3.66	109.58	105.74
2	F	301	NAP	C6A-C5A-N7A	3.60	139.04	132.09
2	D	301	NAP	C2A-N3A-C4A	3.58	120.58	111.83
2	C	301	NAP	N3A-C2A-N1A	-3.58	123.16	128.58
2	G	301	NAP	C4A-C5A-N7A	-3.58	106.49	110.58
2	E	301	NAP	N3A-C2A-N1A	-3.32	123.56	128.58
2	B	301	NAP	C6N-N1N-C2N	-3.32	119.06	121.88
2	A	301	NAP	C5A-N7A-C8A	3.31	108.65	103.45
2	H	301	NAP	C5A-N7A-C8A	3.29	108.62	103.45
2	C	301	NAP	C6N-N1N-C2N	-3.29	119.08	121.88
2	E	301	NAP	C2A-N3A-C4A	3.28	119.85	111.83
2	B	301	NAP	C2A-N3A-C4A	3.25	119.77	111.83
2	D	301	NAP	N3A-C2A-N1A	-3.21	123.72	128.58
2	D	301	NAP	O2B-C2B-C1B	3.18	121.23	110.05
2	D	301	NAP	C5A-N7A-C8A	3.15	108.39	103.45
2	A	301	NAP	N9A-C8A-N7A	-3.12	109.52	113.94
2	H	301	NAP	N9A-C8A-N7A	-3.08	109.57	113.94
2	C	301	NAP	C6A-C5A-N7A	3.05	137.97	132.09
2	G	301	NAP	C2N-C3N-C4N	3.02	121.77	118.26
2	D	301	NAP	O2B-P2B-O1X	-2.97	98.75	109.33
2	F	301	NAP	C5D-C4D-C3D	-2.88	104.86	115.21
2	E	301	NAP	O4D-C4D-C3D	2.87	110.85	105.15
2	B	301	NAP	N3A-C4A-N9A	2.80	131.93	127.17
2	C	301	NAP	C4A-N9A-C8A	2.78	108.66	105.74
2	G	301	NAP	C5A-N7A-C8A	2.78	107.82	103.45
2	C	301	NAP	C2N-C3N-C4N	2.78	121.49	118.26
2	A	301	NAP	C6A-C5A-N7A	2.77	137.43	132.09
2	F	301	NAP	C5A-C4A-N9A	2.76	108.82	105.81
2	G	301	NAP	C6N-N1N-C2N	-2.75	119.54	121.88
2	H	301	NAP	C6A-C5A-N7A	2.75	137.39	132.09
2	F	301	NAP	N3A-C4A-N9A	2.73	131.81	127.17
2	D	301	NAP	O4B-C1B-C2B	-2.69	101.96	106.59
2	G	301	NAP	C2A-N1A-C6A	2.67	123.11	118.73
2	F	301	NAP	C1B-N9A-C8A	2.66	133.00	127.09
2	G	301	NAP	C6A-C5A-N7A	2.65	137.19	132.09
2	F	301	NAP	O2N-PN-O3	-2.64	100.15	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	C5A-N7A-C8A	2.62	107.57	103.45
2	F	301	NAP	C4A-N9A-C1B	-2.62	120.51	126.63
2	B	301	NAP	C2A-N1A-C6A	2.62	123.03	118.73
2	F	301	NAP	O3X-P2B-O2X	2.61	117.60	107.80
2	D	301	NAP	C5B-C4B-C3B	-2.60	105.84	115.21
2	B	301	NAP	C6A-C5A-N7A	2.56	137.03	132.09
2	A	301	NAP	C6N-N1N-C2N	-2.53	119.73	121.88
2	G	301	NAP	P2B-O2B-C2B	-2.52	116.70	123.43
2	G	301	NAP	N9A-C8A-N7A	-2.50	110.39	113.94
2	H	301	NAP	O2A-PA-O1A	2.49	124.05	112.44
2	H	301	NAP	C6N-N1N-C2N	-2.45	119.79	121.88
2	B	301	NAP	C5N-C6N-N1N	2.44	123.71	120.38
2	G	301	NAP	C4B-O4B-C1B	-2.42	104.11	109.47
2	C	301	NAP	O3X-P2B-O2X	2.42	116.88	107.80
2	B	301	NAP	O5B-C5B-C4B	2.40	117.16	108.99
2	E	301	NAP	C5A-C6A-N6A	-2.38	117.39	123.29
2	F	301	NAP	O4D-C4D-C5D	2.35	116.88	109.33
2	F	301	NAP	C5A-N7A-C8A	2.34	107.12	103.45
2	F	301	NAP	O2N-PN-O5D	2.33	118.15	107.57
2	B	301	NAP	O2X-P2B-O1X	2.33	119.91	110.83
2	C	301	NAP	C5N-C4N-C3N	-2.33	118.08	120.36
2	E	301	NAP	C4A-C5A-N7A	-2.33	107.92	110.58
2	E	301	NAP	N6A-C6A-N1A	2.32	123.55	118.38
2	D	301	NAP	O4B-C1B-N9A	2.31	112.53	108.09
2	E	301	NAP	C5N-C6N-N1N	2.30	123.53	120.38
2	C	301	NAP	C5N-C6N-N1N	2.30	123.52	120.38
2	D	301	NAP	C5N-C6N-N1N	2.30	123.52	120.38
2	C	301	NAP	N9A-C8A-N7A	-2.27	110.72	113.94
2	E	301	NAP	N9A-C8A-N7A	-2.27	110.72	113.94
2	H	301	NAP	C2A-N1A-C6A	2.26	122.45	118.73
2	G	301	NAP	C5N-C4N-C3N	-2.22	118.19	120.36
2	E	301	NAP	C5N-C4N-C3N	-2.19	118.21	120.36
2	D	301	NAP	O3-PA-O1A	-2.19	104.12	110.70
2	D	301	NAP	O4B-C4B-C3B	-2.17	100.84	105.15
2	E	301	NAP	C5A-N7A-C8A	2.16	106.84	103.45
2	B	301	NAP	C4A-N9A-C1B	-2.15	121.59	126.63
2	G	301	NAP	O2A-PA-O1A	2.13	122.33	112.44
2	A	301	NAP	C5N-C4N-C3N	-2.11	118.29	120.36
2	C	301	NAP	O4B-C1B-N9A	2.10	112.13	108.09
2	B	301	NAP	O5D-C5D-C4D	-2.10	101.85	108.99
2	E	301	NAP	C2N-C3N-C4N	2.09	120.69	118.26
2	B	301	NAP	O2N-PN-O1N	2.09	122.17	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAP	O5B-C5B-C4B	-2.09	101.88	108.99
2	H	301	NAP	O2B-P2B-O1X	-2.09	101.90	109.33
2	B	301	NAP	C5A-N7A-C8A	2.08	106.71	103.45
2	B	301	NAP	C1B-N9A-C8A	2.08	131.70	127.09
2	F	301	NAP	O2A-PA-O1A	2.07	122.09	112.44
2	D	301	NAP	C6A-C5A-N7A	2.06	136.06	132.09
2	G	301	NAP	O4B-C1B-C2B	-2.05	103.07	106.59
2	C	301	NAP	C4A-N9A-C1B	-2.04	121.87	126.63
2	B	301	NAP	O2B-P2B-O1X	-2.02	102.14	109.33
2	G	301	NAP	O3X-P2B-O2X	2.01	115.35	107.80
2	B	301	NAP	O5B-PA-O1A	2.01	116.90	108.94
2	D	301	NAP	O3X-P2B-O2X	2.01	115.34	107.80

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	PN-O3-PA-O5B
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	C5B-O5B-PA-O3
2	D	301	NAP	C1B-C2B-O2B-P2B
2	D	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5D-O5D-PN-O2N
2	E	301	NAP	C5B-O5B-PA-O2A
2	E	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O2N
2	F	301	NAP	C5D-O5D-PN-O3
2	F	301	NAP	C5D-O5D-PN-O2N
2	H	301	NAP	C5B-O5B-PA-O1A
2	H	301	NAP	C5B-O5B-PA-O2A
2	H	301	NAP	C5B-O5B-PA-O3
3	A	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	302	GOL	O1-C1-C2-C3
3	B	302	GOL	C1-C2-C3-O3
3	B	302	GOL	O2-C2-C3-O3
3	C	302	GOL	O1-C1-C2-C3
3	E	302	GOL	O1-C1-C2-C3
2	B	301	NAP	C3D-C4D-C5D-O5D
2	D	301	NAP	C4B-C5B-O5B-PA
3	A	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
2	D	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3B-C4B-C5B-O5B
2	G	301	NAP	O4B-C4B-C5B-O5B
3	A	302	GOL	C1-C2-C3-O3
3	C	302	GOL	C1-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-O2
3	E	302	GOL	O1-C1-C2-O2
2	H	301	NAP	O4D-C4D-C5D-O5D
2	E	301	NAP	O4B-C4B-C5B-O5B
2	G	301	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C2B-O2B-P2B-O3X
3	A	302	GOL	O2-C2-C3-O3
2	G	301	NAP	C2N-C3N-C7N-O7N
2	F	301	NAP	PN-O3-PA-O5B
2	H	301	NAP	C3D-C4D-C5D-O5D
2	G	301	NAP	C4N-C3N-C7N-O7N
2	G	301	NAP	O4D-C4D-C5D-O5D
2	E	301	NAP	C5B-O5B-PA-O1A
2	E	301	NAP	C5B-O5B-PA-O3
2	G	301	NAP	C4N-C3N-C7N-N7N
2	G	301	NAP	C2N-C3N-C7N-N7N
2	G	301	NAP	C2B-O2B-P2B-O3X
2	H	301	NAP	O4D-C1D-N1N-C6N
2	A	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X
2	F	301	NAP	C2B-O2B-P2B-O1X
2	G	301	NAP	C2B-O2B-P2B-O1X
2	H	301	NAP	PN-O3-PA-O2A
2	H	301	NAP	PN-O3-PA-O5B
2	A	301	NAP	O4B-C4B-C5B-O5B
2	F	301	NAP	C4D-C5D-O5D-PN
2	E	301	NAP	PA-O3-PN-O2N

