



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:12 PM UTC

PDB ID : 4BL5 / pdb_00004bl5
Title : Crystal structure of human GDP-L-fucose synthase with bound NADP and product GDP-L-fucose
Authors : Vollmar, M.; Shafqat, N.; Rojkova, A.; Krojer, T.; Bradley, A.; Raynor, J.W.; Kavanagh, K.; von Delft, F.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.; Oppermann, U.; Yue, W.W.
Deposited on : 2013-05-01
Resolution : 2.60 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](#) ①) were used in the production of this report:

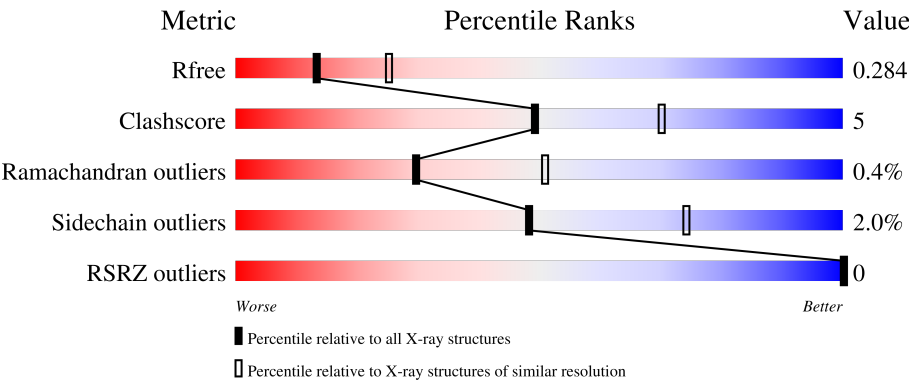
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	336	78% 14% 7%
1	B	336	85% 9% 5%
1	C	336	76% 19%
1	D	336	82% 11% 6%
1	E	336	80% 15% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	336	78%15%7%
1	G	336	83%12%5%
1	H	336	81%13%6%
1	I	336	85%9%. .
1	J	336	84%9%7%
1	K	336	83%10%7%
1	L	336	83%12%. 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29916 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 GDP-L-FUCOSE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2393	1535	404	444	10			
1	B	320	Total	C	N	O	S	0	0	0
			2408	1546	409	443	10			
1	C	321	Total	C	N	O	S	0	0	0
			2453	1576	417	450	10			
1	D	315	Total	C	N	O	S	0	0	0
			2385	1530	403	442	10			
1	E	320	Total	C	N	O	S	0	0	0
			2440	1565	414	451	10			
1	F	313	Total	C	N	O	S	0	0	0
			2377	1528	401	438	10			
1	G	320	Total	C	N	O	S	0	0	0
			2411	1548	406	447	10			
1	H	315	Total	C	N	O	S	0	0	0
			2393	1536	404	443	10			
1	I	321	Total	C	N	O	S	0	0	0
			2443	1567	410	456	10			
1	J	313	Total	C	N	O	S	0	0	0
			2364	1512	405	437	10			
1	K	313	Total	C	N	O	S	0	0	0
			2365	1515	402	438	10			
1	L	320	Total	C	N	O	S	0	0	0
			2407	1544	407	446	10			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q13630
A	-21	HIS	-	expression tag	UNP Q13630
A	-20	HIS	-	expression tag	UNP Q13630
A	-19	HIS	-	expression tag	UNP Q13630
A	-18	HIS	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	HIS	-	expression tag	UNP Q13630
A	-16	HIS	-	expression tag	UNP Q13630
A	-15	SER	-	expression tag	UNP Q13630
A	-14	SER	-	expression tag	UNP Q13630
A	-13	GLY	-	expression tag	UNP Q13630
A	-12	VAL	-	expression tag	UNP Q13630
A	-11	ASP	-	expression tag	UNP Q13630
A	-10	LEU	-	expression tag	UNP Q13630
A	-9	GLY	-	expression tag	UNP Q13630
A	-8	THR	-	expression tag	UNP Q13630
A	-7	GLU	-	expression tag	UNP Q13630
A	-6	ASN	-	expression tag	UNP Q13630
A	-5	LEU	-	expression tag	UNP Q13630
A	-4	TYR	-	expression tag	UNP Q13630
A	-3	PHE	-	expression tag	UNP Q13630
A	-2	GLN	-	expression tag	UNP Q13630
A	-1	SER	-	expression tag	UNP Q13630
B	-22	MET	-	expression tag	UNP Q13630
B	-21	HIS	-	expression tag	UNP Q13630
B	-20	HIS	-	expression tag	UNP Q13630
B	-19	HIS	-	expression tag	UNP Q13630
B	-18	HIS	-	expression tag	UNP Q13630
B	-17	HIS	-	expression tag	UNP Q13630
B	-16	HIS	-	expression tag	UNP Q13630
B	-15	SER	-	expression tag	UNP Q13630
B	-14	SER	-	expression tag	UNP Q13630
B	-13	GLY	-	expression tag	UNP Q13630
B	-12	VAL	-	expression tag	UNP Q13630
B	-11	ASP	-	expression tag	UNP Q13630
B	-10	LEU	-	expression tag	UNP Q13630
B	-9	GLY	-	expression tag	UNP Q13630
B	-8	THR	-	expression tag	UNP Q13630
B	-7	GLU	-	expression tag	UNP Q13630
B	-6	ASN	-	expression tag	UNP Q13630
B	-5	LEU	-	expression tag	UNP Q13630
B	-4	TYR	-	expression tag	UNP Q13630
B	-3	PHE	-	expression tag	UNP Q13630
