



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:26 PM UTC

PDB ID : 6TLK / pdb_00006tlk
Title : Structure of methylene-tetrahydromethanopterin dehydrogenase from *Methylobacterium extorquens* AM1 in an open conformation containing NADP⁺ and methylene-H4MPT
Authors : Wagner, T.; Huang, G.; Demmer, U.; Warkentin, E.; Ermler, U.; Shima, S.
Deposited on : 2019-12-02
Resolution : 1.80 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

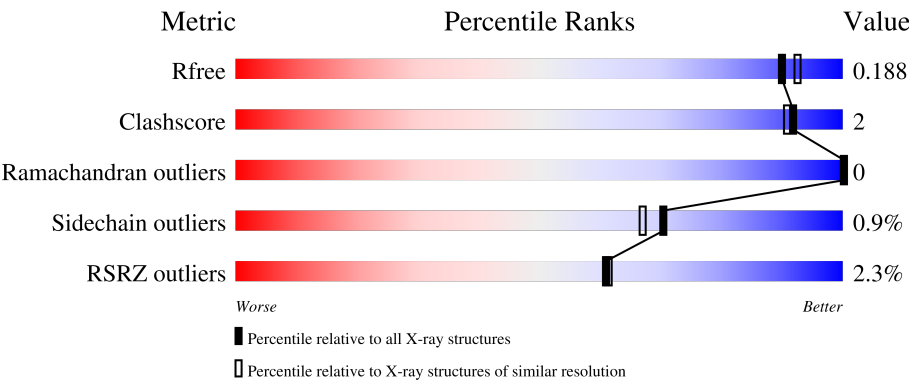
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



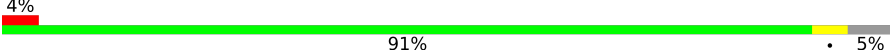
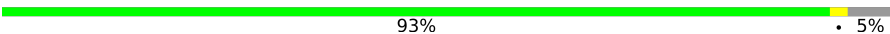
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	303	% 91%5%
1	B	303	91%5%
1	C	303	7%93%5%
1	D	303	%92%5%

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Mol	Chain	Length	Quality of chain
1	E	303	
1	F	303	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	C	402	-	-	X	-
6	CL	D	403	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15166 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 Bifunctional protein MdtA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	2	0
			2113	1333	366	407	7			
1	B	288	Total	C	N	O	S	0	2	0
			2105	1328	364	406	7			
1	C	288	Total	C	N	O	S	0	0	0
			2090	1318	362	403	7			
1	D	288	Total	C	N	O	S	0	1	0
			2096	1322	363	404	7			
1	E	288	Total	C	N	O	S	0	0	0
			2090	1318	362	403	7			
1	F	288	Total	C	N	O	S	0	0	0
			2090	1318	362	403	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	VAL	-	expression tag	UNP P55818
A	290	ASP	-	expression tag	UNP P55818
A	291	LYS	-	expression tag	UNP P55818
A	292	LEU	-	expression tag	UNP P55818
A	293	ALA	-	expression tag	UNP P55818
A	294	ALA	-	expression tag	UNP P55818
A	295	ALA	-	expression tag	UNP P55818
A	296	LEU	-	expression tag	UNP P55818
A	297	GLU	-	expression tag	UNP P55818
A	298	HIS	-	expression tag	UNP P55818
A	299	HIS	-	expression tag	UNP P55818
A	300	HIS	-	expression tag	UNP P55818
A	301	HIS	-	expression tag	UNP P55818
A	302	HIS	-	expression tag	UNP P55818
A	303	HIS	-	expression tag	UNP P55818
B	289	VAL	-	expression tag	UNP P55818
B	290	ASP	-	expression tag	UNP P55818

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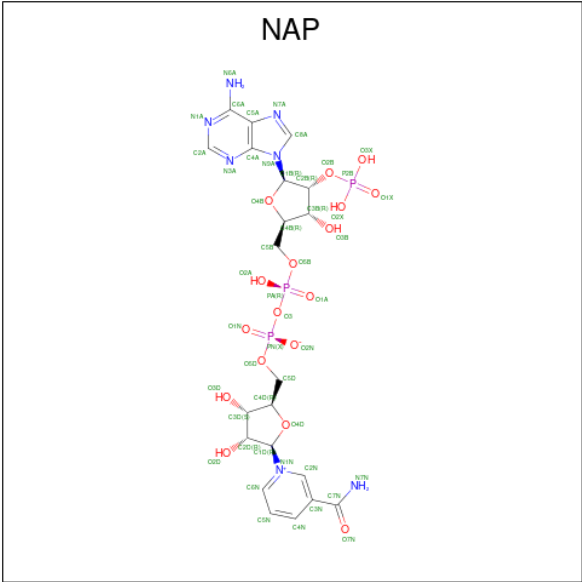
Chain	Residue	Modelled	Actual	Comment	Reference
B	291	LYS	-	expression tag	UNP P55818
B	292	LEU	-	expression tag	UNP P55818
B	293	ALA	-	expression tag	UNP P55818
B	294	ALA	-	expression tag	UNP P55818
B	295	ALA	-	expression tag	UNP P55818
B	296	LEU	-	expression tag	UNP P55818
B	297	GLU	-	expression tag	UNP P55818
B	298	HIS	-	expression tag	UNP P55818
B	299	HIS	-	expression tag	UNP P55818
B	300	HIS	-	expression tag	UNP P55818
B	301	HIS	-	expression tag	UNP P55818
B	302	HIS	-	expression tag	UNP P55818
B	303	HIS	-	expression tag	UNP P55818
C	289	VAL	-	expression tag	UNP P55818
C	290	ASP	-	expression tag	UNP P55818
C	291	LYS	-	expression tag	UNP P55818
C	292	LEU	-	expression tag	UNP P55818
C	293	ALA	-	expression tag	UNP P55818
C	294	ALA	-	expression tag	UNP P55818
C	295	ALA	-	expression tag	UNP P55818
C	296	LEU	-	expression tag	UNP P55818
C	297	GLU	-	expression tag	UNP P55818
C	298	HIS	-	expression tag	UNP P55818
C	299	HIS	-	expression tag	UNP P55818
C	300	HIS	-	expression tag	UNP P55818
C	301	HIS	-	expression tag	UNP P55818
C	302	HIS	-	expression tag	UNP P55818
C	303	HIS	-	expression tag	UNP P55818
D	289	VAL	-	expression tag	UNP P55818
D	290	ASP	-	expression tag	UNP P55818
D	291	LYS	-	expression tag	UNP P55818
D	292	LEU	-	expression tag	UNP P55818
D	293	ALA	-	expression tag	UNP P55818
D	294	ALA	-	expression tag	UNP P55818
D	295	ALA	-	expression tag	UNP P55818
D	296	LEU	-	expression tag	UNP P55818
D	297	GLU	-	expression tag	UNP P55818
D	298	HIS	-	expression tag	UNP P55818
D	299	HIS	-	expression tag	UNP P55818
D	300	HIS	-	expression tag	UNP P55818
D	301	HIS	-	expression tag	UNP P55818
D	302	HIS	-	expression tag	UNP P55818

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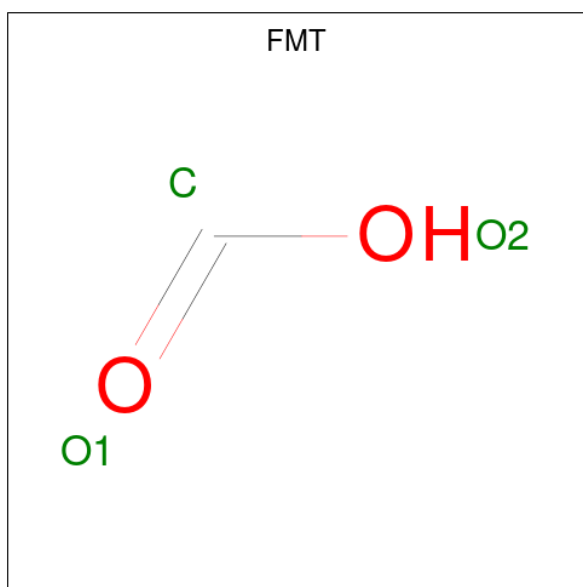
Chain	Residue	Modelled	Actual	Comment	Reference
D	303	HIS	-	expression tag	UNP P55818
E	289	VAL	-	expression tag	UNP P55818
E	290	ASP	-	expression tag	UNP P55818
E	291	LYS	-	expression tag	UNP P55818
E	292	LEU	-	expression tag	UNP P55818
E	293	ALA	-	expression tag	UNP P55818
E	294	ALA	-	expression tag	UNP P55818
E	295	ALA	-	expression tag	UNP P55818
E	296	LEU	-	expression tag	UNP P55818
E	297	GLU	-	expression tag	UNP P55818
E	298	HIS	-	expression tag	UNP P55818
E	299	HIS	-	expression tag	UNP P55818
E	300	HIS	-	expression tag	UNP P55818
E	301	HIS	-	expression tag	UNP P55818
E	302	HIS	-	expression tag	UNP P55818
E	303	HIS	-	expression tag	UNP P55818
F	289	VAL	-	expression tag	UNP P55818
F	290	ASP	-	expression tag	UNP P55818
F	291	LYS	-	expression tag	UNP P55818
F	292	LEU	-	expression tag	UNP P55818
F	293	ALA	-	expression tag	UNP P55818
F	294	ALA	-	expression tag	UNP P55818
F	295	ALA	-	expression tag	UNP P55818
F	296	LEU	-	expression tag	UNP P55818
F	297	GLU	-	expression tag	UNP P55818
F	298	HIS	-	expression tag	UNP P55818
F	299	HIS	-	expression tag	UNP P55818
F	300	HIS	-	expression tag	UNP P55818
F	301	HIS	-	expression tag	UNP P55818
F	302	HIS	-	expression tag	UNP P55818
F	303	HIS	-	expression tag	UNP P55818

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	1
			96	42	14	34	6		

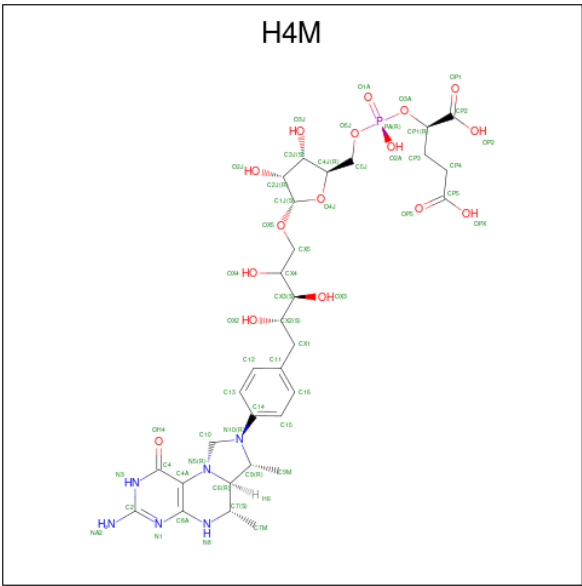
- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		

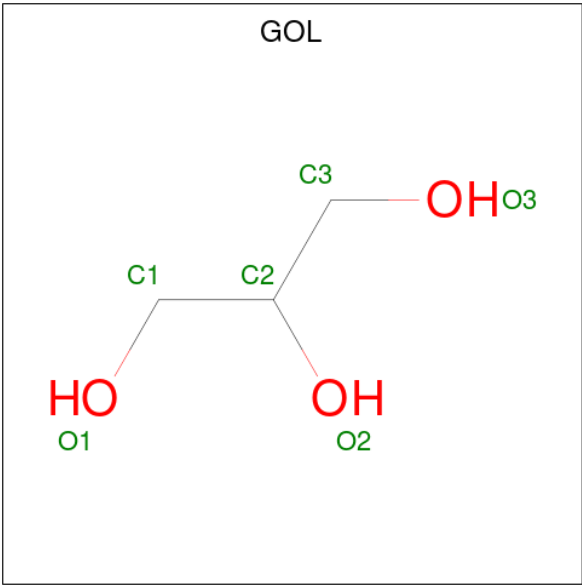
- Molecule 4 is 5,10-DIMETHYLENE TETRAHYDROMETHANOPTERIN (CCD ID: H4M)

(formula: C₃₁H₄₅N₆O₁₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			38	25	6	7		
4	B	1	Total	C	N	O	0	0
			38	25	6	7		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	403	Total O 403 403	0	0
8	B	379	Total O 379 379	0	0
8	C	232	Total O 232 232	0	0
8	D	386	Total O 386 386	0	0
8	E	269	Total O 269 269	0	0
8	F	424	Total O 424 424	0	0

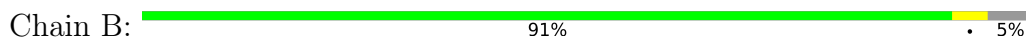
3 Residue-property plots [i](#)

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.