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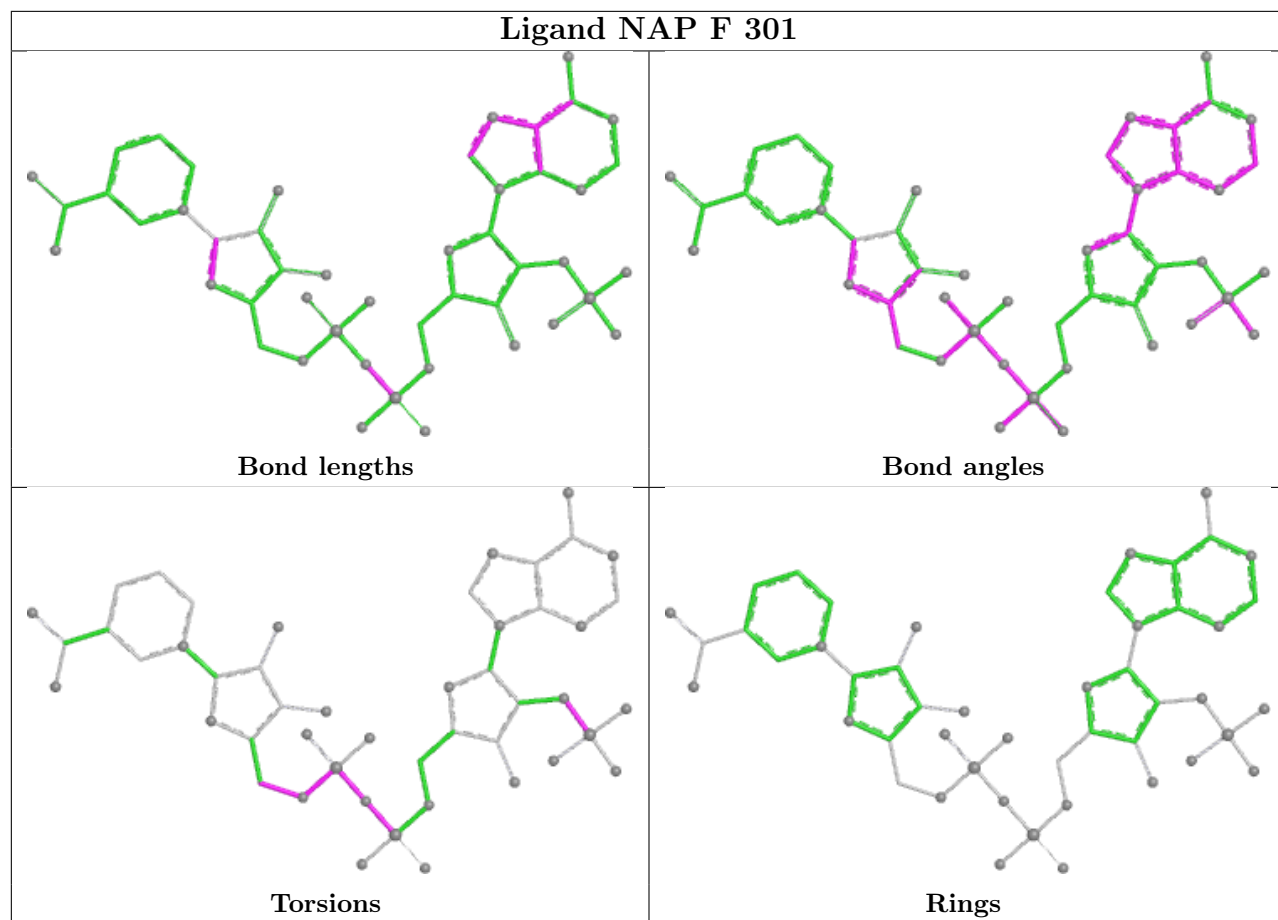
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O2X
2	B	301	NAP	C2B-O2B-P2B-O2X
2	C	301	NAP	C2B-O2B-P2B-O1X
2	E	301	NAP	C2B-O2B-P2B-O1X
2	H	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	PA-O3-PN-O2N
2	F	301	NAP	PA-O3-PN-O2N

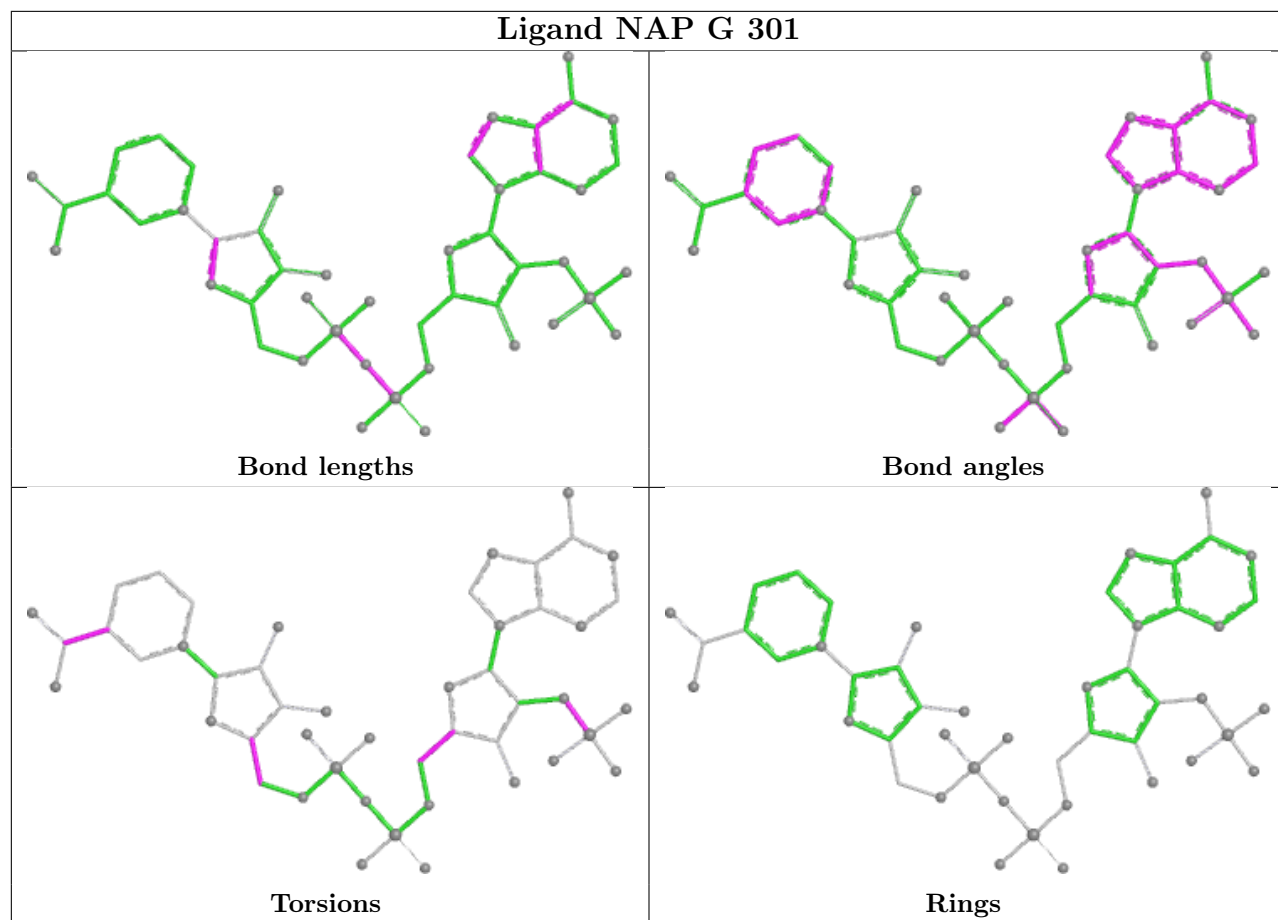
There are no ring outliers.