B	-2	GLN	-	expression tag	UNP Q13630
B	-1	SER	-	expression tag	UNP Q13630
C	-22	MET	-	expression tag	UNP Q13630
C	-21	HIS	-	expression tag	UNP Q13630
C	-20	HIS	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	HIS	-	expression tag	UNP Q13630
C	-18	HIS	-	expression tag	UNP Q13630
C	-17	HIS	-	expression tag	UNP Q13630
C	-16	HIS	-	expression tag	UNP Q13630
C	-15	SER	-	expression tag	UNP Q13630
C	-14	SER	-	expression tag	UNP Q13630
C	-13	GLY	-	expression tag	UNP Q13630
C	-12	VAL	-	expression tag	UNP Q13630
C	-11	ASP	-	expression tag	UNP Q13630
C	-10	LEU	-	expression tag	UNP Q13630
C	-9	GLY	-	expression tag	UNP Q13630
C	-8	THR	-	expression tag	UNP Q13630
C	-7	GLU	-	expression tag	UNP Q13630
C	-6	ASN	-	expression tag	UNP Q13630
C	-5	LEU	-	expression tag	UNP Q13630
C	-4	TYR	-	expression tag	UNP Q13630
C	-3	PHE	-	expression tag	UNP Q13630
C	-2	GLN	-	expression tag	UNP Q13630
C	-1	SER	-	expression tag	UNP Q13630
D	-22	MET	-	expression tag	UNP Q13630
D	-21	HIS	-	expression tag	UNP Q13630
D	-20	HIS	-	expression tag	UNP Q13630
D	-19	HIS	-	expression tag	UNP Q13630
D	-18	HIS	-	expression tag	UNP Q13630
D	-17	HIS	-	expression tag	UNP Q13630
D	-16	HIS	-	expression tag	UNP Q13630
D	-15	SER	-	expression tag	UNP Q13630
D	-14	SER	-	expression tag	UNP Q13630
D	-13	GLY	-	expression tag	UNP Q13630
D	-12	VAL	-	expression tag	UNP Q13630
D	-11	ASP	-	expression tag	UNP Q13630
D	-10	LEU	-	expression tag	UNP Q13630
D	-9	GLY	-	expression tag	UNP Q13630
D	-8	THR	-	expression tag	UNP Q13630
D	-7	GLU	-	expression tag	UNP Q13630
D	-6	ASN	-	expression tag	UNP Q13630
D	-5	LEU	-	expression tag	UNP Q13630
D	-4	TYR	-	expression tag	UNP Q13630
D	-3	PHE	-	expression tag	UNP Q13630
D	-2	GLN	-	expression tag	UNP Q13630
D	-1	SER	-	expression tag	UNP Q13630
E	-22	MET	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	HIS	-	expression tag	UNP Q13630
E	-20	HIS	-	expression tag	UNP Q13630
E	-19	HIS	-	expression tag	UNP Q13630
E	-18	HIS	-	expression tag	UNP Q13630
E	-17	HIS	-	expression tag	UNP Q13630
E	-16	HIS	-	expression tag	UNP Q13630
E	-15	SER	-	expression tag	UNP Q13630
E	-14	SER	-	expression tag	UNP Q13630
E	-13	GLY	-	expression tag	UNP Q13630
E	-12	VAL	-	expression tag	UNP Q13630
E	-11	ASP	-	expression tag	UNP Q13630
E	-10	LEU	-	expression tag	UNP Q13630
E	-9	GLY	-	expression tag	UNP Q13630
E	-8	THR	-	expression tag	UNP Q13630
E	-7	GLU	-	expression tag	UNP Q13630
E	-6	ASN	-	expression tag	UNP Q13630
E	-5	LEU	-	expression tag	UNP Q13630
E	-4	TYR	-	expression tag	UNP Q13630
E	-3	PHE	-	expression tag	UNP Q13630
E	-2	GLN	-	expression tag	UNP Q13630
E	-1	SER	-	expression tag	UNP Q13630
F	-22	MET	-	expression tag	UNP Q13630
F	-21	HIS	-	expression tag	UNP Q13630
F	-20	HIS	-	expression tag	UNP Q13630
F	-19	HIS	-	expression tag	UNP Q13630
F	-18	HIS	-	expression tag	UNP Q13630
F	-17	HIS	-	expression tag	UNP Q13630
F	-16	HIS	-	expression tag	UNP Q13630
F	-15	SER	-	expression tag	UNP Q13630
F	-14	SER	-	expression tag	UNP Q13630
F	-13	GLY	-	expression tag	UNP Q13630
F	-12	VAL	-	expression tag	UNP Q13630
F	-11	ASP	-	expression tag	UNP Q13630
F	-10	LEU	-	expression tag	UNP Q13630
F	-9	GLY	-	expression tag	UNP Q13630
F	-8	THR	-	expression tag	UNP Q13630
F	-7	GLU	-	expression tag	UNP Q13630
F	-6	ASN	-	expression tag	UNP Q13630
F	-5	LEU	-	expression tag	UNP Q13630
F	-4	TYR	-	expression tag	UNP Q13630