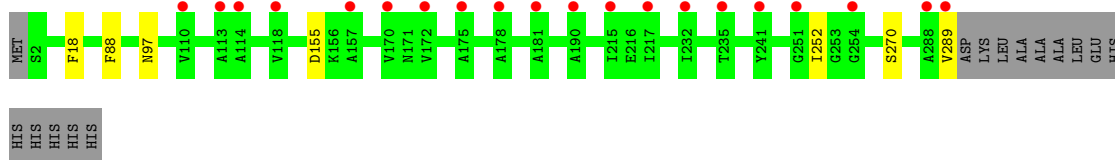
- Molecule 1: Bifunctional protein MdtA



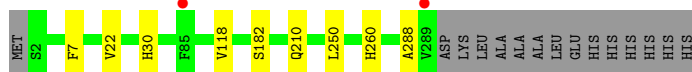
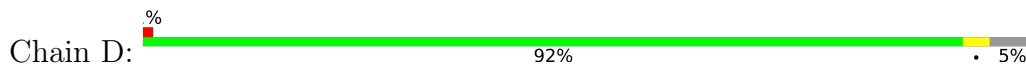
- Molecule 1: Bifunctional protein MdtA



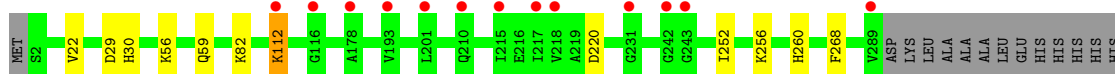
- Molecule 1: Bifunctional protein MdtA



- Molecule 1: Bifunctional protein MdtA



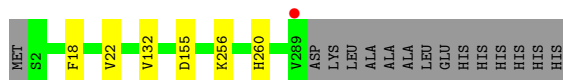
- Molecule 1: Bifunctional protein MdtA



HIS

- Molecule 1: Bifunctional protein MdtA

Chain F: 93% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.92Å 149.27Å 78.56Å 90.00° 93.64° 90.00°	Depositor
Resolution (Å)	26.35 – 1.80 26.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (26.35-1.80) 98.8 (26.35-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.166 , 0.201 (Not available) , 0.188	Depositor DCC
R_{free} test set	7909 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15166	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, FMT, H4M, 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	0.76	0/2148	1.03	3/2893 (0.1%)
1	B	0.71	0/2140	1.01	3/2883 (0.1%)
1	C	0.65	0/2122	1.07	3/2860 (0.1%)
1	D	0.76	0/2131	1.05	4/2872 (0.1%)
1	E	0.72	0/2122	1.06	4/2860 (0.1%)
1	F	0.74	0/2122	1.03	1/2860 (0.0%)
All	All	0.72	0/12785	1.04	18/17228 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ASP	CA-CB-CG	6.87	119.47	112.60
1	C	155	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	155	ASP	CA-CB-CG	6.71	119.31	112.60
1	F	155	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	220	ASP	CA-CB-CG	6.14	118.74	112.60
1	E	252	ILE	CA-C-N	6.02	126.67	119.98
1	E	252	ILE	C-N-CA	6.02	126.67	119.98
1	D	288	ALA	CA-C-N	5.99	132.48	121.70
1	D	288	ALA	C-N-CA	5.99	132.48	121.70
1	D	118	VAL	N-CA-C	-5.83	107.06	112.43
1	A	276	ASP	CA-CB-CG	5.51	118.11	112.60
1	E	220	ASP	CA-CB-CG	5.24	117.83	112.60
1	C	252	ILE	CA-C-N	5.19	126.62	120.14
1	C	252	ILE	C-N-CA	5.19	126.62	120.14
1	B	7	PHE	CA-CB-CG	-5.14	108.66	113.80
1	D	7	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	290	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	268	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2113	0	2124	8	0
1	B	2105	0	2113	5	0
1	C	2090	0	2095	5	0
1	D	2096	0	2103	5	0
1	E	2090	0	2095	6	0
1	F	2090	0	2095	6	0
2	A	48	0	25	2	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	96	0	50	4	0
3	A	6	0	2	0	0
3	C	6	0	2	0	0
3	D	3	0	1	0	0
3	E	15	0	5	0	0
3	F	9	0	3	0	0
4	A	38	0	32	4	0
4	B	38	0	32	3	0
5	C	12	0	16	6	0
5	E	6	0	8	0	0
5	F	18	0	24	4	0
6	D	1	0	0	3	0
7	F	1	0	0	0	0
8	A	403	0	0	3	0
8	B	379	0	0	0	0
8	C	232	0	0	2	0
8	D	386	0	0	1	0
8	E	269	0	0	0	0
8	F	424	0	0	2	0
All	All	15166	0	12925	41	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 2.

All (41) 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)
2:A:401:NAP:O7N	4:A:404:H4M:H16	1.67	0.93
1:B:18:PHE:CE2	4:B:402:H4M:H15	2.21	0.76
2:F:401[B]:NAP:H2N	8:F:518:HOH:O	1.90	0.71
1:B:22:VAL:HG13	1:B:261:ARG:HG3	1.75	0.68
1:C:18:PHE:CD1	5:C:402:GOL:H31	2.28	0.67
2:A:401:NAP:C7N	4:A:404:H4M:H16	2.28	0.63
2:B:401:NAP:O7N	4:B:402:H4M:H16	2.01	0.59
1:C:289:VAL:HG12	1:C:289:VAL:O	2.02	0.59
1:A:2:SER:HB3	8:A:501:HOH:O	2.04	0.56
1:A:18:PHE:CE2	4:A:404:H4M:H15	2.40	0.56
1:B:18:PHE:CZ	4:B:402:H4M:H15	2.40	0.56
1:A:289:VAL:O	1:A:289:VAL:HG13	2.07	0.54
2:F:401[A]:NAP:H4N	5:F:403:GOL:H31	1.90	0.54
1:C:88:PHE:CZ	5:C:403:GOL:H32	2.45	0.51
1:D:30:HIS:ND1	6:D:403:CL:CL	2.72	0.50
1:B:206:GLN:HG3	1:B:210:GLN:OE1	2.12	0.50
1:F:22:VAL:HG11	1:F:260:HIS:CG	2.49	0.47
1:F:18:PHE:CD1	5:F:403:GOL:H2	2.49	0.47
1:D:22:VAL:HG11	1:D:260:HIS:CG	2.49	0.47
6:D:403:CL:CL	8:D:526:HOH:O	2.58	0.46
1:A:18:PHE:CZ	4:A:404:H4M:H15	2.50	0.46
1:F:256:LYS:NZ	2:F:401[B]:NAP:O7N	2.41	0.46
1:A:4[A]:LYS:NZ	8:A:502:HOH:O	2.49	0.46
1:B:22:VAL:HG11	1:B:260:HIS:CG	2.52	0.45
1:D:250:LEU:HD21	5:F:404:GOL:H12	1.98	0.45
1:A:22:VAL:HG11	1:A:260:HIS:CG	2.52	0.44
1:F:132:VAL:HG21	2:F:401[A]:NAP:H6N	1.99	0.44
1:E:56:LYS:O	1:E:59:GLN:HG2	2.18	0.44
1:C:97:ASN:C	5:C:402:GOL:H2	2.43	0.44
5:C:402:GOL:H12	8:C:641:HOH:O	2.17	0.43
1:E:22:VAL:HG11	1:E:260:HIS:CG	2.53	0.43
1:E:112:LYS:HD2	1:E:112:LYS:C	2.44	0.42
1:D:30:HIS:CE1	1:E:29:ASP:O	2.73	0.41
1:C:97:ASN:O	5:C:402:GOL:H2	2.20	0.41
6:D:403:CL:CL	1:E:30:HIS:ND1	2.72	0.41
1:A:2:SER:N	8:A:505:HOH:O	2.53	0.41
1:A:218:VAL:HB	1:A:229:ILE:HD13	2.03	0.41
5:C:402:GOL:H32	8:C:566:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:LYS:NZ	8:F:506:HOH:O	2.52	0.41
1:D:30:HIS:HE1	1:E:29:ASP:O	2.04	0.41
1:F:18:PHE:CG	5:F:403:GOL:H2	2.56	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	289/303 (95%)	284 (98%)	5 (2%)	0	100	100
1	B	288/303 (95%)	284 (99%)	4 (1%)	0	100	100
1	C	286/303 (94%)	281 (98%)	5 (2%)	0	100	100
1	D	287/303 (95%)	283 (99%)	4 (1%)	0	100	100
1	E	286/303 (94%)	280 (98%)	6 (2%)	0	100	100
1	F	286/303 (94%)	281 (98%)	5 (2%)	0	100	100
All	All	1722/1818 (95%)	1693 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/217 (96%)	205 (99%)	3 (1%)	59	52
1	B	207/217 (95%)	205 (99%)	2 (1%)	68	64
1	C	205/217 (94%)	204 (100%)	1 (0%)	81	80
1	D	206/217 (95%)	203 (98%)	3 (2%)	57	49
1	E	205/217 (94%)	202 (98%)	3 (2%)	57	49
1	F	205/217 (94%)	205 (100%)	0	100	100
All	All	1236/1302 (95%)	1224 (99%)	12 (1%)	70	64

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	A	270	SER
1	A	289	VAL
1	B	256	LYS
1	B	289	VAL
1	C	270	SER
1	D	182	SER
1	D	210[A]	GLN
1	D	210[B]	GLN
1	E	82	LYS
1	E	112	LYS
1	E	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	206	GLN
1	A	224	GLN
1	B	97	ASN
1	C	158	GLN
1	E	210	GLN
1	E	211	ASN
1	F	224	GLN