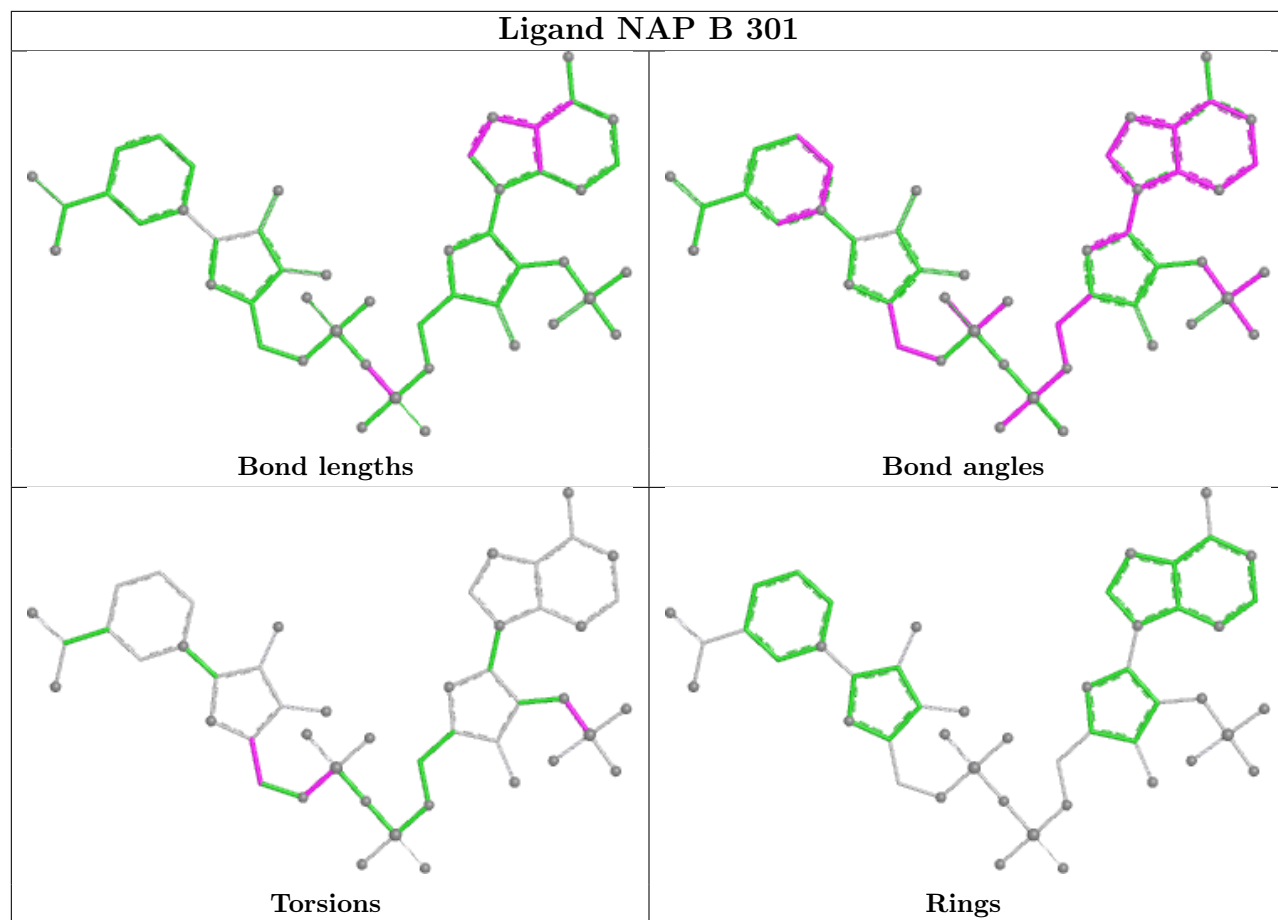
9 monomers are involved in 35 short contacts:

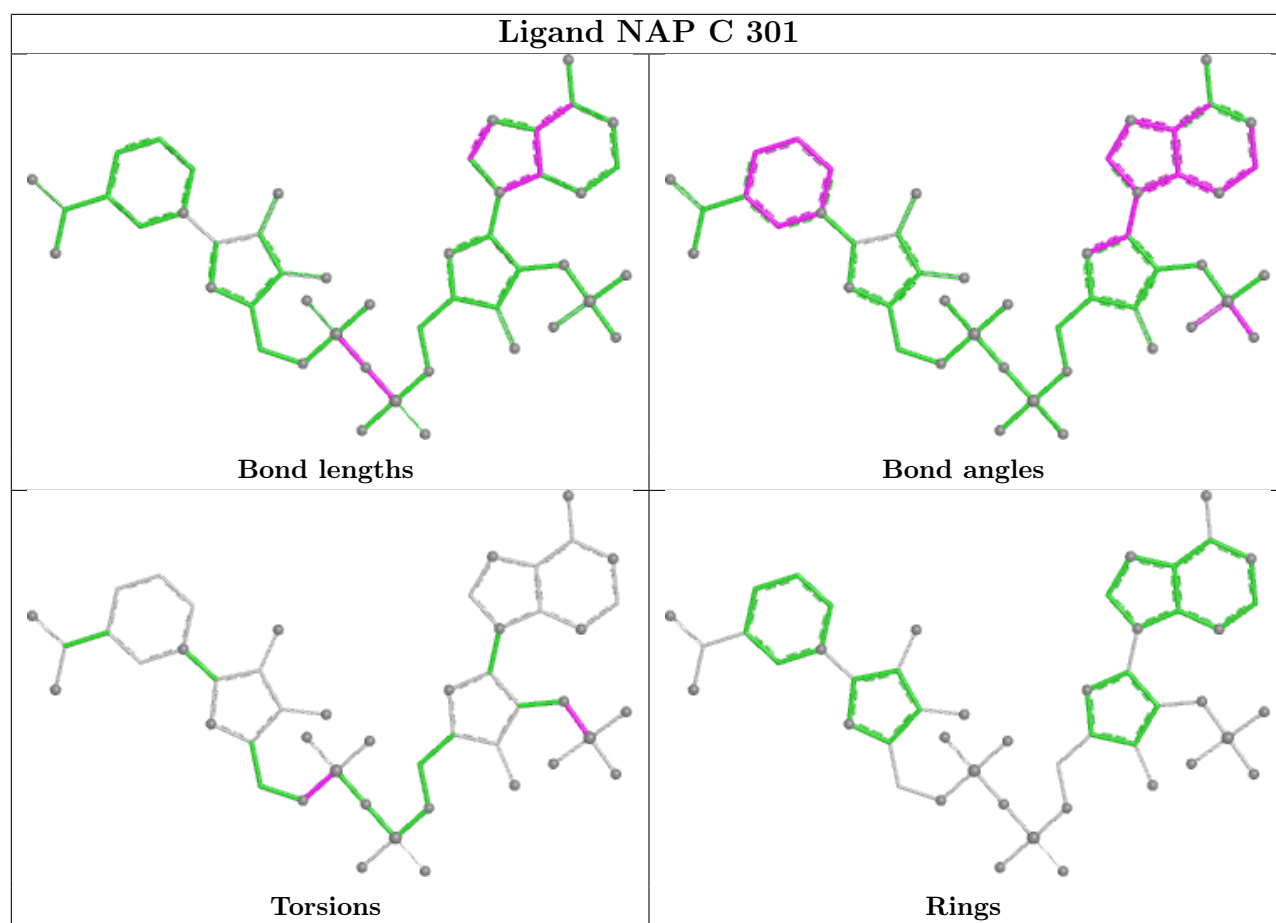
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	NAP	7	0
2	G	301	NAP	6	0
2	B	301	NAP	5	0
2	C	301	NAP	1	0
2	A	301	NAP	1	0
2	H	301	NAP	6	0
3	A	302	GOL	1	0
2	D	301	NAP	4	0
2	E	301	NAP	4	0

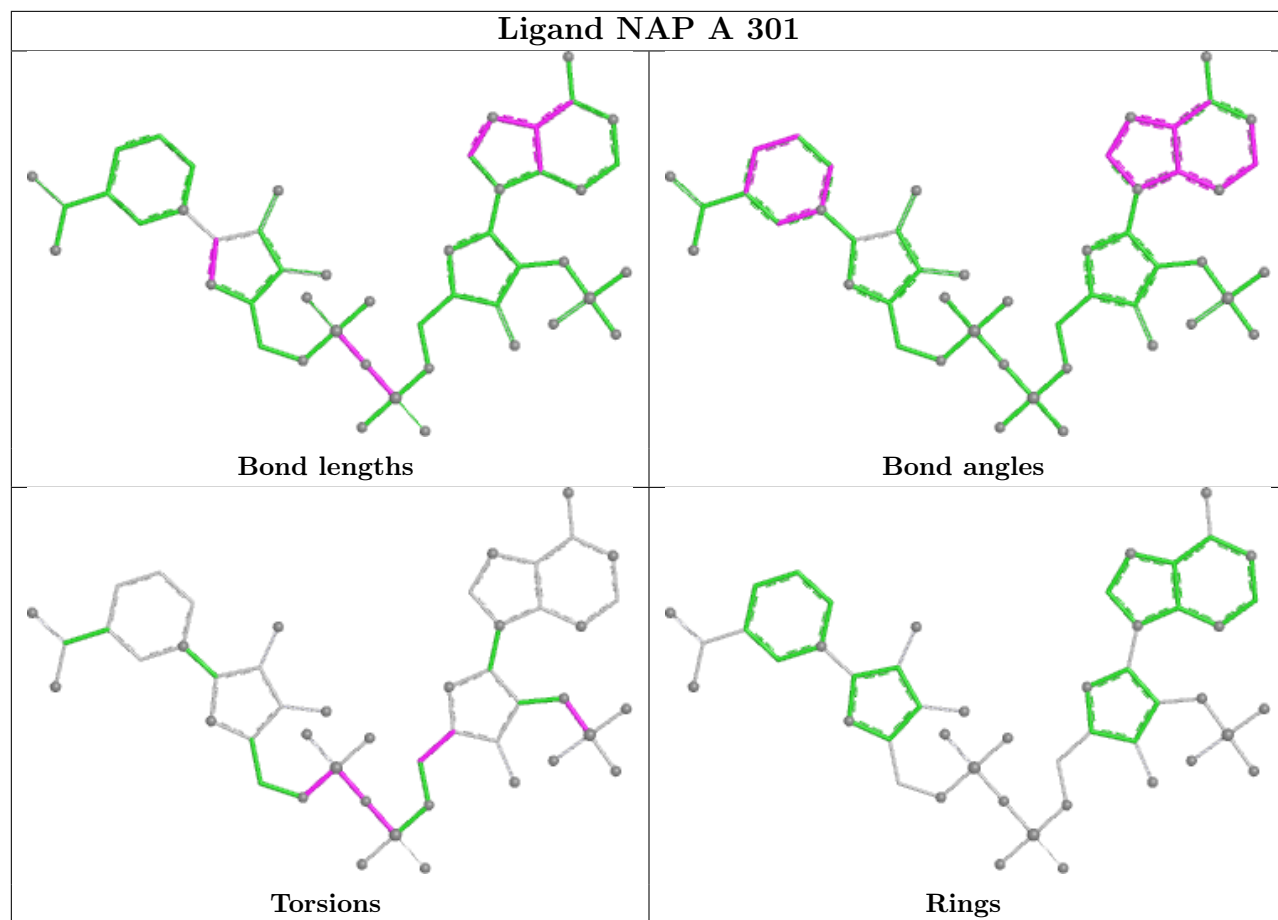
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