F	-3	PHE	-	expression tag	UNP Q13630
F	-2	GLN	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	SER	-	expression tag	UNP Q13630
G	-22	MET	-	expression tag	UNP Q13630
G	-21	HIS	-	expression tag	UNP Q13630
G	-20	HIS	-	expression tag	UNP Q13630
G	-19	HIS	-	expression tag	UNP Q13630
G	-18	HIS	-	expression tag	UNP Q13630
G	-17	HIS	-	expression tag	UNP Q13630
G	-16	HIS	-	expression tag	UNP Q13630
G	-15	SER	-	expression tag	UNP Q13630
G	-14	SER	-	expression tag	UNP Q13630
G	-13	GLY	-	expression tag	UNP Q13630
G	-12	VAL	-	expression tag	UNP Q13630
G	-11	ASP	-	expression tag	UNP Q13630
G	-10	LEU	-	expression tag	UNP Q13630
G	-9	GLY	-	expression tag	UNP Q13630
G	-8	THR	-	expression tag	UNP Q13630
G	-7	GLU	-	expression tag	UNP Q13630
G	-6	ASN	-	expression tag	UNP Q13630
G	-5	LEU	-	expression tag	UNP Q13630
G	-4	TYR	-	expression tag	UNP Q13630
G	-3	PHE	-	expression tag	UNP Q13630
G	-2	GLN	-	expression tag	UNP Q13630
G	-1	SER	-	expression tag	UNP Q13630
H	-22	MET	-	expression tag	UNP Q13630
H	-21	HIS	-	expression tag	UNP Q13630
H	-20	HIS	-	expression tag	UNP Q13630
H	-19	HIS	-	expression tag	UNP Q13630
H	-18	HIS	-	expression tag	UNP Q13630
H	-17	HIS	-	expression tag	UNP Q13630
H	-16	HIS	-	expression tag	UNP Q13630
H	-15	SER	-	expression tag	UNP Q13630
H	-14	SER	-	expression tag	UNP Q13630
H	-13	GLY	-	expression tag	UNP Q13630
H	-12	VAL	-	expression tag	UNP Q13630
H	-11	ASP	-	expression tag	UNP Q13630
H	-10	LEU	-	expression tag	UNP Q13630
H	-9	GLY	-	expression tag	UNP Q13630
H	-8	THR	-	expression tag	UNP Q13630
H	-7	GLU	-	expression tag	UNP Q13630
H	-6	ASN	-	expression tag	UNP Q13630
H	-5	LEU	-	expression tag	UNP Q13630
H	-4	TYR	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	PHE	-	expression tag	UNP Q13630
H	-2	GLN	-	expression tag	UNP Q13630
H	-1	SER	-	expression tag	UNP Q13630
I	-22	MET	-	expression tag	UNP Q13630
I	-21	HIS	-	expression tag	UNP Q13630
I	-20	HIS	-	expression tag	UNP Q13630
I	-19	HIS	-	expression tag	UNP Q13630
I	-18	HIS	-	expression tag	UNP Q13630
I	-17	HIS	-	expression tag	UNP Q13630
I	-16	HIS	-	expression tag	UNP Q13630
I	-15	SER	-	expression tag	UNP Q13630
I	-14	SER	-	expression tag	UNP Q13630
I	-13	GLY	-	expression tag	UNP Q13630
I	-12	VAL	-	expression tag	UNP Q13630
I	-11	ASP	-	expression tag	UNP Q13630
I	-10	LEU	-	expression tag	UNP Q13630
I	-9	GLY	-	expression tag	UNP Q13630
I	-8	THR	-	expression tag	UNP Q13630
I	-7	GLU	-	expression tag	UNP Q13630
I	-6	ASN	-	expression tag	UNP Q13630
I	-5	LEU	-	expression tag	UNP Q13630
I	-4	TYR	-	expression tag	UNP Q13630
I	-3	PHE	-	expression tag	UNP Q13630
I	-2	GLN	-	expression tag	UNP Q13630
I	-1	SER	-	expression tag	UNP Q13630
J	-22	MET	-	expression tag	UNP Q13630
J	-21	HIS	-	expression tag	UNP Q13630
J	-20	HIS	-	expression tag	UNP Q13630
J	-19	HIS	-	expression tag	UNP Q13630
J	-18	HIS	-	expression tag	UNP Q13630
J	-17	HIS	-	expression tag	UNP Q13630
J	-16	HIS	-	expression tag	UNP Q13630
J	-15	SER	-	expression tag	UNP Q13630
J	-14	SER	-	expression tag	UNP Q13630
J	-13	GLY	-	expression tag	UNP Q13630
J	-12	VAL	-	expression tag	UNP Q13630
J	-11	ASP	-	expression tag	UNP Q13630
J	-10	LEU	-	expression tag	UNP Q13630
J	-9	GLY	-	expression tag	UNP Q13630
J	-8	THR	-	expression tag	UNP Q13630
J	-7	GLU	-	expression tag	UNP Q13630
J	-6	ASN	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