5.3.3 RNA ⓘ

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](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMT	D	402	-	2,2,2	0.84	0	1,1,1	0.48	0
3	FMT	C	405	-	2,2,2	0.76	0	1,1,1	0.46	0
2	NAP	F	401[A]	-	50,52,52	1.49	6 (12%)	71,80,80	1.79	16 (22%)
3	FMT	C	404	-	2,2,2	0.71	0	1,1,1	0.62	0
5	GOL	E	402	-	5,5,5	0.16	0	5,5,5	0.24	0
3	FMT	F	408	-	2,2,2	0.73	0	1,1,1	0.62	0
2	NAP	F	401[B]	-	50,52,52	1.49	7 (14%)	71,80,80	1.74	14 (19%)
2	NAP	B	401	-	50,52,52	1.75	14 (28%)	71,80,80	1.76	15 (21%)
3	FMT	A	403	-	2,2,2	0.72	0	1,1,1	0.57	0
2	NAP	C	401	-	50,52,52	1.71	9 (18%)	71,80,80	1.81	15 (21%)
3	FMT	F	407	-	2,2,2	0.80	0	1,1,1	0.66	0
2	NAP	D	401	-	50,52,52	1.53	7 (14%)	71,80,80	1.78	16 (22%)
3	FMT	E	406	-	2,2,2	0.76	0	1,1,1	0.58	0
5	GOL	F	405	-	5,5,5	0.09	0	5,5,5	0.64	0
5	GOL	F	403	-	5,5,5	0.12	0	5,5,5	0.49	0
4	H4M	B	402	-	40,42,58	4.95	4 (10%)	44,62,86	1.89	12 (27%)
2	NAP	E	401	-	50,52,52	1.61	12 (24%)	71,80,80	1.68	13 (18%)
3	FMT	E	407	-	2,2,2	0.70	0	1,1,1	0.64	0
3	FMT	A	402	-	2,2,2	0.77	0	1,1,1	0.47	0
5	GOL	C	403	-	5,5,5	0.21	0	5,5,5	0.54	0
4	H4M	A	404	-	40,42,58	4.75	4 (10%)	44,62,86	1.76	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	402	-	5,5,5	0.14	0	5,5,5	0.58	0
3	FMT	E	405	-	2,2,2	0.77	0	1,1,1	0.49	0
3	FMT	E	404	-	2,2,2	0.71	0	1,1,1	0.66	0
2	NAP	A	401	-	50,52,52	1.58	7 (14%)	71,80,80	1.77	14 (19%)
5	GOL	F	404	-	5,5,5	0.06	0	5,5,5	0.28	0
3	FMT	F	406	-	2,2,2	0.76	0	1,1,1	0.52	0
3	FMT	E	403	-	2,2,2	0.71	0	1,1,1	0.56	0

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
5	GOL	C	402	-	-	4/4/4/4	-
5	GOL	F	405	-	-	2/4/4/4	-
2	NAP	F	401[A]	-	-	2/35/67/67	0/5/5/5
5	GOL	F	403	-	-	0/4/4/4	-
2	NAP	B	401	-	-	3/35/67/67	0/5/5/5
2	NAP	A	401	-	-	2/35/67/67	0/5/5/5
4	H4M	B	402	-	-	4/21/59/85	0/5/5/5
2	NAP	E	401	-	-	3/35/67/67	0/5/5/5
2	NAP	C	401	-	-	2/35/67/67	0/5/5/5
5	GOL	E	402	-	-	2/4/4/4	-
5	GOL	F	404	-	-	2/4/4/4	-
5	GOL	C	403	-	-	4/4/4/4	-
2	NAP	D	401	-	-	1/35/67/67	0/5/5/5
4	H4M	A	404	-	-	4/21/59/85	0/5/5/5
2	NAP	F	401[B]	-	-	9/35/67/67	0/5/5/5

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	H4M	C10-N5	-29.74	1.26	1.45
4	A	404	H4M	C10-N5	-28.47	1.27	1.45
4	B	402	H4M	C10-N10	-7.83	1.27	1.45
4	A	404	H4M	C10-N10	-7.62	1.27	1.45
2	A	401	NAP	C5A-C4A	5.75	1.49	1.39
2	D	401	NAP	C5A-C4A	5.51	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	C5A-C4A	5.45	1.48	1.39
2	C	401	NAP	C6N-N1N	5.41	1.47	1.35
2	D	401	NAP	C6N-N1N	5.34	1.47	1.35
2	F	401[A]	NAP	C6N-N1N	5.15	1.47	1.35
2	F	401[B]	NAP	C6N-N1N	5.06	1.46	1.35
2	F	401[B]	NAP	C5A-C4A	5.06	1.48	1.39
2	F	401[A]	NAP	C5A-C4A	5.04	1.48	1.39
2	A	401	NAP	C6N-N1N	5.04	1.46	1.35
2	C	401	NAP	PN-O3	4.33	1.64	1.59
2	E	401	NAP	C5A-C4A	4.19	1.46	1.39
2	B	401	NAP	C5A-C4A	4.17	1.46	1.39
2	E	401	NAP	PN-O3	-3.86	1.55	1.59
2	B	401	NAP	PA-O3	-3.67	1.55	1.59
2	B	401	NAP	C4A-N9A	-3.51	1.30	1.37
2	B	401	NAP	C5A-N7A	-3.51	1.32	1.39
2	F	401[A]	NAP	C6N-C5N	3.43	1.45	1.38
2	C	401	NAP	C6N-C5N	3.40	1.45	1.38
2	F	401[B]	NAP	C6N-C5N	3.39	1.45	1.38
2	A	401	NAP	C5A-C6A	3.29	1.50	1.41
2	A	401	NAP	C6N-C5N	3.23	1.45	1.38
2	C	401	NAP	PA-O3	3.16	1.62	1.59
2	C	401	NAP	C5A-C6A	3.15	1.49	1.41
2	D	401	NAP	C6N-C5N	3.09	1.45	1.38
2	B	401	NAP	PN-O2N	-2.95	1.41	1.55
2	F	401[B]	NAP	C5A-C6A	2.93	1.49	1.41
2	F	401[A]	NAP	C5A-C6A	2.93	1.49	1.41
2	D	401	NAP	C5A-C6A	2.92	1.49	1.41
2	B	401	NAP	P2B-O3X	-2.84	1.44	1.54
4	A	404	H4M	OX5-C1J	2.78	1.44	1.40
2	E	401	NAP	C5A-C6A	2.75	1.48	1.41
2	B	401	NAP	P2B-O2X	-2.70	1.44	1.54
2	E	401	NAP	C4A-N9A	-2.65	1.32	1.37
2	E	401	NAP	C5A-N7A	-2.56	1.34	1.39
2	E	401	NAP	O7N-C7N	-2.56	1.19	1.24
2	A	401	NAP	PA-O3	2.55	1.62	1.59
2	B	401	NAP	C5A-C6A	2.51	1.48	1.41
2	B	401	NAP	O4D-C4D	-2.50	1.39	1.45
4	B	402	H4M	OX5-C1J	2.48	1.44	1.40
2	E	401	NAP	C2N-N1N	-2.46	1.32	1.35
2	B	401	NAP	PN-O3	-2.45	1.56	1.59
2	A	401	NAP	PN-O3	2.44	1.62	1.59
2	B	401	NAP	PA-O2A	-2.43	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401[A]	NAP	PA-O3	2.42	1.62	1.59
2	C	401	NAP	O4D-C1D	2.40	1.44	1.40
2	D	401	NAP	C5A-N7A	-2.36	1.34	1.39
2	D	401	NAP	PN-O3	2.34	1.62	1.59
2	E	401	NAP	PN-O2N	-2.32	1.44	1.55
2	B	401	NAP	O4B-C4B	-2.30	1.39	1.45
2	F	401[B]	NAP	C5A-N7A	-2.29	1.34	1.39
2	B	401	NAP	O7N-C7N	-2.28	1.19	1.24
2	B	401	NAP	C8A-N9A	-2.27	1.33	1.37
2	F	401[A]	NAP	C5A-N7A	-2.24	1.35	1.39
2	E	401	NAP	PA-O3	-2.24	1.57	1.59
2	F	401[B]	NAP	PA-O3	2.24	1.61	1.59
2	E	401	NAP	O4D-C4D	-2.22	1.40	1.45
4	A	404	H4M	C4A-C4	2.21	1.49	1.43
2	E	401	NAP	P2B-O3X	-2.21	1.46	1.54
2	C	401	NAP	C5A-N7A	-2.19	1.35	1.39
2	A	401	NAP	C8A-N7A	2.18	1.35	1.31
2	E	401	NAP	C8A-N9A	-2.16	1.33	1.37
2	C	401	NAP	C4A-N9A	-2.04	1.33	1.37
2	D	401	NAP	C4A-N9A	-2.04	1.33	1.37
4	B	402	H4M	C4A-C4	2.03	1.48	1.43
2	F	401[B]	NAP	C8A-N7A	2.02	1.35	1.31