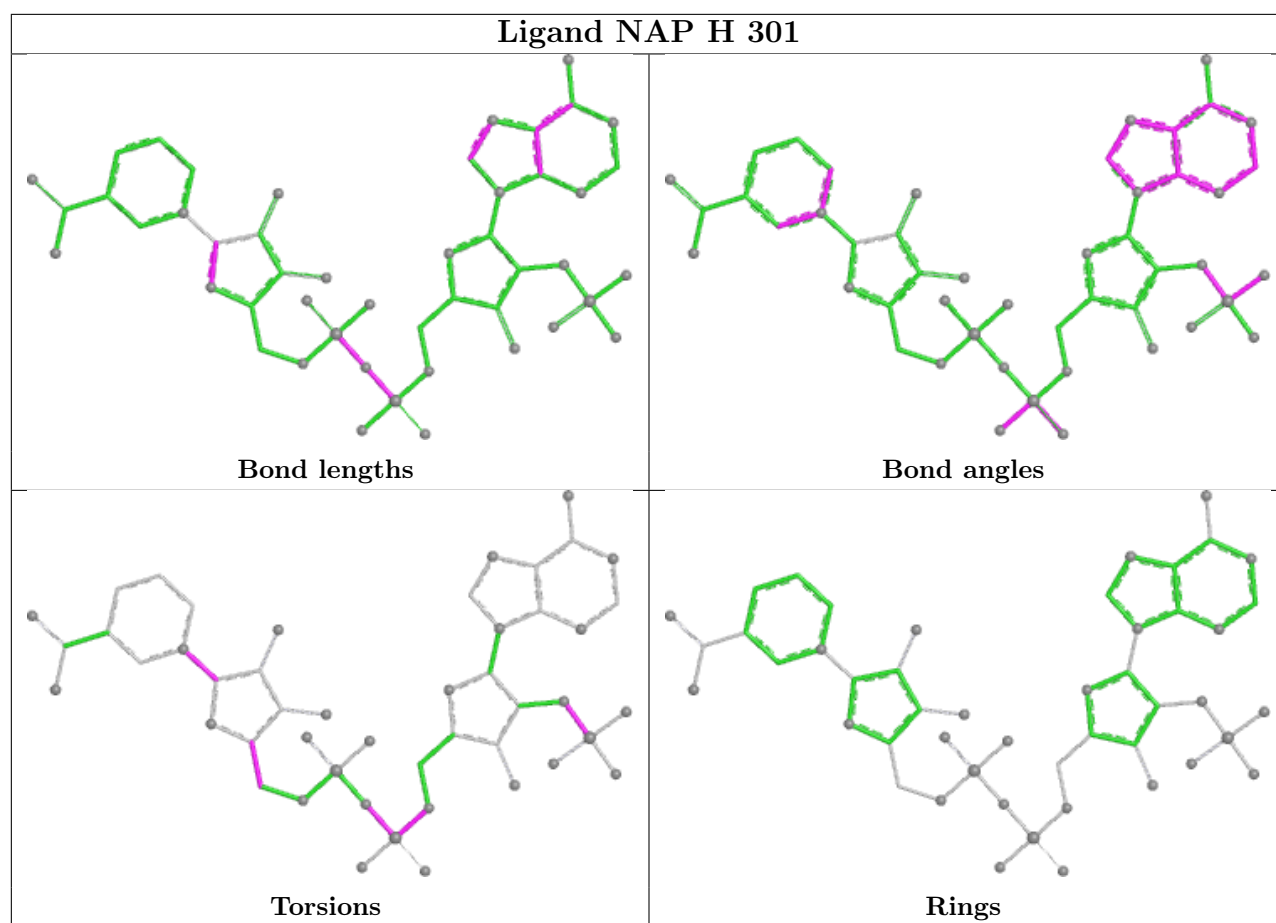


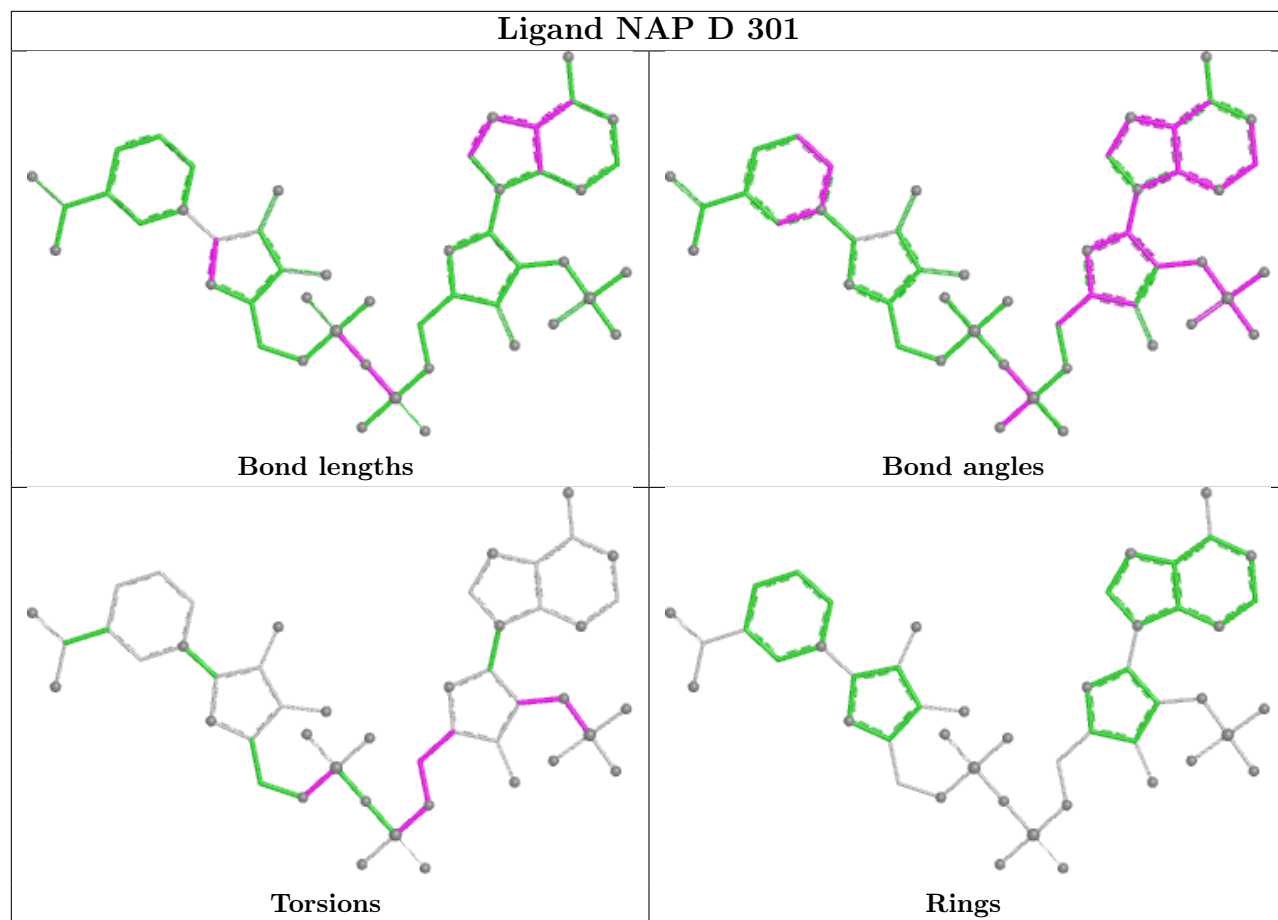


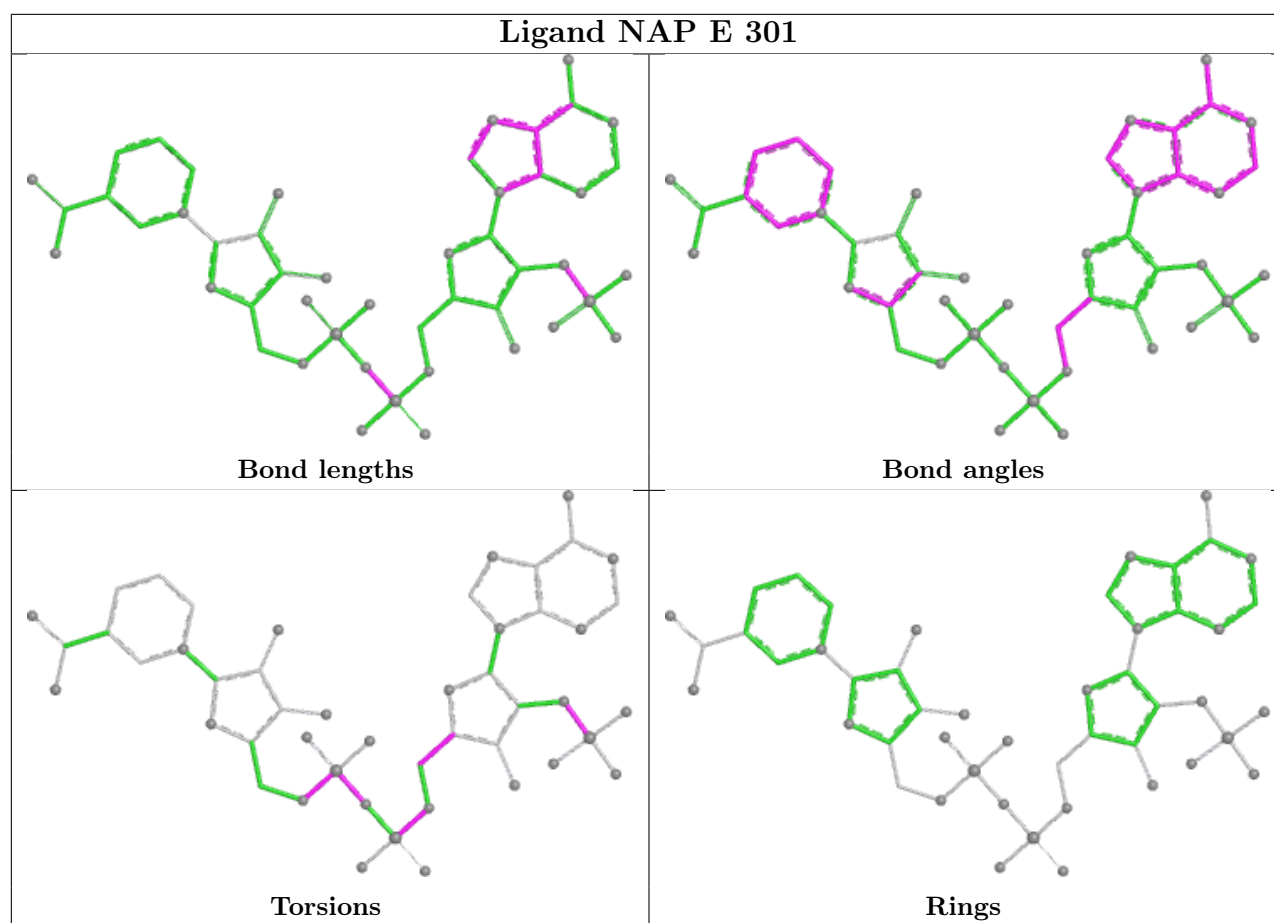












5.7 Other polymers [i](#)

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	249/262 (95%)	1.89	80 (32%) 1 1	1, 53, 92, 145	7 (2%)
1	B	249/262 (95%)	2.15	96 (38%) 1 0	1, 54, 88, 163	11 (4%)
1	C	249/262 (95%)	1.98	89 (35%) 1 0	1, 61, 101, 165	8 (3%)
1	D	249/262 (95%)	1.92	95 (38%) 1 0	31, 54, 88, 151	7 (2%)
1	E	249/262 (95%)	1.91	72 (28%) 1 1	1, 46, 84, 176	7 (2%)
1	F	249/262 (95%)	1.75	67 (26%) 1 1	1, 47, 83, 139	7 (2%)
1	G	249/262 (95%)	2.32	111 (44%) 0 0	1, 57, 89, 139	8 (3%)
1	H	249/262 (95%)	1.57	67 (26%) 1 1	29, 50, 80, 146	6 (2%)
All	All	1992/2096 (95%)	1.94	677 (33%) 1 1	1, 53, 92, 176	61 (3%)

All (677) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	GLN	26.7
1	G	193	SER	25.0
1	F	193	SER	23.3
1	G	191	GLN	22.7
1	B	195	GLN	21.5
1	E	193	SER	21.3
1	C	193	SER	19.4
1	E	196	GLU	18.3
1	G	196	GLU	18.3
1	A	193	SER	17.6
1	E	200	GLU	17.4
1	B	193	SER	16.9
1	B	194	THR	13.0
1	H	191	GLN	11.3
1	A	204	LYS	11.0
1	C	188	ILE	10.8