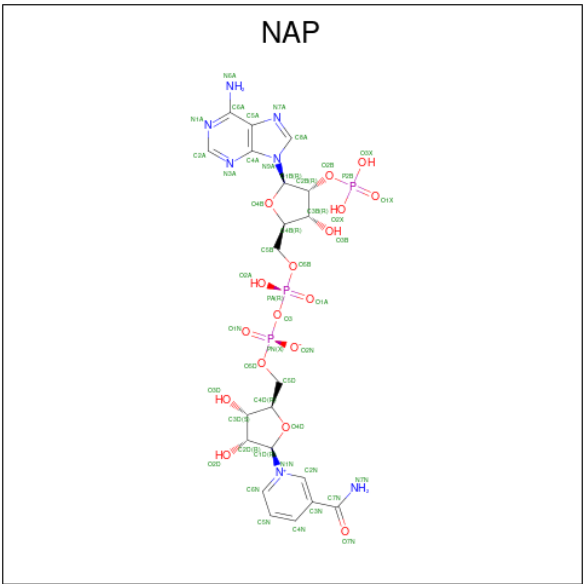
Chain	Residue	Modelled	Actual	Comment	Reference
J	-5	LEU	-	expression tag	UNP Q13630
J	-4	TYR	-	expression tag	UNP Q13630
J	-3	PHE	-	expression tag	UNP Q13630
J	-2	GLN	-	expression tag	UNP Q13630
J	-1	SER	-	expression tag	UNP Q13630
K	-22	MET	-	expression tag	UNP Q13630
K	-21	HIS	-	expression tag	UNP Q13630
K	-20	HIS	-	expression tag	UNP Q13630
K	-19	HIS	-	expression tag	UNP Q13630
K	-18	HIS	-	expression tag	UNP Q13630
K	-17	HIS	-	expression tag	UNP Q13630
K	-16	HIS	-	expression tag	UNP Q13630
K	-15	SER	-	expression tag	UNP Q13630
K	-14	SER	-	expression tag	UNP Q13630
K	-13	GLY	-	expression tag	UNP Q13630
K	-12	VAL	-	expression tag	UNP Q13630
K	-11	ASP	-	expression tag	UNP Q13630
K	-10	LEU	-	expression tag	UNP Q13630
K	-9	GLY	-	expression tag	UNP Q13630
K	-8	THR	-	expression tag	UNP Q13630
K	-7	GLU	-	expression tag	UNP Q13630
K	-6	ASN	-	expression tag	UNP Q13630
K	-5	LEU	-	expression tag	UNP Q13630
K	-4	TYR	-	expression tag	UNP Q13630
K	-3	PHE	-	expression tag	UNP Q13630
K	-2	GLN	-	expression tag	UNP Q13630
K	-1	SER	-	expression tag	UNP Q13630
L	-22	MET	-	expression tag	UNP Q13630
L	-21	HIS	-	expression tag	UNP Q13630
L	-20	HIS	-	expression tag	UNP Q13630
L	-19	HIS	-	expression tag	UNP Q13630
L	-18	HIS	-	expression tag	UNP Q13630
L	-17	HIS	-	expression tag	UNP Q13630
L	-16	HIS	-	expression tag	UNP Q13630
L	-15	SER	-	expression tag	UNP Q13630
L	-14	SER	-	expression tag	UNP Q13630
L	-13	GLY	-	expression tag	UNP Q13630
L	-12	VAL	-	expression tag	UNP Q13630
L	-11	ASP	-	expression tag	UNP Q13630
L	-10	LEU	-	expression tag	UNP Q13630
L	-9	GLY	-	expression tag	UNP Q13630
L	-8	THR	-	expression tag	UNP Q13630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	GLU	-	expression tag	UNP Q13630
L	-6	ASN	-	expression tag	UNP Q13630
L	-5	LEU	-	expression tag	UNP Q13630
L	-4	TYR	-	expression tag	UNP Q13630
L	-3	PHE	-	expression tag	UNP Q13630
L	-2	GLN	-	expression tag	UNP Q13630
L	-1	SER	-	expression tag	UNP Q13630