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401[A]	NAP	C5N-C6N-N1N	-5.54	112.82	120.38
2	F	401[A]	NAP	C5A-C4A-N3A	-5.34	119.37	126.72
2	D	401	NAP	C5N-C6N-N1N	-5.31	113.14	120.38
2	F	401[B]	NAP	C5A-C4A-N3A	-5.30	119.42	126.72
4	B	402	H4M	C7-C6-N5	-5.26	103.37	108.61
2	C	401	NAP	C3N-C7N-N7N	5.17	124.11	117.74
2	B	401	NAP	C5A-C4A-N3A	-5.14	119.64	126.72
2	E	401	NAP	C5A-C4A-N3A	-5.04	119.78	126.72
2	F	401[B]	NAP	N3A-C4A-N9A	4.99	135.65	127.17
4	B	402	H4M	C8A-C4A-N5	-4.96	113.12	119.80
2	F	401[A]	NAP	N3A-C4A-N9A	4.94	135.57	127.17
4	A	404	H4M	C2-N1-C8A	4.92	122.05	113.36
2	A	401	NAP	O7N-C7N-N7N	-4.83	115.64	122.62
2	E	401	NAP	N3A-C4A-N9A	4.72	135.20	127.17
2	A	401	NAP	C3N-C7N-N7N	4.70	123.53	117.74
4	A	404	H4M	C4A-C4-N3	4.56	118.96	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAP	C4A-N9A-C8A	4.56	110.52	105.74
2	A	401	NAP	C5A-C4A-N3A	-4.49	120.54	126.72
2	A	401	NAP	C4A-N9A-C8A	4.46	110.42	105.74
2	A	401	NAP	N3A-C4A-N9A	4.43	134.71	127.17
2	C	401	NAP	N3A-C4A-N9A	4.41	134.66	127.17
2	C	401	NAP	C5A-C4A-N3A	-4.18	120.96	126.72
2	D	401	NAP	C2A-N1A-C6A	4.18	125.59	118.73
2	C	401	NAP	N3A-C2A-N1A	-4.17	122.28	128.58
4	B	402	H4M	C2-N1-C8A	4.11	120.61	113.36
2	B	401	NAP	O7N-C7N-N7N	-4.08	116.73	122.62
2	B	401	NAP	N3A-C2A-N1A	-4.06	122.44	128.58
2	F	401[B]	NAP	C4A-N9A-C8A	4.05	109.99	105.74
2	B	401	NAP	C4D-O4D-C1D	3.99	113.58	109.92
2	F	401[A]	NAP	C4A-N9A-C8A	3.93	109.87	105.74
2	B	401	NAP	C2A-N3A-C4A	3.92	121.42	111.83
2	C	401	NAP	C2A-N1A-C6A	3.78	124.93	118.73
2	E	401	NAP	C2A-N3A-C4A	3.69	120.85	111.83
2	B	401	NAP	N3A-C4A-N9A	3.69	133.44	127.17
2	E	401	NAP	O7N-C7N-C3N	-3.66	115.12	119.60
2	D	401	NAP	C5A-C4A-N3A	-3.65	121.69	126.72
2	D	401	NAP	N3A-C2A-N1A	-3.64	123.07	128.58
2	D	401	NAP	C6N-N1N-C2N	3.63	124.97	121.88
2	E	401	NAP	C4A-N9A-C8A	3.63	109.55	105.74
2	B	401	NAP	C4A-C5A-N7A	-3.62	106.44	110.58
4	A	404	H4M	C6-C9-N10	-3.61	99.89	102.55
2	F	401[A]	NAP	C2A-N3A-C4A	3.61	120.65	111.83
2	F	401[A]	NAP	N3A-C2A-N1A	-3.58	123.16	128.58
2	E	401	NAP	C3N-C7N-N7N	3.58	122.15	117.74
2	F	401[B]	NAP	C2A-N3A-C4A	3.57	120.55	111.83
2	F	401[B]	NAP	N3A-C2A-N1A	-3.55	123.21	128.58
2	F	401[B]	NAP	C5N-C6N-N1N	-3.49	115.62	120.38
2	E	401	NAP	N3A-C2A-N1A	-3.45	123.36	128.58
2	D	401	NAP	C3N-C7N-N7N	3.40	121.93	117.74
2	F	401[A]	NAP	C4A-C5A-N7A	-3.39	106.71	110.58
2	D	401	NAP	O7N-C7N-N7N	-3.38	117.73	122.62
2	D	401	NAP	N6A-C6A-N1A	3.36	125.86	118.38
2	A	401	NAP	C4A-C5A-N7A	-3.35	106.75	110.58
2	C	401	NAP	O7N-C7N-N7N	-3.34	117.79	122.62
2	A	401	NAP	N3A-C2A-N1A	-3.31	123.57	128.58
2	D	401	NAP	C4A-C5A-N7A	-3.31	106.80	110.58
2	D	401	NAP	C5N-C4N-C3N	3.31	123.62	120.36
2	D	401	NAP	N3A-C4A-N9A	3.30	132.78	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401[B]	NAP	C4A-C5A-N7A	-3.30	106.81	110.58
2	C	401	NAP	C2A-N3A-C4A	3.27	119.82	111.83
2	A	401	NAP	C2A-N3A-C4A	3.21	119.67	111.83
2	C	401	NAP	C4A-C5A-N7A	-3.15	106.99	110.58
2	B	401	NAP	C3N-C7N-N7N	3.10	121.56	117.74
2	D	401	NAP	C4A-N9A-C8A	3.01	108.90	105.74
2	A	401	NAP	C5A-N7A-C8A	2.97	108.12	103.45
2	B	401	NAP	C6A-C5A-N7A	2.95	137.78	132.09
4	A	404	H4M	C7M-C7-N8	-2.90	106.67	109.44
2	A	401	NAP	C6A-C5A-N7A	2.88	137.63	132.09
4	B	402	H4M	C4A-C4-N3	2.87	115.99	110.94
4	A	404	H4M	C8A-C4A-N5	-2.86	115.94	119.80
2	A	401	NAP	N9A-C8A-N7A	-2.84	109.90	113.94
4	B	402	H4M	OX5-CX5-CX4	2.82	115.76	109.29
2	A	401	NAP	C5N-C6N-N1N	-2.82	116.54	120.38
4	A	404	H4M	OH4-C4-C4A	-2.78	120.79	127.62
2	F	401[A]	NAP	C5A-N7A-C8A	2.78	107.81	103.45
4	B	402	H4M	OX4-CX4-CX3	2.75	115.69	109.25
2	F	401[B]	NAP	C5A-N7A-C8A	2.75	107.77	103.45
2	E	401	NAP	C2B-C1B-N9A	-2.75	109.23	113.75
2	E	401	NAP	C6A-C5A-N7A	2.73	137.36	132.09
2	F	401[A]	NAP	O7N-C7N-N7N	-2.72	118.69	122.62
2	C	401	NAP	C5A-N7A-C8A	2.71	107.72	103.45
4	A	404	H4M	C4J-O4J-C1J	2.71	112.30	107.57
4	B	402	H4M	C9-C6-N5	-2.70	99.83	102.36
4	A	404	H4M	OX5-C1J-O4J	2.67	117.12	110.95
2	E	401	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
2	C	401	NAP	C6A-C5A-N7A	2.66	137.23	132.09
2	A	401	NAP	C2A-N1A-C6A	2.63	123.05	118.73
2	C	401	NAP	C5N-C6N-N1N	-2.63	116.80	120.38
4	B	402	H4M	OH4-C4-C4A	-2.61	121.22	127.62
2	B	401	NAP	C2B-C1B-N9A	-2.59	109.48	113.75
2	E	401	NAP	O2A-PA-O3	2.57	114.23	107.27
2	B	401	NAP	O2N-PN-O3	2.54	114.14	107.27
2	D	401	NAP	C2A-N3A-C4A	2.54	118.03	111.83
2	F	401[A]	NAP	O7N-C7N-C3N	2.53	122.69	119.60
2	F	401[B]	NAP	C6N-N1N-C2N	-2.51	119.74	121.88
2	B	401	NAP	C4A-N9A-C8A	2.51	108.37	105.74
2	B	401	NAP	C2A-N1A-C6A	2.51	122.85	118.73
2	F	401[B]	NAP	N9A-C8A-N7A	-2.50	110.39	113.94
2	C	401	NAP	N9A-C8A-N7A	-2.50	110.39	113.94
2	F	401[A]	NAP	N9A-C8A-N7A	-2.47	110.43	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	H4M	OX4-CX4-CX3	2.46	115.00	109.25
2	F	401[B]	NAP	C2A-N1A-C6A	2.45	122.76	118.73
4	B	402	H4M	CX1-C11-C16	-2.44	116.37	120.90
2	C	401	NAP	C2B-C1B-N9A	-2.43	109.75	113.75
2	F	401[A]	NAP	C2A-N1A-C6A	2.43	122.73	118.73
2	D	401	NAP	C5A-N7A-C8A	2.38	107.19	103.45
4	B	402	H4M	C4J-O4J-C1J	2.35	111.68	107.57
2	B	401	NAP	O2A-PA-O3	2.33	113.58	107.27
2	A	401	NAP	C6N-N1N-C2N	-2.33	119.89	121.88
4	B	402	H4M	CX4-CX3-CX2	2.32	117.43	113.57
2	E	401	NAP	C2A-N1A-C6A	2.30	122.50	118.73
2	B	401	NAP	C5A-N7A-C8A	2.29	107.05	103.45
2	C	401	NAP	O2N-PN-O3	2.23	113.29	107.27
2	F	401[B]	NAP	C2N-C3N-C4N	2.22	120.84	118.26
4	A	404	H4M	OX5-CX5-CX4	2.22	114.37	109.29
2	F	401[B]	NAP	N6A-C6A-N1A	2.21	123.30	118.38
2	F	401[A]	NAP	C6A-C5A-N7A	2.19	136.32	132.09
2	F	401[A]	NAP	N6A-C6A-N1A	2.17	123.21	118.38
2	D	401	NAP	C6A-C5A-N7A	2.15	136.24	132.09
2	F	401[B]	NAP	C6A-C5A-N7A	2.15	136.24	132.09
2	F	401[A]	NAP	C6N-N1N-C2N	2.13	123.69	121.88
2	F	401[A]	NAP	C4B-O4B-C1B	-2.11	104.81	109.47
4	B	402	H4M	NA2-C2-N3	2.09	121.17	116.76
2	D	401	NAP	O4B-C4B-C3B	-2.07	101.04	105.15
2	E	401	NAP	C5A-N7A-C8A	2.03	106.65	103.45

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAP	O4D-C1D-N1N-C6N
2	F	401[B]	NAP	O4D-C1D-N1N-C2N
2	F	401[B]	NAP	O4D-C1D-N1N-C6N
2	F	401[B]	NAP	C2D-C1D-N1N-C2N
2	F	401[B]	NAP	C2D-C1D-N1N-C6N
4	B	402	H4M	O4J-C1J-OX5-CX5
5	C	403	GOL	O1-C1-C2-O2
5	C	403	GOL	C1-C2-C3-O3
5	E	402	GOL	C1-C2-C3-O3
2	F	401[B]	NAP	C2N-C3N-C7N-N7N
2	F	401[B]	NAP	C2N-C3N-C7N-O7N
5	C	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	C	402	GOL	C1-C2-C3-O3
5	C	403	GOL	O1-C1-C2-C3
5	F	405	GOL	O1-C1-C2-C3
5	C	402	GOL	O1-C1-C2-O2
5	E	402	GOL	O2-C2-C3-O3
5	F	405	GOL	O1-C1-C2-O2
2	F	401[B]	NAP	C4N-C3N-C7N-O7N
2	F	401[B]	NAP	C4N-C3N-C7N-N7N
4	B	402	H4M	OX4-CX4-CX5-OX5
5	C	403	GOL	O2-C2-C3-O3
5	F	404	GOL	O2-C2-C3-O3
4	A	404	H4M	C16-C11-CX1-CX2
4	A	404	H4M	OX4-CX4-CX5-OX5
4	B	402	H4M	C16-C11-CX1-CX2
2	E	401	NAP	C5D-O5D-PN-O1N
4	A	404	H4M	C12-C11-CX1-CX2
4	B	402	H4M	C12-C11-CX1-CX2
2	A	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	C2B-O2B-P2B-O1X
2	C	401	NAP	C2B-O2B-P2B-O1X
2	D	401	NAP	C2B-O2B-P2B-O1X
2	E	401	NAP	C2B-O2B-P2B-O1X
2	F	401[A]	NAP	C2B-O2B-P2B-O1X
5	C	402	GOL	O2-C2-C3-O3
2	F	401[A]	NAP	C4N-C3N-C7N-N7N
2	E	401	NAP	C2B-O2B-P2B-O3X
5	F	404	GOL	O1-C1-C2-O2
2	B	401	NAP	C2B-O2B-P2B-O1X
2	F	401[B]	NAP	C2B-O2B-P2B-O1X
4	A	404	H4M	CX4-CX5-OX5-C1J

There are no ring outliers.

10 monomers are involved in 20 short contacts:

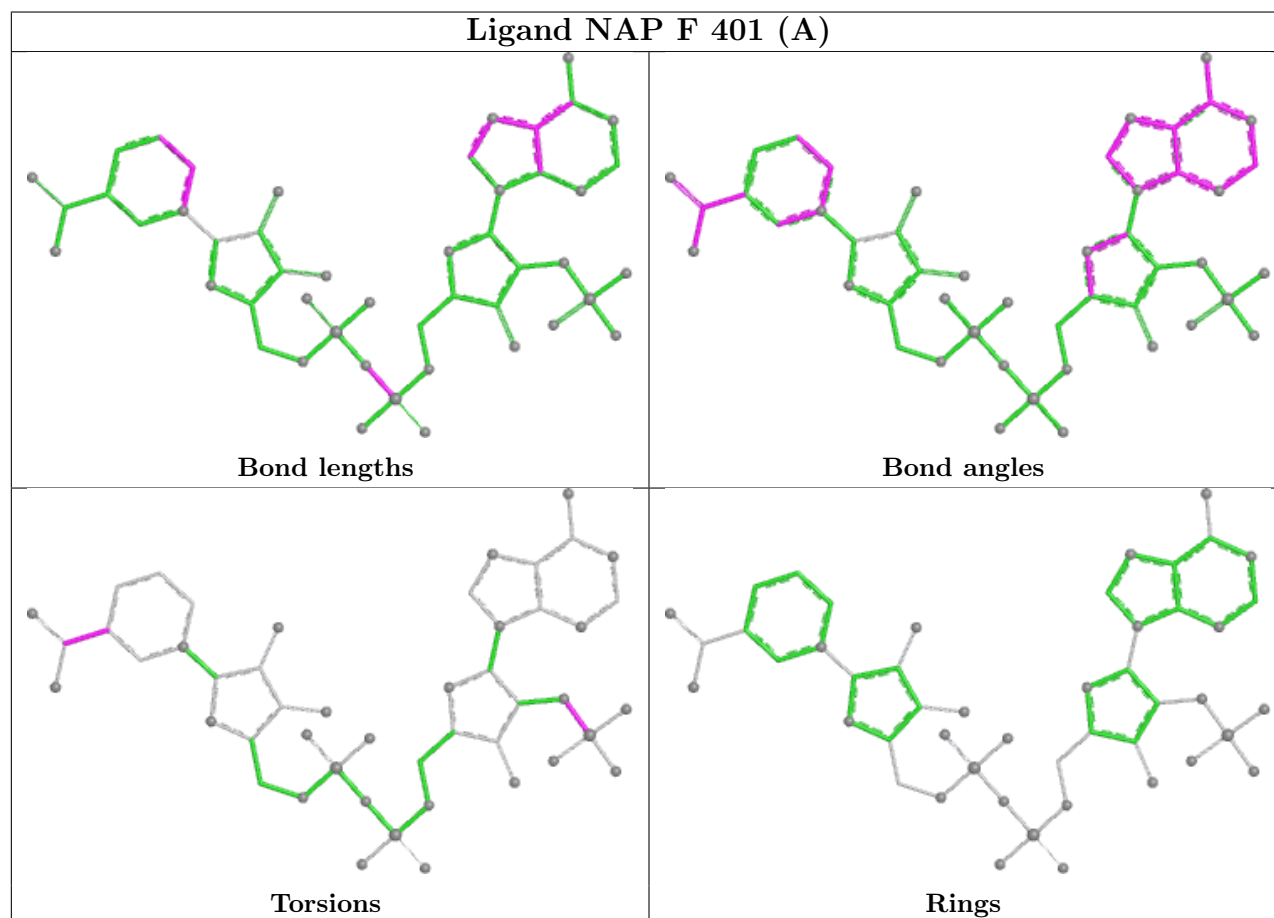
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401[A]	NAP	2	0
2	F	401[B]	NAP	2	0
2	B	401	NAP	1	0
5	F	403	GOL	3	0
4	B	402	H4M	3	0