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Mol	Chain	Res	Type	RSRZ
1	B	190	ASN	10.4
1	G	197	GLU	10.4
1	B	202	ARG	10.0
1	D	200	GLU	9.8
1	A	202	ARG	9.3
1	C	195	GLN	9.0
1	A	195	GLN	8.9
1	G	195	GLN	8.9
1	B	200	GLU	8.8
1	D	195	GLN	8.7
1	G	204	LYS	8.3
1	A	199	ASP	8.3
1	H	196	GLU	8.2
1	D	196	GLU	8.1
1	F	194	THR	8.0
1	H	200	GLU	7.9
1	E	195	GLN	7.8
1	B	197	GLU	7.7
1	F	196	GLU	7.6
1	F	195	GLN	7.6
1	G	194	THR	7.4
1	C	196	GLU	7.4
1	D	193	SER	7.3
1	G	199	ASP	7.2
1	C	194	THR	7.1
1	C	189	GLU	7.1
1	B	196	GLU	7.0
1	B	189	GLU	6.7
1	F	204	LYS	6.7
1	D	205	PHE	6.6
1	G	208	ALA	6.5
1	E	194	THR	6.5
1	C	199	ASP	6.5
1	B	204	LYS	6.5
1	A	187	ILE	6.4
1	E	188	ILE	6.4
1	A	200	GLU	6.2
1	H	193	SER	6.1
1	A	196	GLU	6.0
1	E	80	SER	6.0
1	H	195	GLN	5.9
1	F	199	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	79	GLY	5.8
1	B	129	GLY	5.8
1	E	204	LYS	5.7
1	B	6	ASN	5.6
1	G	53	ASN	5.6
1	D	51	GLY	5.5
1	E	2	TYR	5.5
1	C	201	LEU	5.4
1	H	205	PHE	5.4
1	E	34	PHE	5.4
1	B	30	GLY	5.4
1	G	20	LEU	5.4
1	F	197	GLU	5.3
1	B	188	ILE	5.3
1	B	192	VAL	5.3
1	G	188	ILE	5.2
1	E	79	GLY	5.2
1	E	184	ASP	5.2
1	A	52	ARG	5.1
1	G	2	TYR	5.1
1	H	111	ASN	5.1
1	B	130	GLY	5.1
1	F	2	TYR	5.0
1	B	127	ARG	5.0
1	F	1	ALA	5.0
1	A	89	GLY	4.9
1	B	198	ALA	4.9
1	E	1	ALA	4.8
1	H	76	GLU	4.8
1	B	90	ALA	4.7
1	A	188	ILE	4.7
1	G	83	VAL	4.7
1	F	75	ARG	4.7
1	C	184	ASP	4.7
1	E	205	PHE	4.7
1	F	6	ASN	4.7
1	B	113	ARG	4.6
1	G	88	SER	4.6
1	G	192	VAL	4.6
1	A	14	GLY	4.6
1	H	90	ALA	4.5
1	E	191	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	198	ALA	4.5
1	E	84	LEU	4.5
1	F	151	SER	4.5
1	C	208	ALA	4.4
1	D	184	ASP	4.4
1	C	1	ALA	4.4
1	D	208	ALA	4.4
1	H	194	THR	4.3
1	C	187	ILE	4.3
1	A	194	THR	4.3
1	E	149	THR	4.3
1	G	187	ILE	4.2
1	B	75	ARG	4.2
1	D	101	PRO	4.2
1	G	61	VAL	4.2
1	G	236	ALA	4.2
1	D	192	VAL	4.1
1	F	33	VAL	4.1
1	D	14	GLY	4.1
1	F	192	VAL	4.1
1	F	79	GLY	4.1
1	B	59	ALA	4.1
1	C	192	VAL	4.0
1	G	91	ILE	4.0
1	B	185	THR	4.0
1	F	205	PHE	4.0
1	G	7	LYS	4.0
1	D	151	SER	3.9
1	A	75	ARG	3.9
1	G	127	ARG	3.9
1	F	190	ASN	3.9
1	B	80	SER	3.9
1	E	187	ILE	3.9
1	C	148	ASP	3.9
1	B	201	LEU	3.8
1	H	192	VAL	3.8
1	F	198	ALA	3.8
1	G	131	SER	3.8
1	D	43	LEU	3.8
1	G	201	LEU	3.8
1	D	199	ASP	3.8
1	G	54	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	86	ALA	3.8
1	F	155	ALA	3.8
1	E	197	GLU	3.8
1	H	1	ALA	3.8
1	D	16	SER	3.7
1	B	132	VAL	3.7
1	A	104	TYR	3.7
1	G	43	LEU	3.7
1	B	8	THR	3.7
1	G	34	PHE	3.7
1	B	165	THR	3.7
1	A	184	ASP	3.7
1	H	184	ASP	3.7
1	D	198	ALA	3.6
1	A	79	GLY	3.6
1	F	127	ARG	3.6
1	A	189	GLU	3.6
1	D	99	ILE	3.6
1	F	54	VAL	3.6
1	D	90	ALA	3.6
1	B	205	PHE	3.6
1	D	100	THR	3.6
1	A	153	ALA	3.6
1	A	137	SER	3.6
1	G	202	ARG	3.6
1	H	140	GLY	3.6
1	A	80	SER	3.6
1	E	137	SER	3.6
1	G	71	TYR	3.6
1	A	78	ARG	3.5
1	C	198	ALA	3.5
1	D	207	ALA	3.5
1	A	111	ASN	3.5
1	E	75	ARG	3.5
1	G	44	GLU	3.5
1	F	201	LEU	3.5
1	A	139	ALA	3.5
1	A	76	GLU	3.5
1	C	202	ARG	3.5
1	D	52	ARG	3.5
1	H	2	TYR	3.5
1	G	183	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	76	GLU	3.4
1	H	40	ARG	3.4
1	D	75	ARG	3.4
1	A	77	GLN	3.4
1	A	201	LEU	3.4
1	G	10	VAL	3.4
1	F	23	ALA	3.4
1	G	82	ASP	3.4
1	B	78	ARG	3.4
1	B	203	ALA	3.4
1	A	73	ILE	3.4
1	F	179	SER	3.4
1	H	159	SER	3.4
1	D	194	THR	3.4
1	A	6	ASN	3.3
1	A	192	VAL	3.3
1	E	189	GLU	3.3
1	G	58	LYS	3.3
1	G	121	LYS	3.3
1	G	206	ALA	3.3
1	D	105	ASP	3.3
1	C	52	ARG	3.3
1	D	175	VAL	3.3
1	F	74	VAL	3.3
1	B	72	ALA	3.3
1	D	136	SER	3.3
1	G	232	SER	3.3
1	F	88	SER	3.3
1	G	106	ARG	3.2
1	C	71	TYR	3.2
1	F	136	SER	3.2
1	E	202	ARG	3.2
1	B	137	SER	3.2
1	C	203	ALA	3.2
1	G	28	ALA	3.2
1	G	205	PHE	3.2
1	F	77	GLN	3.2
1	G	120	GLN	3.2
1	F	30	GLY	3.2
1	D	150	TYR	3.2
1	B	105	ASP	3.2
1	H	198	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	141	VAL	3.2
1	E	83	VAL	3.2
1	D	189	GLU	3.2
1	E	217	PRO	3.2
1	E	32	TYR	3.1
1	A	113	ARG	3.1
1	G	222	ALA	3.1
1	B	85	PHE	3.1
1	C	175	VAL	3.1
1	H	54	VAL	3.1
1	F	248	GLN	3.1
1	H	244	GLY	3.1
1	E	125	LEU	3.1
1	A	236	ALA	3.1
1	E	229	SER	3.1
1	D	190	ASN	3.1
1	C	70	LEU	3.1
1	B	146	ALA	3.1
1	C	205	PHE	3.1
1	G	33	VAL	3.1
1	C	73	ILE	3.1
1	D	202	ARG	3.1
1	A	90	ALA	3.1
1	A	205	PHE	3.1
1	A	37	GLY	3.1
1	C	13	GLY	3.1
1	G	14	GLY	3.1
1	G	218	GLU	3.1
1	D	110	VAL	3.0
1	D	80	SER	3.0
1	E	52	ARG	3.0
1	E	78	ARG	3.0
1	A	239	GLU	3.0
1	E	185	THR	3.0
1	A	1	ALA	3.0
1	B	33	VAL	3.0
1	G	27	VAL	3.0
1	G	85	PHE	3.0
1	C	233	SER	3.0
1	E	230	ASP	3.0
1	F	80	SER	3.0
1	D	191	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	188	ILE	3.0
1	A	102	GLU	3.0
1	B	187	ILE	3.0
1	A	131	SER	3.0
1	C	65	GLU	3.0
1	D	40	ARG	3.0
1	B	53	ASN	3.0
1	C	151	SER	3.0
1	E	127	ARG	2.9
1	H	52	ARG	2.9
1	C	150	TYR	2.9
1	C	186	PRO	2.9
1	A	198	ALA	2.9
1	B	10	VAL	2.9
1	C	119	VAL	2.9
1	C	121	LYS	2.9
1	B	114	GLY	2.9
1	B	82	ASP	2.9
1	C	90	ALA	2.9
1	G	59	ALA	2.9
1	G	73	ILE	2.9
1	H	99	ILE	2.9
1	G	225	LEU	2.9
1	B	237	GLY	2.9
1	H	151	SER	2.9
1	A	214	VAL	2.9
1	B	117	PHE	2.9
1	F	187	ILE	2.9
1	D	201	LEU	2.9
1	F	5	LEU	2.9
1	D	6	ASN	2.9
1	E	6	ASN	2.9
1	G	87	ASN	2.9
1	A	119	VAL	2.9
1	G	138	VAL	2.9
1	B	40	ARG	2.9
1	D	103	HIS	2.9
1	B	55	THR	2.9
1	A	84	LEU	2.9
1	D	168	LEU	2.9
1	A	191	GLN	2.8
1	C	15	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	156	ALA	2.8
1	C	34	PHE	2.8
1	E	53	ASN	2.8
1	F	78	ARG	2.8
1	G	6	ASN	2.8
1	E	199	ASP	2.8
1	C	50	ILE	2.8
1	F	14	GLY	2.8
1	G	63	LYS	2.8
1	C	197	GLU	2.8
1	H	42	GLU	2.8
1	D	104	TYR	2.8
1	C	228	ALA	2.8
1	F	59	ALA	2.8
1	C	85	PHE	2.8
1	D	34	PHE	2.8
1	D	87	ASN	2.8
1	D	82	ASP	2.8
1	F	128	ASP	2.8
1	G	13	GLY	2.8
1	B	2	TYR	2.8
1	A	156	ALA	2.8
1	G	221	ALA	2.8
1	H	190	ASN	2.8
1	B	109	ASP	2.8
1	D	76	GLU	2.8
1	G	69	ARG	2.8
1	D	59	ALA	2.8
1	G	21	ALA	2.8
1	A	127	ARG	2.7
1	E	192	VAL	2.7
1	D	91	ILE	2.7
1	D	111	ASN	2.7
1	A	151	SER	2.7
1	A	212	GLY	2.7
1	B	88	SER	2.7
1	B	151	SER	2.7