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



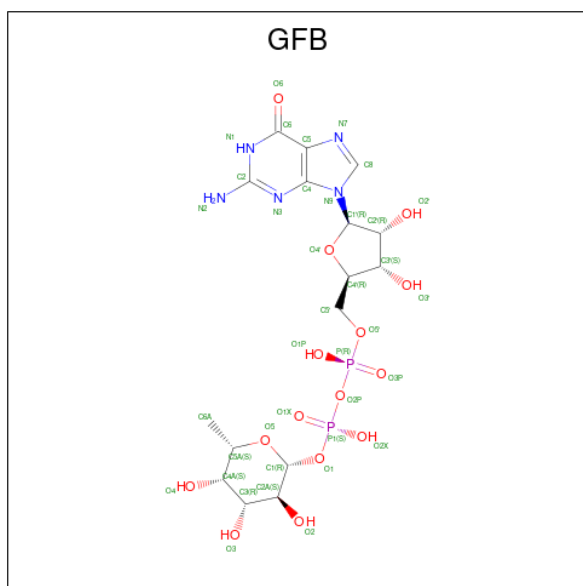
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-BETA-L-FUCOPYRANOSE (CCD ID: GFB) (formula: $C_{16}H_{25}N_5O_{15}P_2$).



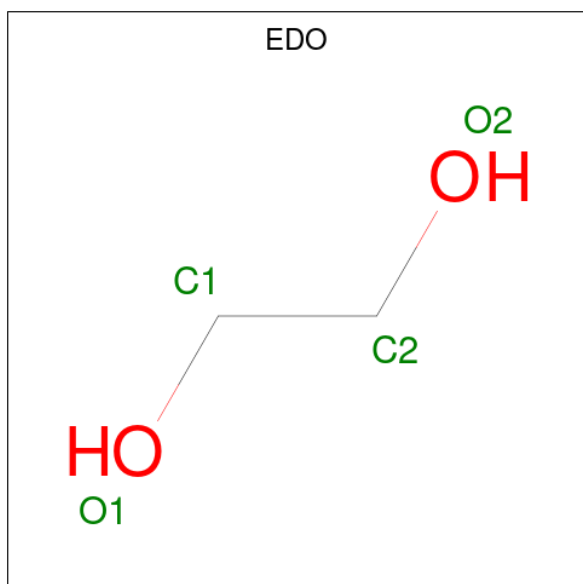
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	C	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	E	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	F	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	H	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	I	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	J	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	K	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	L	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