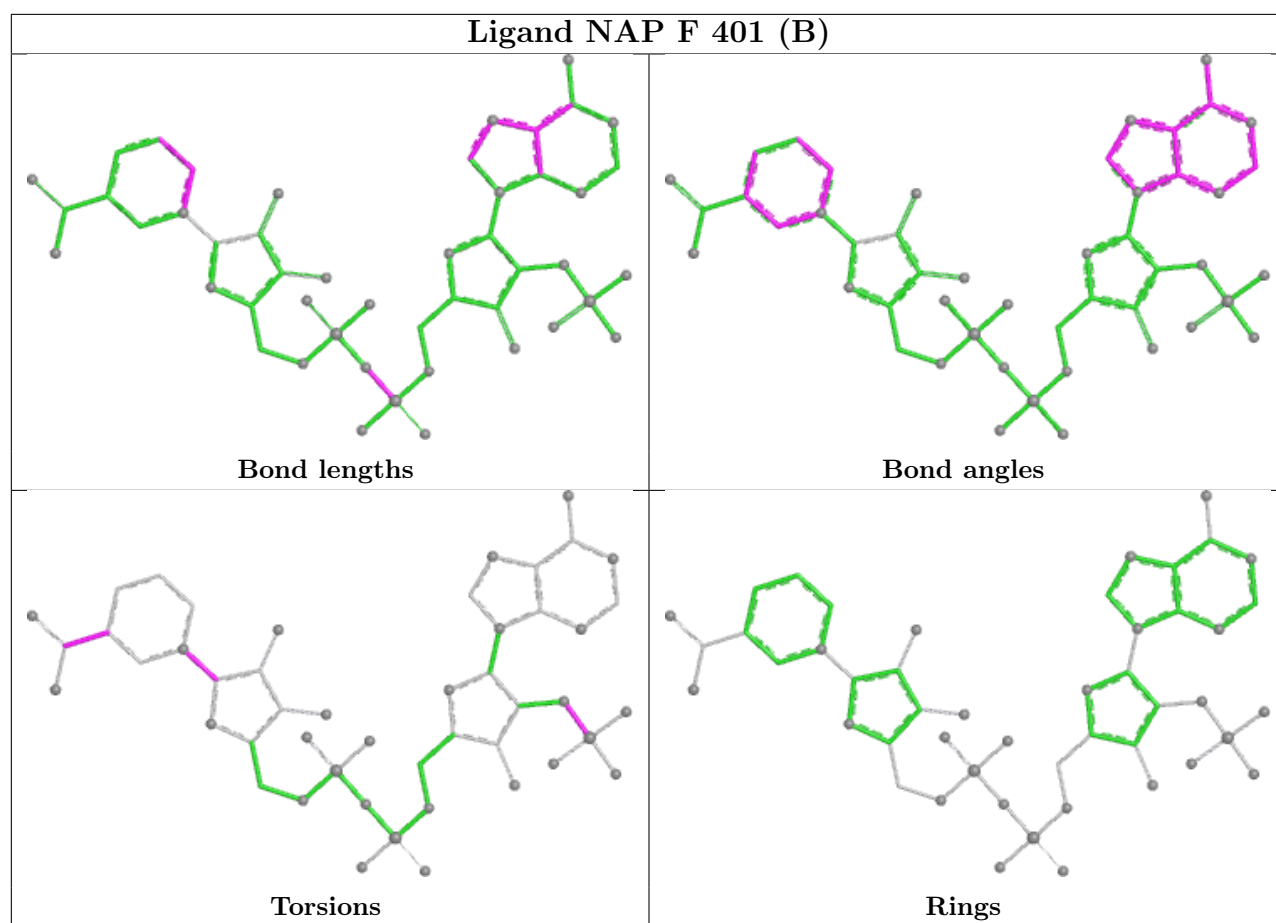
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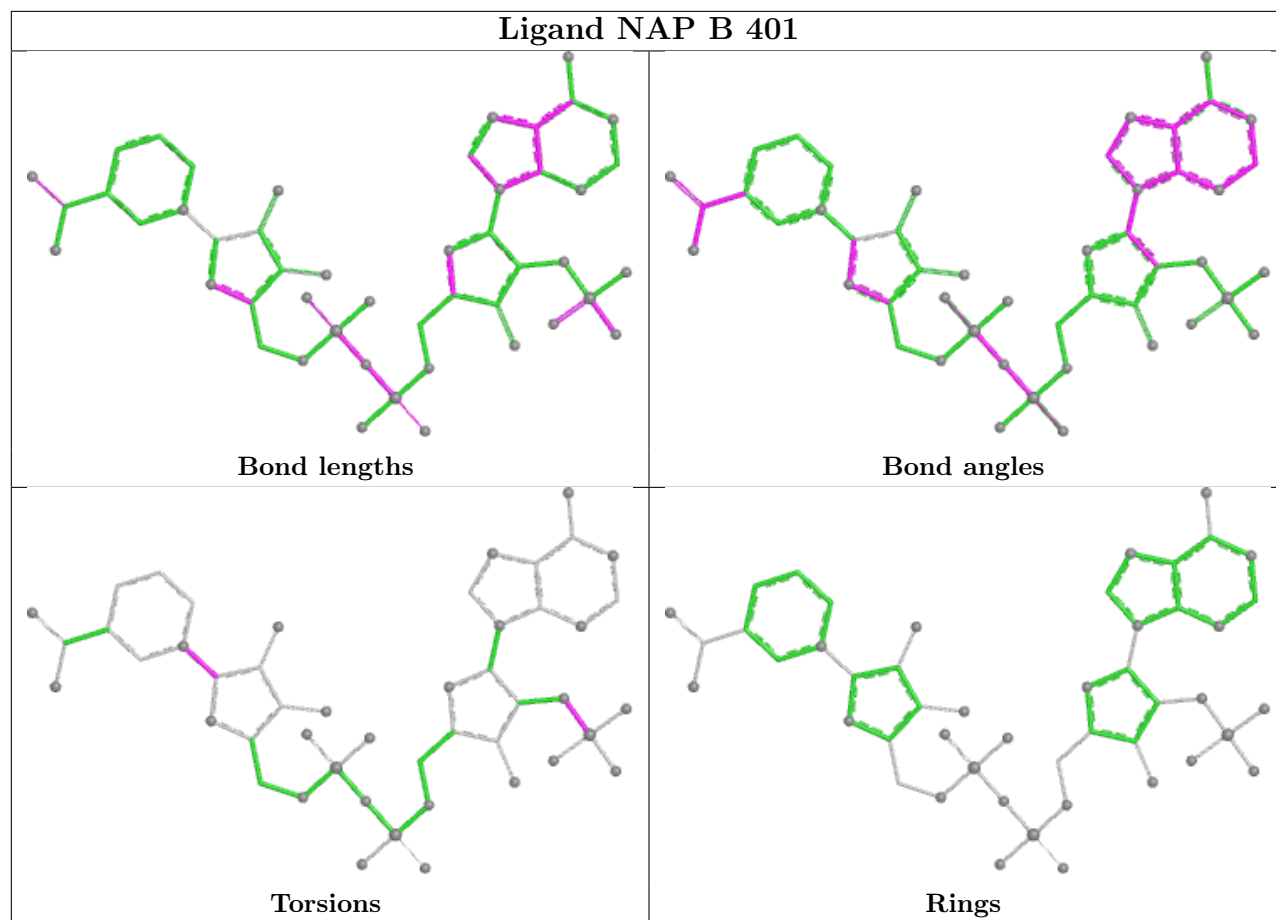
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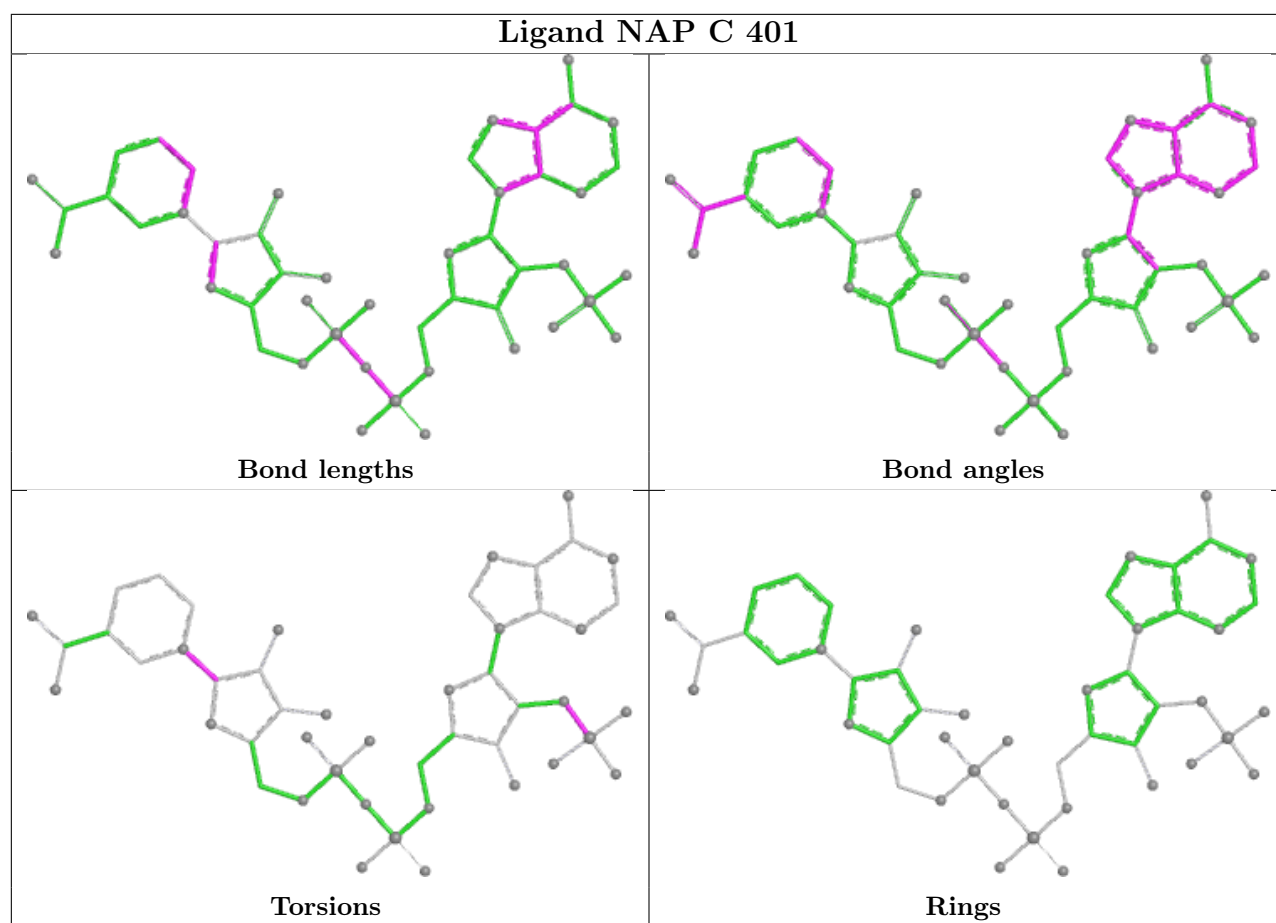
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	GOL	1	0
4	A	404	H4M	4	0
5	C	402	GOL	5	0
2	A	401	NAP	2	0
5	F	404	GOL	1	0