1	G	51	GLY	2.7
1	H	69	ARG	2.7
1	E	156	ALA	2.7
1	E	201	LEU	2.7
1	G	223	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	32	TYR	2.7
1	E	190	ASN	2.7
1	B	101	PRO	2.7
1	G	157	VAL	2.7
1	A	222	ALA	2.7
1	B	125	LEU	2.7
1	D	32	TYR	2.7
1	B	52	ARG	2.7
1	G	12	THR	2.7
1	H	109	ASP	2.7
1	D	83	VAL	2.7
1	A	64	LEU	2.7
1	D	134	LEU	2.7
1	C	32	TYR	2.7
1	C	79	GLY	2.7
1	B	191	GLN	2.7
1	G	50	ILE	2.6
1	C	117	PHE	2.6
1	C	236	ALA	2.6
1	F	34	PHE	2.6
1	B	124	PRO	2.6
1	B	76	GLU	2.6
1	D	128	ASP	2.6
1	E	7	LYS	2.6
1	E	246	LEU	2.6
1	H	152	ALA	2.6
1	H	7	LYS	2.6
1	G	48	ALA	2.6
1	H	177	ALA	2.6
1	B	19	GLY	2.6
1	D	186	PRO	2.6
1	E	245	GLY	2.6
1	C	63	LYS	2.6
1	H	175	VAL	2.6
1	D	97	GLU	2.6
1	A	122	ALA	2.6
1	G	16	SER	2.6
1	H	113	ARG	2.6
1	E	234	TYR	2.6
1	F	186	PRO	2.6
1	G	150	TYR	2.6
1	A	74	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	50	ILE	2.6
1	F	18	ILE	2.6
1	H	50	ILE	2.6
1	H	93	GLN	2.6
1	A	86	ALA	2.6
1	G	1	ALA	2.6
1	D	127	ARG	2.5
1	D	88	SER	2.5
1	D	41	LYS	2.5
1	A	13	GLY	2.5
1	C	89	GLY	2.5
1	D	17	GLY	2.5
1	D	185	THR	2.5
1	C	69	ARG	2.5
1	B	131	SER	2.5
1	G	30	GLY	2.5
1	C	45	GLN	2.5
1	C	135	THR	2.5
1	D	45	GLN	2.5
1	A	155	ALA	2.5
1	G	156	ALA	2.5
1	C	111	ASN	2.5
1	B	126	LEU	2.5
1	G	237	GLY	2.5
1	H	14	GLY	2.5
1	C	61	VAL	2.5
1	E	27	VAL	2.5
1	C	44	GLU	2.5
1	D	107	THR	2.5
1	C	106	ARG	2.5
1	C	127	ARG	2.5
1	H	158	ARG	2.5
1	D	68	ASP	2.5
1	C	179	SER	2.5
1	G	186	PRO	2.5
1	D	37	GLY	2.5
1	H	130	GLY	2.5
1	A	138	VAL	2.5
1	B	119	VAL	2.5
1	E	104	TYR	2.5
1	G	189	GLU	2.5
1	A	203	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	69	ARG	2.5
1	D	113	ARG	2.5
1	G	9	ALA	2.5
1	G	56	ALA	2.5
1	G	198	ALA	2.5
1	H	87	ASN	2.5
1	A	186	PRO	2.4
1	B	91	ILE	2.4
1	C	116	ILE	2.4
1	D	187	ILE	2.4
1	D	188	ILE	2.4
1	B	170	GLY	2.4
1	E	14	GLY	2.4
1	F	37	GLY	2.4
1	E	179	SER	2.4
1	F	137	SER	2.4
1	F	3	ARG	2.4
1	G	65	GLU	2.4
1	B	1	ALA	2.4
1	C	93	GLN	2.4
1	E	221	ALA	2.4
1	D	62	THR	2.4
1	C	4	LEU	2.4
1	E	123	LEU	2.4
1	F	4	LEU	2.4
1	H	199	ASP	2.4
1	E	224	VAL	2.4
1	H	235	VAL	2.4
1	A	229	SER	2.4
1	F	153	ALA	2.4
1	H	147	HIS	2.4
1	C	115	LEU	2.4
1	B	110	VAL	2.4
1	C	214	VAL	2.4
1	D	19	GLY	2.4
1	F	132	VAL	2.4
1	G	132	VAL	2.4
1	D	204	LYS	2.4
1	G	90	ALA	2.4
1	E	214	VAL	2.4
1	F	108	PHE	2.4
1	F	177	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	2.4
1	H	88	SER	2.4
1	H	165	THR	2.4
1	D	96	LEU	2.4
1	F	134	LEU	2.4
1	H	187	ILE	2.4
1	A	15	ASN	2.3
1	A	154	LYS	2.3
1	E	212	GLY	2.3
1	E	152	ALA	2.3
1	E	203	ALA	2.3
1	G	47	ALA	2.3
1	C	104	TYR	2.3
1	C	123	LEU	2.3
1	D	36	VAL	2.3
1	G	39	ARG	2.3
1	G	178	VAL	2.3
1	G	114	GLY	2.3
1	C	28	ALA	2.3
1	D	48	ALA	2.3
1	C	172	SER	2.3
1	A	61	VAL	2.3
1	E	108	PHE	2.3
1	F	28	ALA	2.3
1	G	161	ALA	2.3
1	G	148	ASP	2.3
1	A	16	SER	2.3
1	C	35	ILE	2.3
1	H	91	ILE	2.3
1	C	185	THR	2.3
1	H	119	VAL	2.3
1	B	51	GLY	2.3
1	G	15	ASN	2.3
1	B	228	ALA	2.3
1	D	42	GLU	2.3
1	E	76	GLU	2.3
1	E	139	ALA	2.3
1	H	207	ALA	2.3
1	A	148	ASP	2.3
1	G	96	LEU	2.3
1	G	220	LEU	2.3
1	H	41	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	173	ILE	2.3
1	C	183	ILE	2.3
1	C	137	SER	2.3
1	E	106	ARG	2.3
1	G	8	THR	2.3
1	C	2	TYR	2.3
1	B	54	VAL	2.3
1	B	244	GLY	2.3
1	B	65	GLU	2.2
1	B	208	ALA	2.2
1	C	53	ASN	2.2
1	C	221	ALA	2.2
1	E	177	ALA	2.2
1	H	161	ALA	2.2
1	H	201	LEU	2.2
1	F	45	GLN	2.2
1	B	118	THR	2.2
1	G	209	THR	2.2
1	E	10	VAL	2.2
1	H	27	VAL	2.2
1	C	122	ALA	2.2
1	D	53	ASN	2.2
1	F	126	LEU	2.2
1	B	60	ASP	2.2
1	D	66	ASP	2.2
1	F	230	ASP	2.2
1	G	52	ARG	2.2
1	A	163	THR	2.2
1	A	209	THR	2.2
1	H	112	VAL	2.2
1	A	30	GLY	2.2
1	A	146	ALA	2.2
1	B	63	LYS	2.2
1	B	97	GLU	2.2
1	B	139	ALA	2.2
1	B	156	ALA	2.2
1	D	220	LEU	2.2
1	H	153	ALA	2.2
1	B	111	ASN	2.2
1	A	99	ILE	2.2
1	D	11	ILE	2.2
1	E	73	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	45	GLN	2.2
1	F	178	VAL	2.2
1	H	110	VAL	2.2
1	G	55	THR	2.2
1	G	100	THR	2.2
1	B	17	GLY	2.2
1	B	172	SER	2.2
1	E	30	GLY	2.2
1	H	26	PHE	2.2
1	E	96	LEU	2.2
1	F	125	LEU	2.2
1	H	222	ALA	2.2
1	A	40	ARG	2.2
1	H	106	ARG	2.2
1	C	231	ASP	2.2
1	D	74	VAL	2.2
1	G	119	VAL	2.2
1	G	180	PRO	2.2
1	H	231	ASP	2.2
1	C	118	THR	2.2
1	F	95	THR	2.2
1	F	165	THR	2.2
1	H	55	THR	2.2
1	A	2	TYR	2.2
1	D	159	SER	2.2
1	A	228	ALA	2.2
1	B	152	ALA	2.2
1	D	152	ALA	2.2
1	D	116	ILE	2.1
1	B	176	ASN	2.1
1	F	111	ASN	2.1
1	A	57	VAL	2.1
1	B	74	VAL	2.1
1	C	54	VAL	2.1
1	H	157	VAL	2.1
1	A	100	THR	2.1
1	A	118	THR	2.1
1	H	204	LYS	2.1
1	B	89	GLY	2.1
1	H	17	GLY	2.1
1	B	5	LEU	2.1
1	F	26	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	153	ALA	2.1
1	D	72	ALA	2.1
1	D	153	ALA	2.1
1	C	99	ILE	2.1
1	G	18	ILE	2.1
1	B	77	GLN	2.1
1	B	87	ASN	2.1
1	E	74	VAL	2.1
1	E	82	ASP	2.1
1	F	143	GLY	2.1
1	B	108	PHE	2.1
1	D	85	PHE	2.1
1	D	211	LEU	2.1
1	C	31	ALA	2.1
1	C	161	ALA	2.1
1	D	203	ALA	2.1
1	G	78	ARG	2.1
1	H	28	ALA	2.1
1	G	99	ILE	2.1
1	F	191	GLN	2.1
1	F	147	HIS	2.1
1	H	176	ASN	2.1
1	A	5	LEU	2.1
1	A	143	GLY	2.1
1	D	181	GLY	2.1
1	H	212	GLY	2.1
1	B	107	THR	2.1
1	E	182	ALA	2.1
1	G	203	ALA	2.1
1	G	228	ALA	2.1
1	D	2	TYR	2.1
1	C	232	SER	2.1
1	B	112	VAL	2.1
1	E	138	VAL	2.1
1	F	112	VAL	2.1
1	G	154	LYS	2.1
1	B	246	LEU	2.1
1	B	149	THR	2.1
1	D	247	THR	2.1
1	E	153	ALA	2.1
1	E	173	ILE	2.1
1	G	46	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	122	ALA	2.1
1	H	56	ALA	2.1
1	C	88	SER	2.0
1	C	83	VAL	2.0
1	D	119	VAL	2.0
1	A	124	PRO	2.0
1	G	5	LEU	2.0
1	C	3	ARG	2.0
1	G	212	GLY	2.0
1	F	81	ILE	2.0
1	G	11	ILE	2.0
1	G	81	ILE	2.0
1	C	21	ALA	2.0
1	C	47	ALA	2.0
1	D	197	GLU	2.0
1	G	97	GLU	2.0
1	G	164	TRP	2.0
1	C	10	VAL	2.0
1	C	147	HIS	2.0
1	D	248	GLN	2.0
1	F	83	VAL	2.0
1	A	67	LEU	2.0
1	B	70	LEU	2.0
1	C	64	LEU	2.0
1	G	64	LEU	2.0
1	C	40	ARG	2.0
1	F	52	ARG	2.0
1	B	133	ILE	2.0
1	D	1	ALA	2.0
1	D	44	GLU	2.0
1	D	65	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 oligosaccharides in this entry.