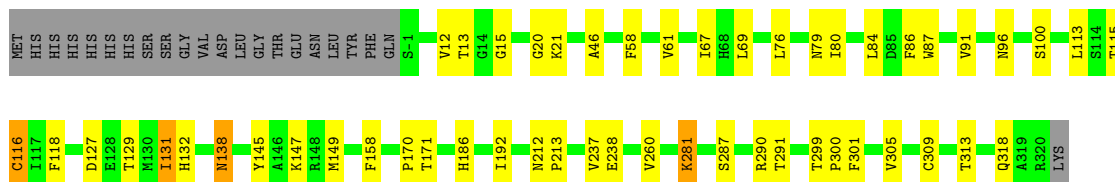
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total 6	O 6	0	0
5	D	7	Total 7	O 7	0	0
5	E	4	Total 4	O 4	0	0
5	F	2	Total 2	O 2	0	0
5	H	2	Total 2	O 2	0	0
5	J	2	Total 2	O 2	0	0
5	K	1	Total 1	O 1	0	0
5	L	3	Total 3	O 3	0	0

3 Residue-property plots

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

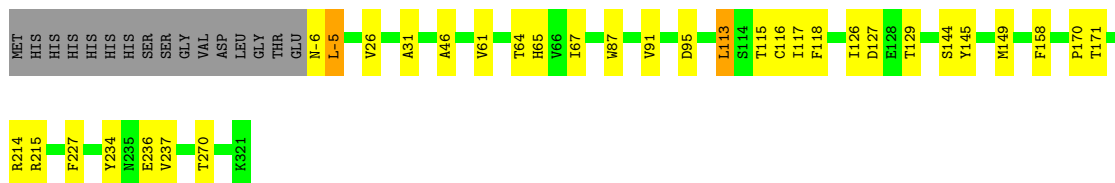
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain A: 



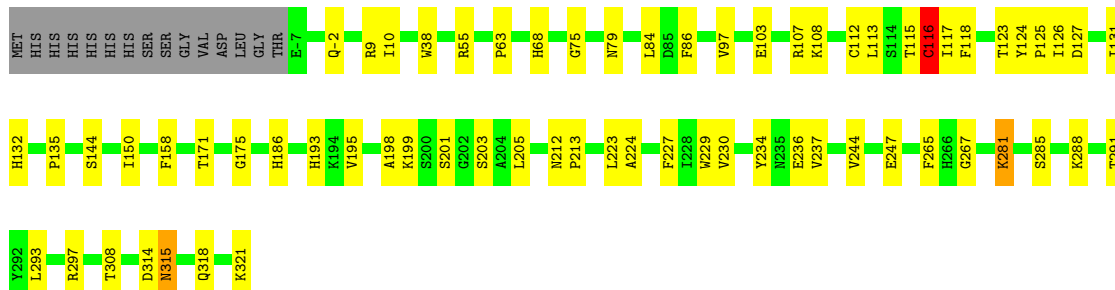
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain B: 



• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain C: 



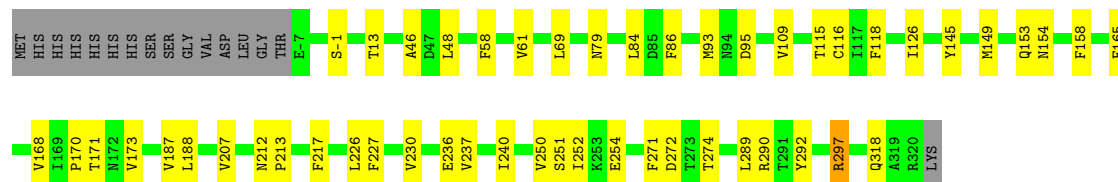
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain D: 



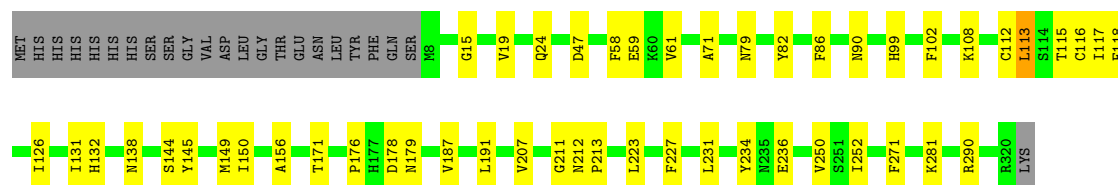
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain E: 80% 15% 5%