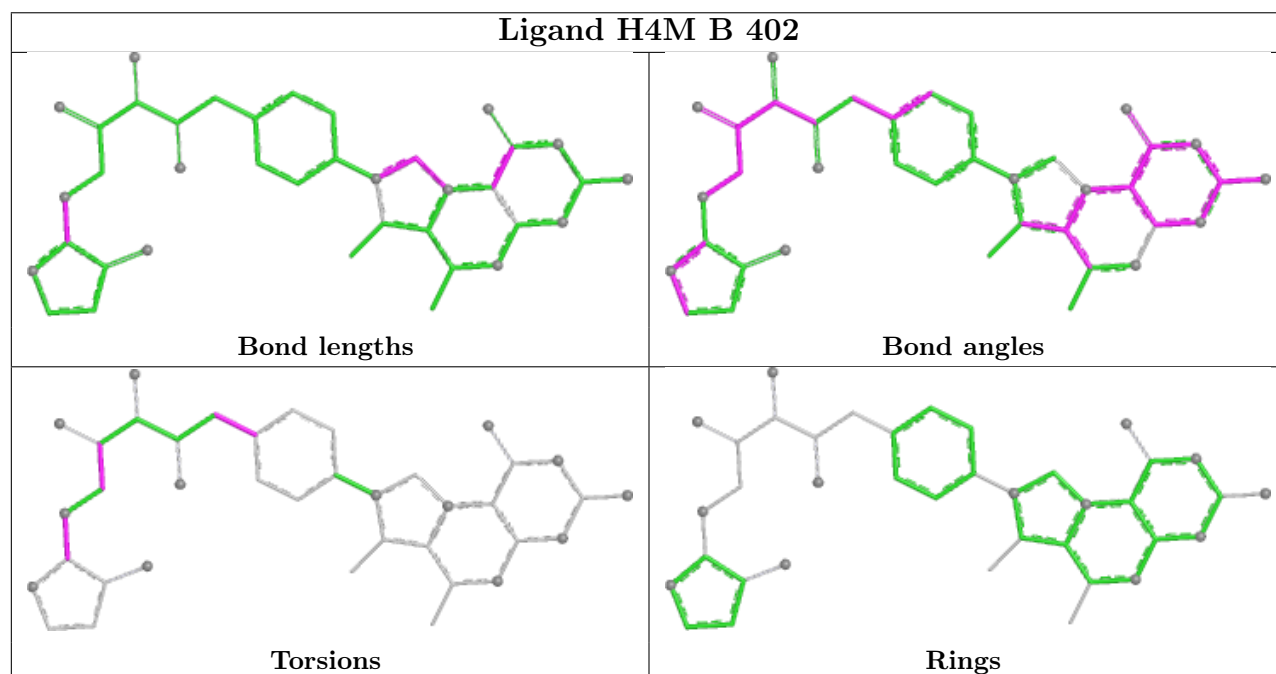
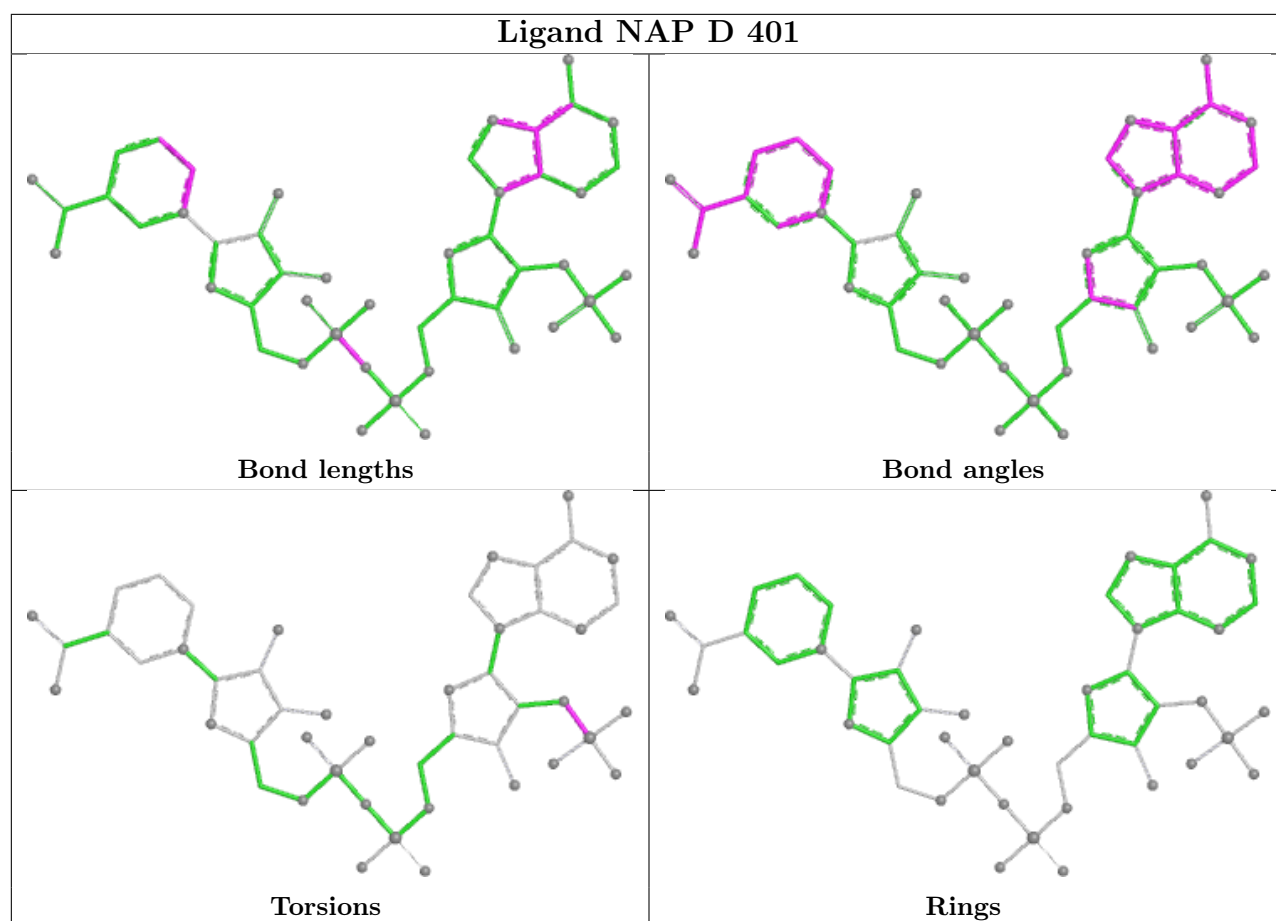
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