6.4 Ligands

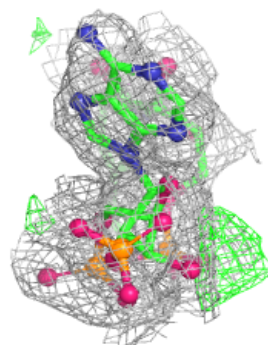
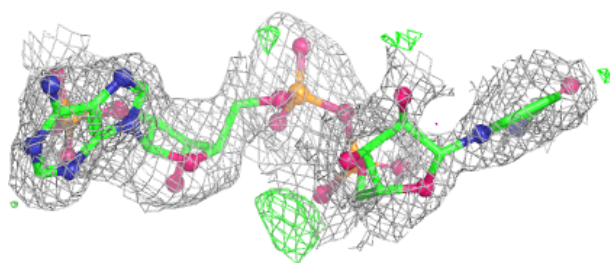
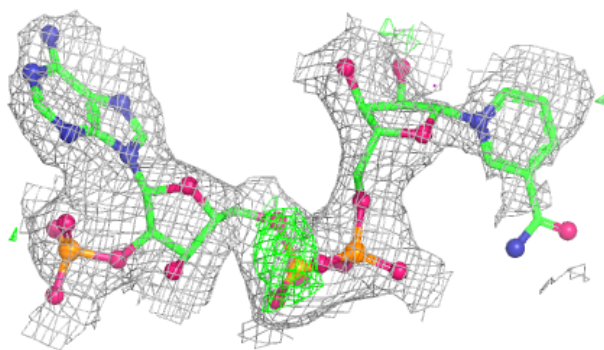
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	302	6/6	0.71	0.23	68,76,84,96	0
3	GOL	E	302	6/6	0.78	0.22	46,61,72,72	0
2	NAP	D	301	48/48	0.83	0.16	54,71,107,132	0
2	NAP	G	301	48/48	0.84	0.16	47,66,79,79	0
2	NAP	A	301	48/48	0.86	0.15	41,63,74,84	0
3	GOL	C	302	6/6	0.86	0.18	63,72,74,78	0
3	GOL	A	302	6/6	0.86	0.13	61,61,63,64	0
2	NAP	E	301	48/48	0.87	0.14	43,56,66,68	0
2	NAP	F	301	48/48	0.88	0.15	34,48,61,74	0
2	NAP	C	301	48/48	0.88	0.14	55,69,78,85	0
2	NAP	H	301	48/48	0.90	0.15	47,73,98,109	0
2	NAP	B	301	48/48	0.91	0.12	37,56,76,87	0

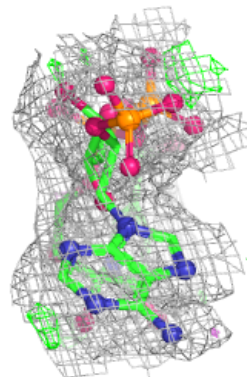
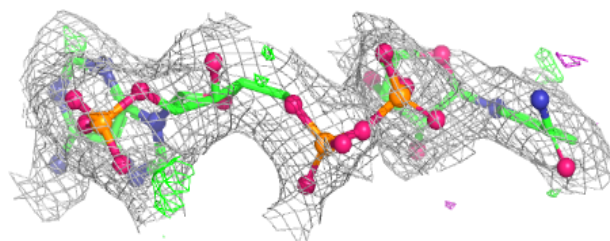
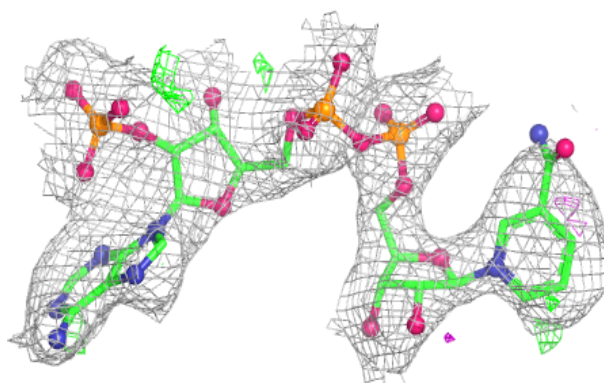
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