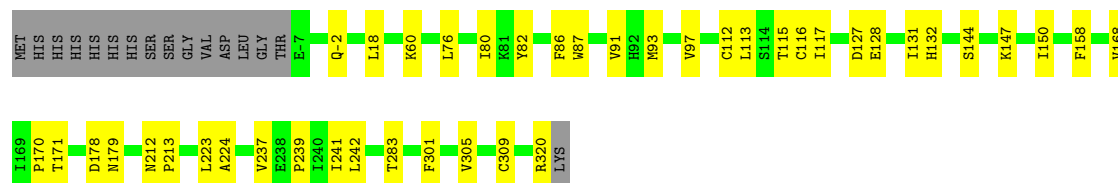
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain F: 78% 15% 7%



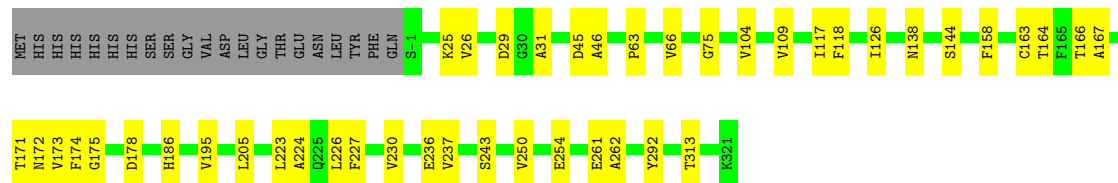
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain G: 83% 12% 5%



• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain H: 81% 13% 6%



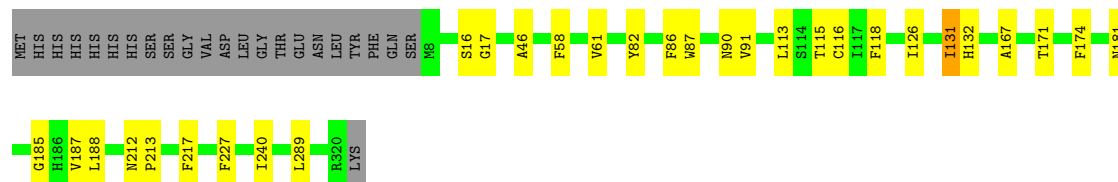
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain I: 85% 9% 6%



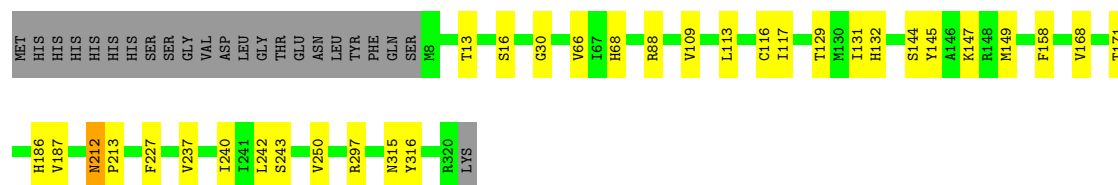
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain J: 84% 9% 7%



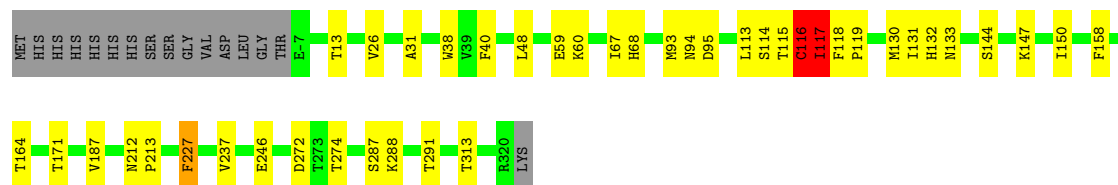
• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain K: 83% 10% 7%



• Molecule 1: GDP-L-FUCOSE SYNTHASE

Chain L: 83% 12% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.41Å 90.48Å 147.52Å 72.54° 72.64° 60.14°	Depositor
Resolution (Å)	29.66 – 2.60 29.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.66-2.60) 94.6 (29.66-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.222 , 0.286 0.225 , 0.284	Depositor DCC
R_{free} test set	5700 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.206 for -h+k,-h,-h+l 0.206 for -k,h-k,-k+l 0.079 for h,h-k,h-l 0.078 for -h+k,k,k-l 0.078 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29916	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% 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: EDO, NAP, GFB