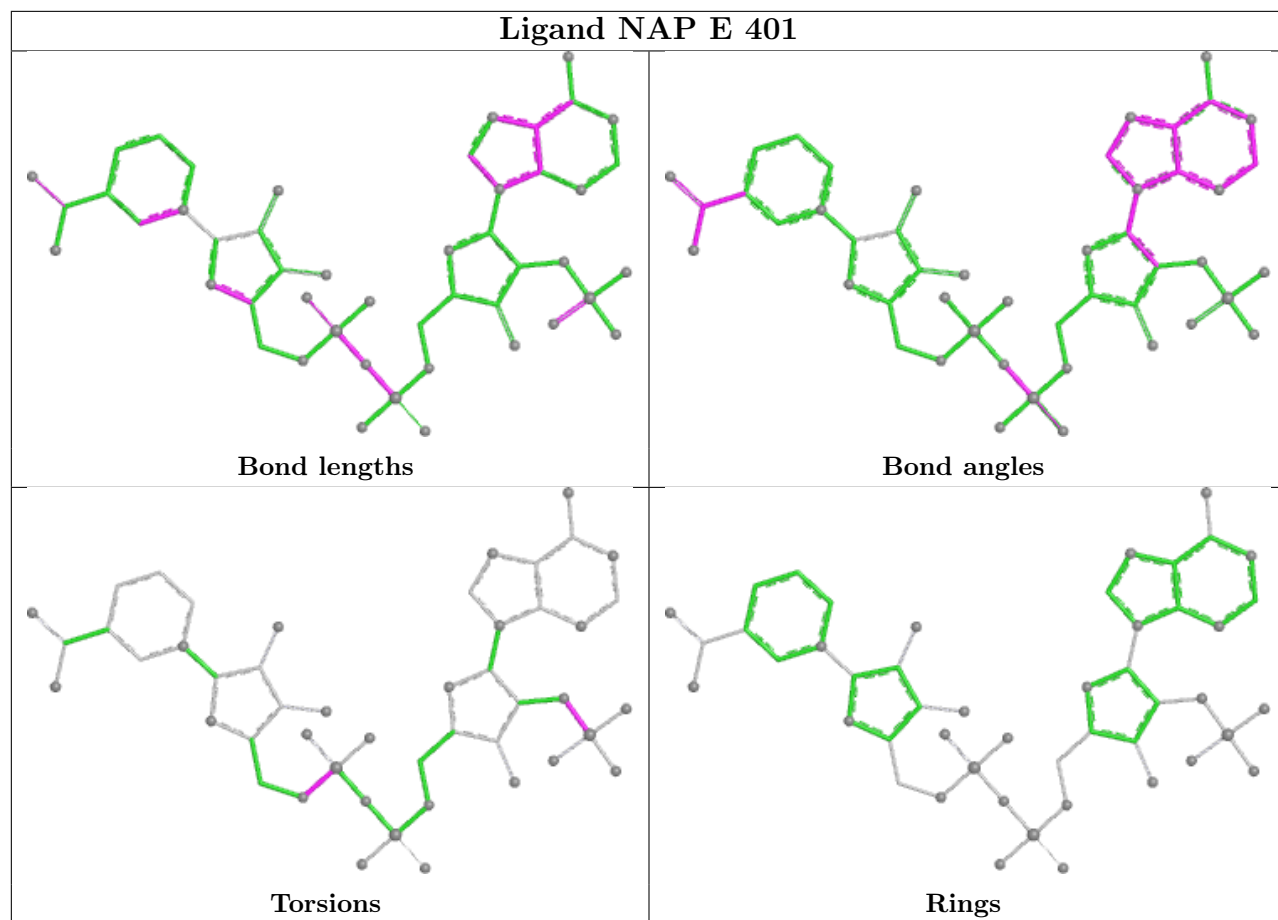




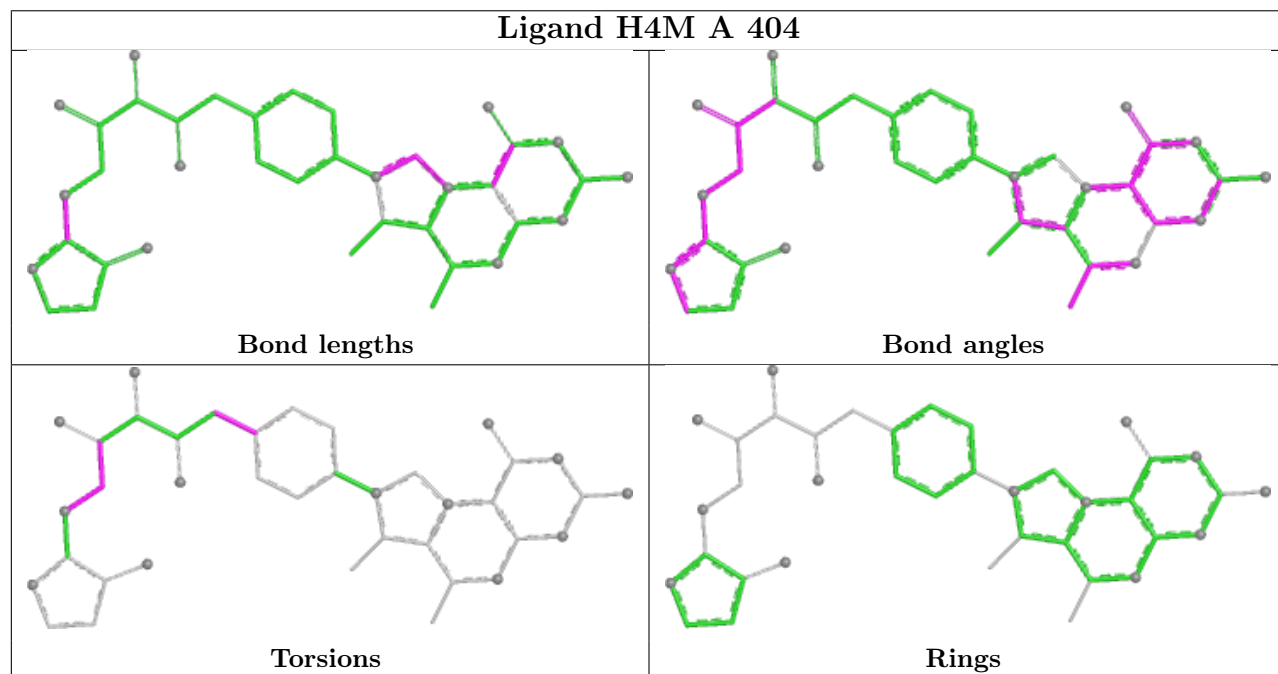


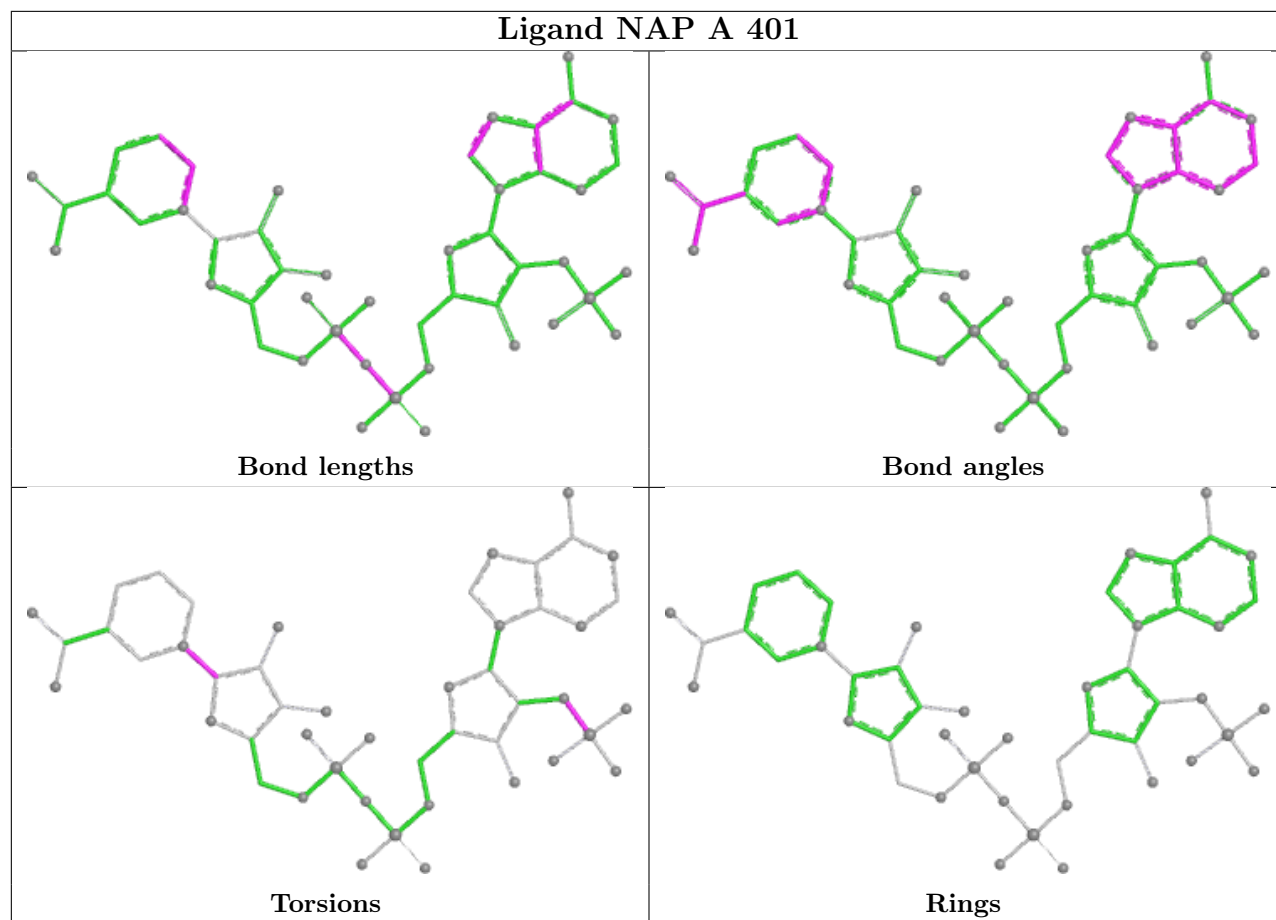


Ligand NAP E 401



Ligand H4M A 404





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	289/303 (95%)	-0.50	2 (0%) 84 85	11, 26, 43, 59	2 (0%)
1	B	288/303 (95%)	-0.34	1 (0%) 90 90	15, 30, 51, 67	2 (0%)
1	C	288/303 (95%)	0.47	20 (6%) 23 21	22, 45, 80, 99	0
1	D	288/303 (95%)	-0.39	2 (0%) 84 85	17, 27, 50, 66	1 (0%)
1	E	288/303 (95%)	0.26	13 (4%) 38 37	19, 39, 75, 90	0
1	F	288/303 (95%)	-0.57	1 (0%) 90 90	17, 26, 44, 58	0
All	All	1729/1818 (95%)	-0.18	39 (2%) 61 61	11, 30, 66, 99	5 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	ILE	4.0
1	D	85	PHE	4.0
1	C	175	ALA	3.8
1	E	116	GLY	3.7
1	E	201	LEU	3.5
1	E	289	VAL	3.5
1	C	289	VAL	3.2
1	E	242	GLY	3.1
1	F	289	VAL	3.1
1	D	289	VAL	3.0
1	A	290	ASP	3.0
1	C	217	ILE	2.9
1	C	110	VAL	2.8
1	B	289	VAL	2.8
1	C	172	VAL	2.8
1	C	170	VAL	2.6
1	E	218	VAL	2.6
1	C	113	ALA	2.6
1	C	118	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	251	GLY	2.5
1	C	235	THR	2.5
1	C	157	ALA	2.4
1	C	215	ILE	2.4
1	C	241	TYR	2.3
1	E	178	ALA	2.3
1	C	114	ALA	2.2
1	C	181	ALA	2.2
1	C	232	ILE	2.2
1	E	112	LYS	2.2
1	E	231	GLY	2.1
1	C	190	ALA	2.1
1	C	254	GLY	2.1
1	E	193	VAL	2.1
1	E	243	GLY	2.1
1	C	288	ALA	2.1
1	A	85	PHE	2.1
1	E	210	GLN	2.1
1	E	217	ILE	2.0
1	C	178	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	F	406	3/3	0.62	0.17	67,67,68,69	0
5	GOL	C	403	6/6	0.73	0.12	36,38,41,44	0
5	GOL	F	405	6/6	0.76	0.15	50,52,57,59	0

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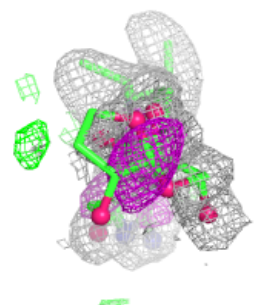
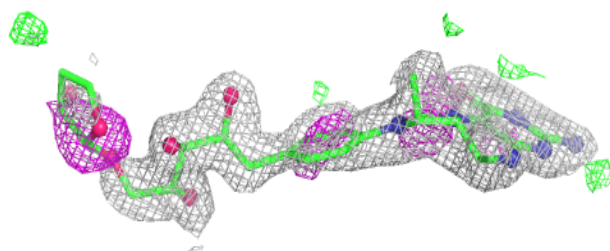
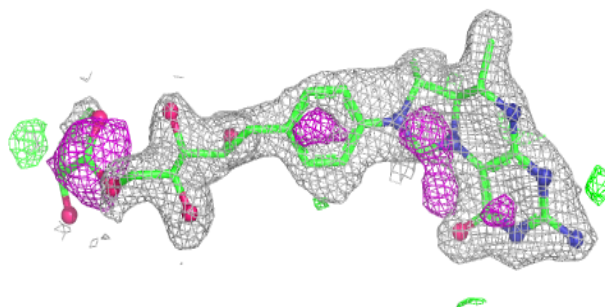
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMT	C	405	3/3	0.79	0.15	60,60,64,65	0
5	GOL	C	402	6/6	0.79	0.14	41,45,48,51	0
3	FMT	E	404	3/3	0.80	0.15	56,56,61,62	0
5	GOL	E	402	6/6	0.82	0.11	31,36,37,38	0
3	FMT	E	406	3/3	0.82	0.15	65,65,66,67	0
3	FMT	F	408	3/3	0.83	0.10	68,68,68,69	0
5	GOL	F	404	6/6	0.83	0.11	49,53,58,59	0
4	H4M	A	404	38/54	0.83	0.12	32,50,85,86	0
4	H4M	B	402	38/54	0.84	0.13	28,51,90,92	0
3	FMT	E	407	3/3	0.84	0.22	59,59,60,62	0
3	FMT	C	404	3/3	0.85	0.20	60,60,62,64	0
3	FMT	D	402	3/3	0.86	0.10	44,44,48,51	0
3	FMT	A	402	3/3	0.87	0.16	43,43,52,55	0
3	FMT	A	403	3/3	0.88	0.12	54,54,64,68	0
3	FMT	F	407	3/3	0.88	0.13	39,39,46,54	0
3	FMT	E	405	3/3	0.90	0.12	40,40,49,53	0
5	GOL	F	403	6/6	0.90	0.11	31,50,56,56	0
3	FMT	E	403	3/3	0.91	0.20	44,44,50,51	0
6	CL	D	403	1/1	0.91	0.12	57,57,57,57	0
7	MG	F	402	1/1	0.92	0.09	53,53,53,53	0
2	NAP	E	401	48/48	0.94	0.08	31,43,56,60	0
2	NAP	C	401	48/48	0.95	0.08	29,44,59,60	0
2	NAP	F	401[B]	48/48	0.96	0.07	24,28,34,35	48
2	NAP	F	401[A]	48/48	0.96	0.07	24,29,35,38	48
2	NAP	B	401	48/48	0.97	0.06	27,32,41,50	0
2	NAP	A	401	48/48	0.97	0.06	22,33,43,54	0
2	NAP	D	401	48/48	0.99	0.04	17,22,39,47	0

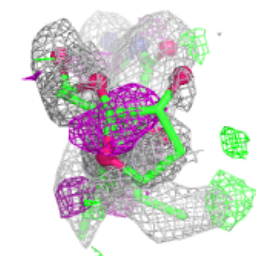
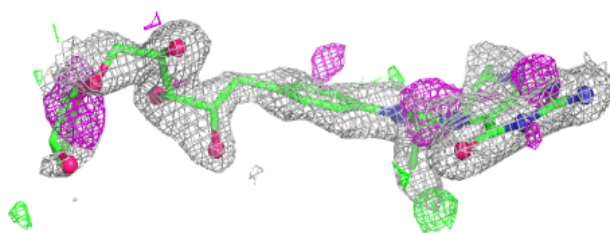
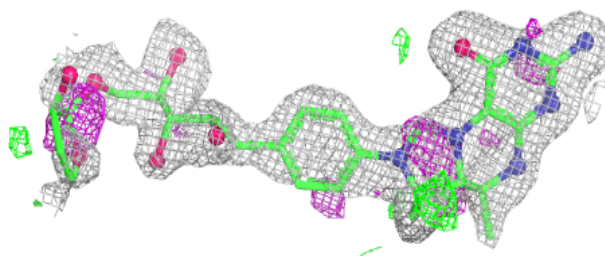
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H4M A 404:

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

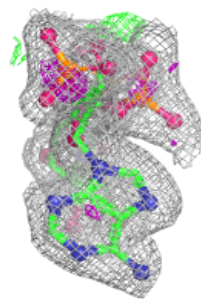
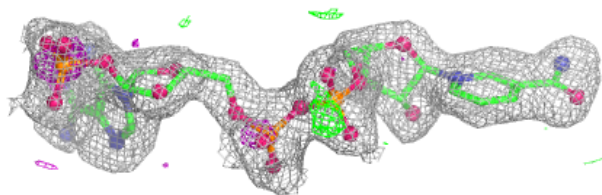
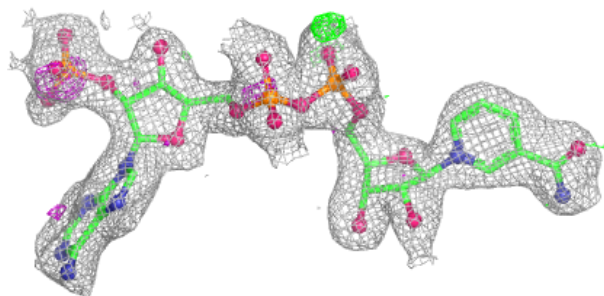
**Electron density around H4M B 402:**

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

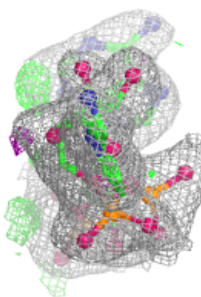
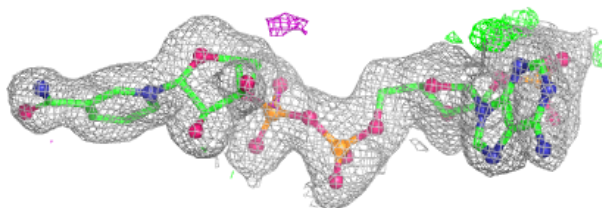
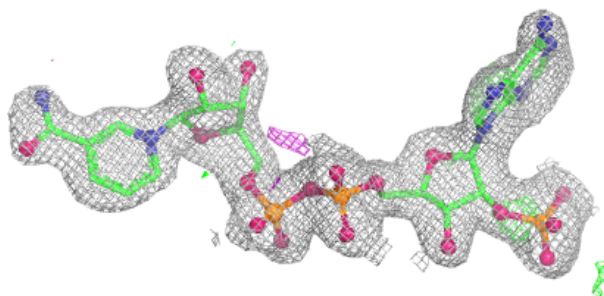


Electron density around NAP E 401:

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

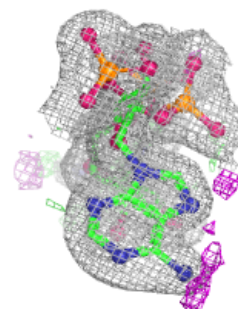
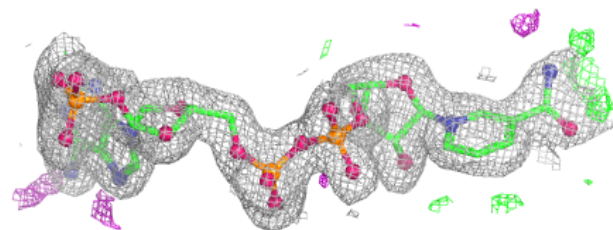
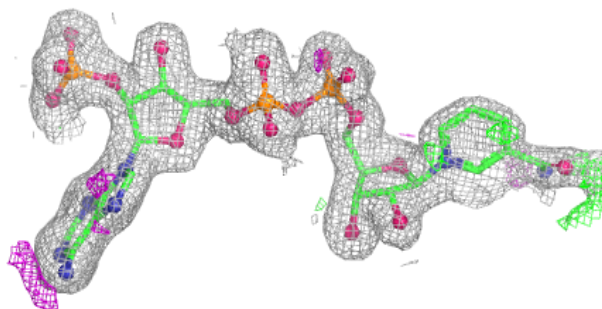
**Electron density around NAP C 401:**

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

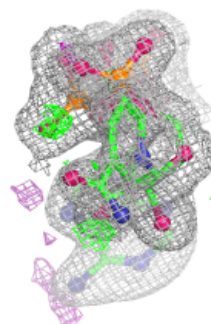
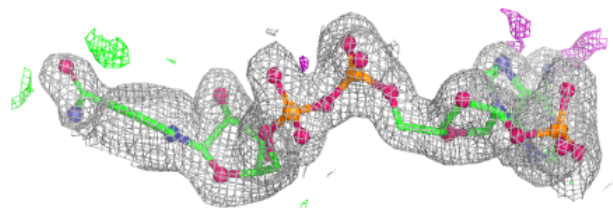
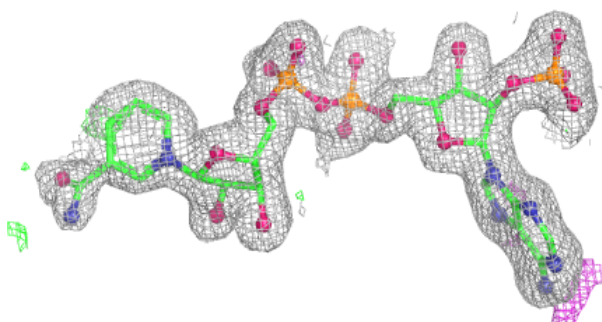


Electron density around NAP F 401 (B):

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

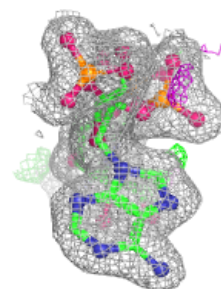
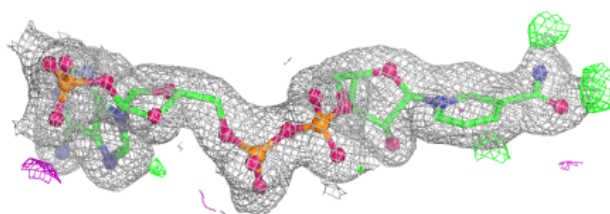
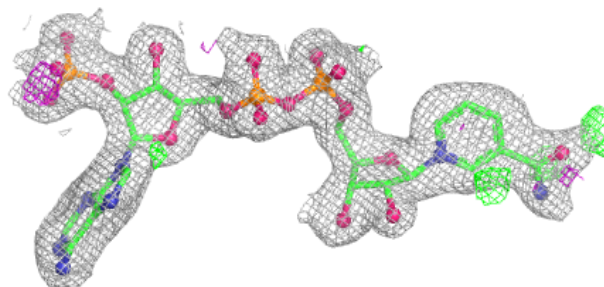
**Electron density around NAP F 401 (A):**

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

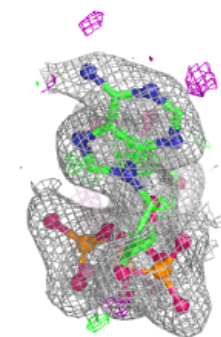
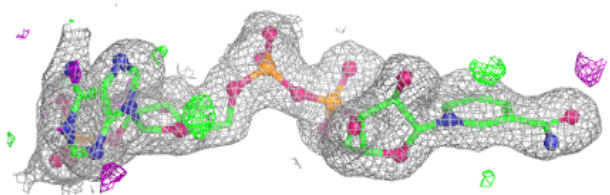
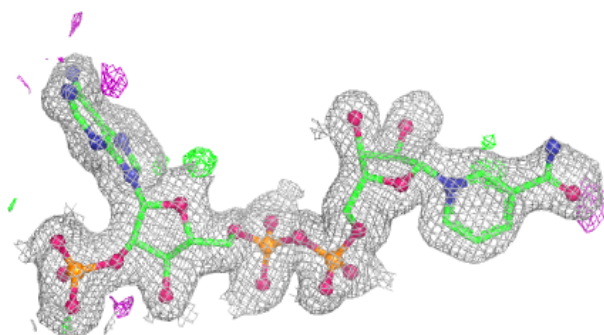


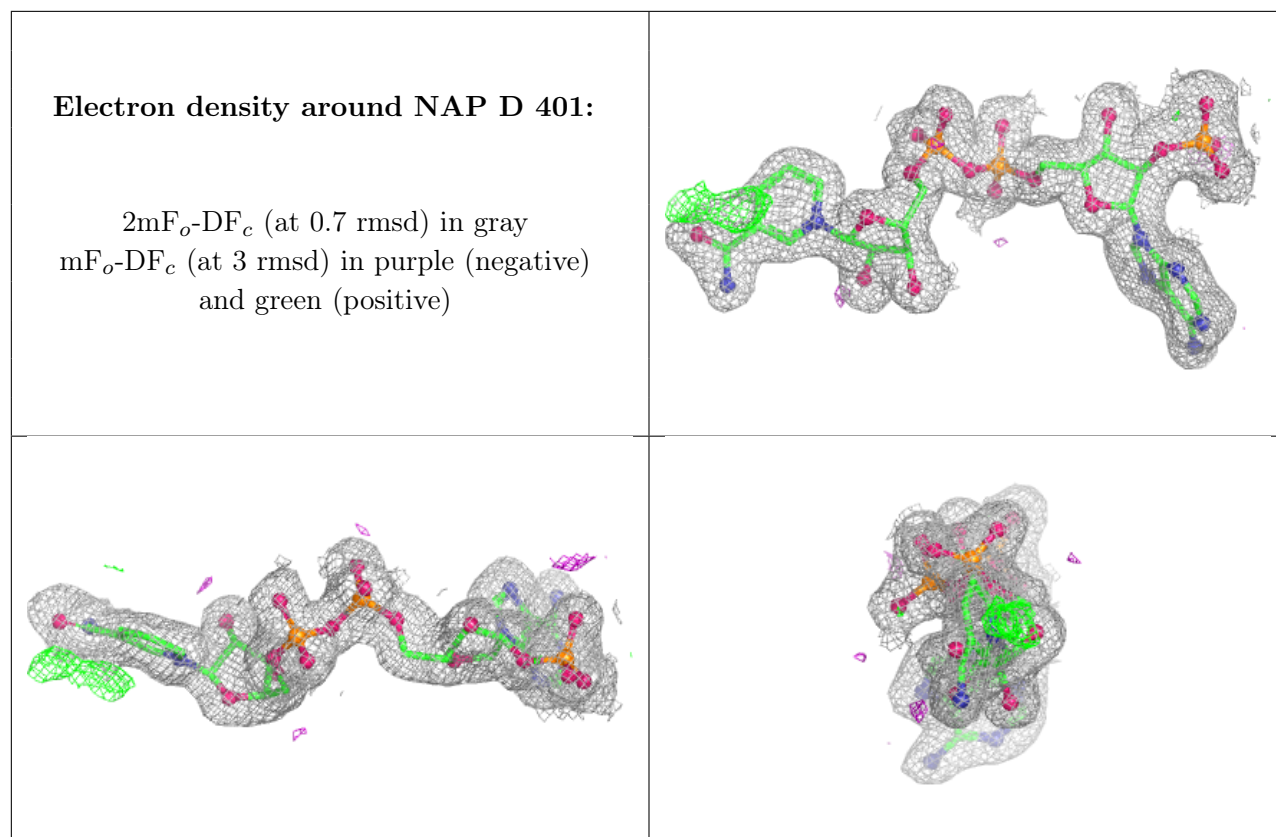
Electron density around NAP B 401:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.