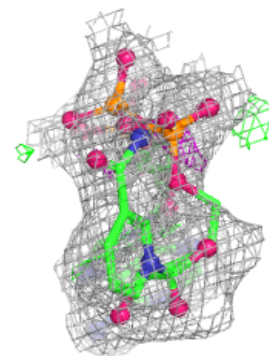
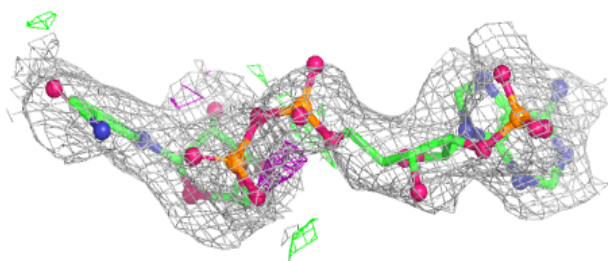
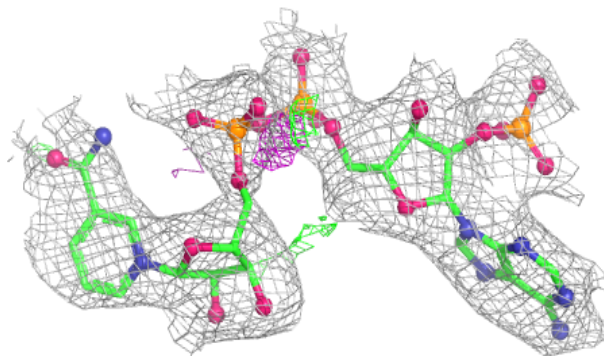
**Electron density around NAP G 301:**

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

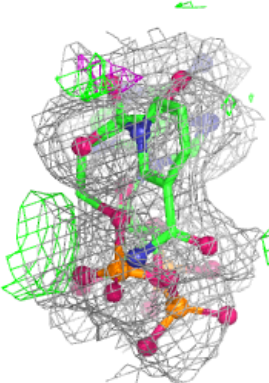
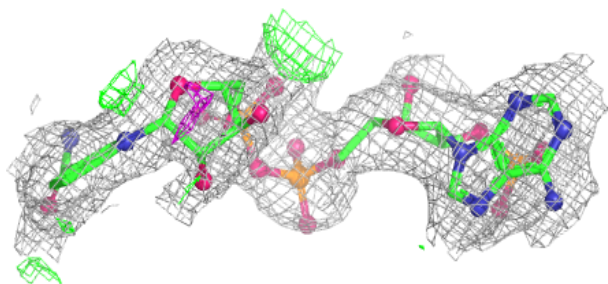
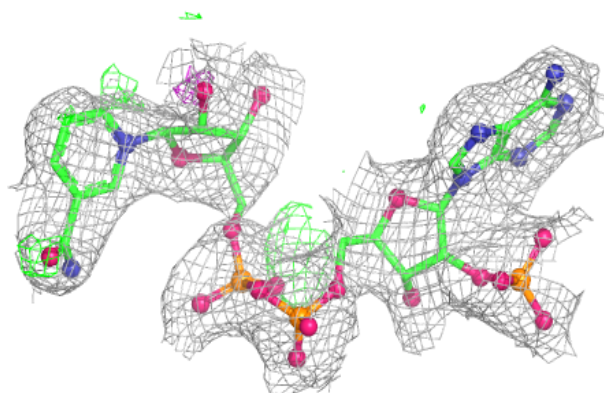


Electron density around NAP A 301:

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

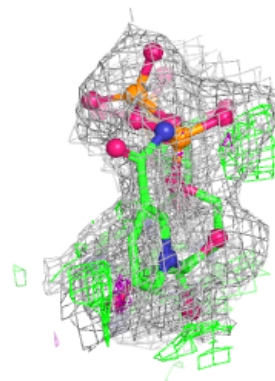
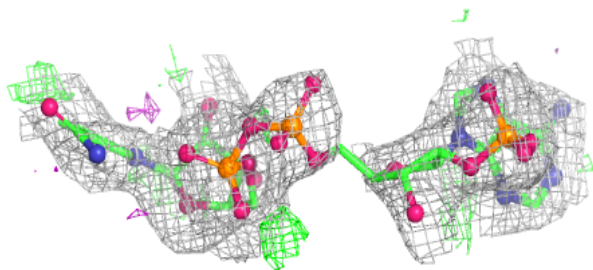
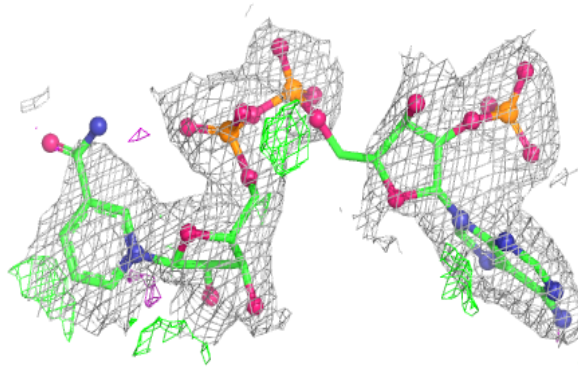
**Electron density around NAP E 301:**

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

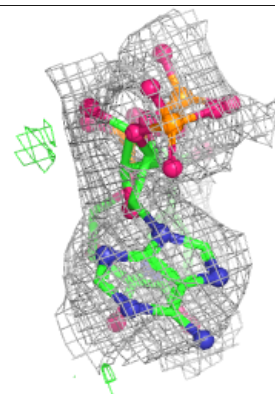
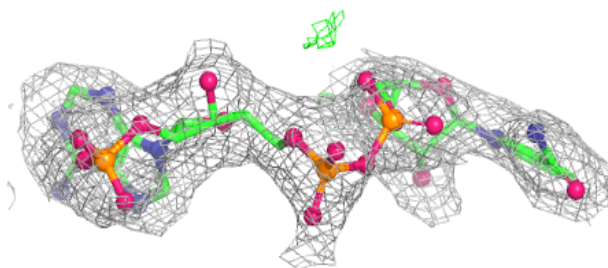
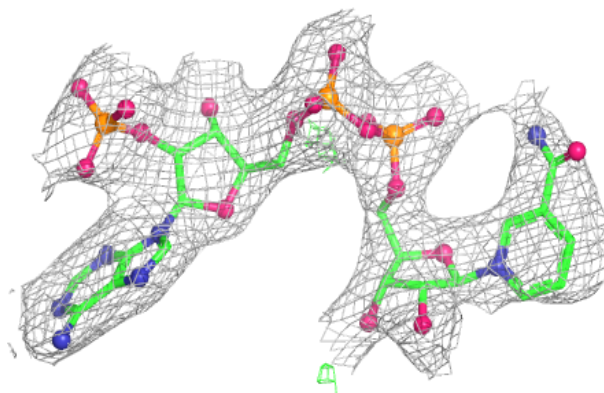


Electron density around NAP F 301:

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

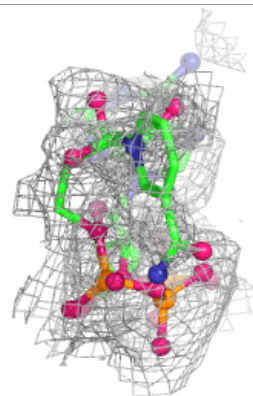
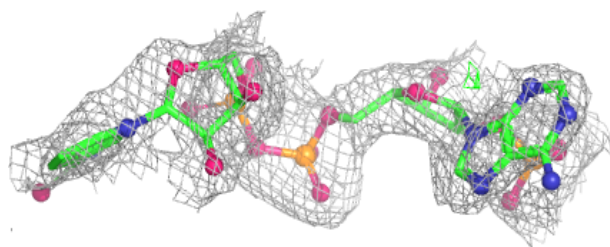
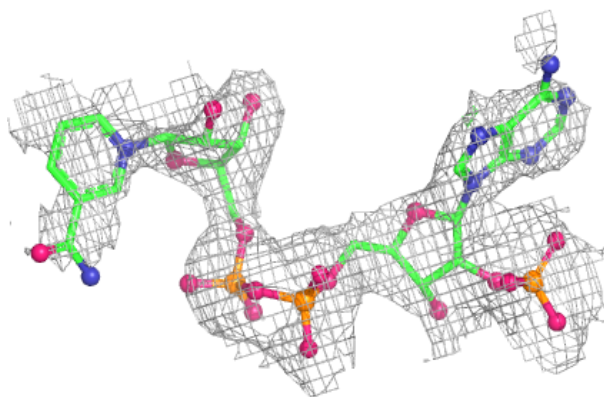
**Electron density around NAP C 301:**

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

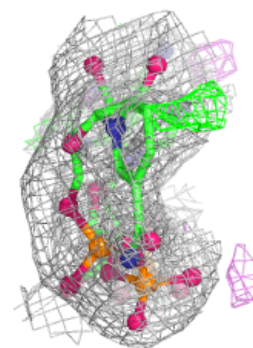
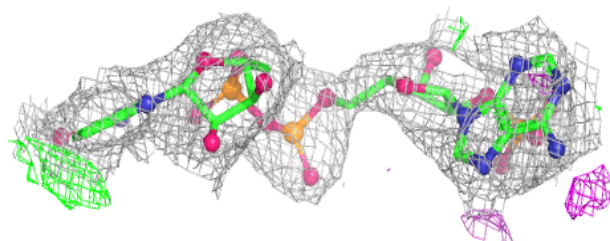
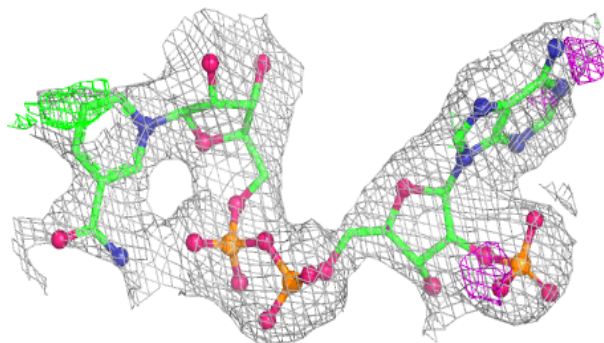


Electron density around NAP H 301:

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

**Electron density around NAP B 301:**

$2mF_o-DF_c$ (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.