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	0.70	0/2456	0.92	2/3351 (0.1%)
1	B	0.69	0/2472	0.92	1/3376 (0.0%)
1	C	0.69	0/2517	0.91	3/3432 (0.1%)
1	D	0.70	0/2448	0.92	2/3345 (0.1%)
1	E	0.68	0/2504	0.91	0/3418
1	F	0.68	0/2440	0.92	1/3331 (0.0%)
1	G	0.68	0/2476	0.90	0/3385
1	H	0.64	0/2456	0.91	0/3353
1	I	0.65	0/2507	0.90	2/3423 (0.1%)
1	J	0.63	0/2427	0.90	2/3313 (0.1%)
1	K	0.62	0/2428	0.85	2/3317 (0.1%)
1	L	0.61	0/2471	0.86	1/3378 (0.0%)
All	All	0.66	0/29602	0.90	16/40422 (0.0%)

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	C	0	1
1	L	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	212	ASN	CA-C-N	-6.54	113.22	119.89
1	K	212	ASN	C-N-CA	-6.54	113.22	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	TYR	N-CA-C	6.42	119.10	110.88
1	I	131	ILE	N-CA-C	5.87	117.31	110.62
1	C	116	CYS	CB-CA-C	-5.82	101.08	110.74
1	J	131	ILE	N-CA-C	5.78	117.21	110.62
1	A	131	ILE	N-CA-C	5.70	117.12	110.62
1	D	122	THR	N-CA-C	5.68	117.71	109.07
1	D	259	VAL	CB-CA-C	-5.44	104.79	112.14
1	C	135	PRO	O-C-N	5.40	123.69	121.15
1	C	244	VAL	N-CA-C	-5.24	104.29	110.21
1	L	117	ILE	N-CA-CB	-5.24	106.45	112.21
1	J	82	TYR	N-CA-C	5.19	117.10	110.61
1	A	116	CYS	CB-CA-C	-5.17	100.14	110.42
1	I	61	VAL	N-CA-C	-5.07	103.06	109.80
1	B	61	VAL	N-CA-C	-5.03	103.10	109.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	CYS	Peptide
1	L	116	CYS	Peptide

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	2393	0	2231	27	0
1	B	2408	0	2206	20	0
1	C	2453	0	2291	35	1
1	D	2385	0	2200	21	0
1	E	2440	0	2260	30	0
1	F	2377	0	2205	28	0
1	G	2411	0	2191	27	0
1	H	2393	0	2214	24	0
1	I	2443	0	2251	20	0
1	J	2364	0	2162	17	0
1	K	2365	0	2165	19	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2407	0	2190	30	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	2	0
2	G	48	0	25	1	0
2	H	48	0	25	0	0
2	I	48	0	25	2	0
2	J	48	0	25	2	0
2	K	48	0	25	3	0
2	L	48	0	25	0	0
3	A	38	0	23	3	0
3	B	38	0	23	4	0
3	C	38	0	23	4	0
3	D	38	0	23	5	0
3	E	38	0	23	5	0
3	F	38	0	23	4	0
3	G	38	0	23	8	0
3	H	38	0	23	3	0
3	I	38	0	23	3	0
3	J	38	0	23	3	0
3	K	38	0	23	4	0
3	L	38	0	23	5	0
4	F	4	0	6	0	0
5	A	11	0	0	1	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0
5	D	7	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	3	0	0	0	0
All	All	29916	0	27148	307	1

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 5.

All (307) 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:G:116:CYS:SG	3:G:902:GFB:H2A	2.14	0.87
1:E:236:GLU:OE2	1:E:292:TYR:OH	1.96	0.83
1:C:108:LYS:NZ	1:C:234:TYR:O	2.14	0.80
1:L:117:ILE:HG12	1:L:144:SER:HA	1.65	0.79
1:F:115:THR:HG21	1:F:171:THR:HG22	1.65	0.78
1:E:116:CYS:SG	3:E:902:GFB:H6AA	2.24	0.77
1:C:55:ARG:NE	1:C:103:GLU:OE2	2.19	0.75
1:L:116:CYS:SG	3:L:902:GFB:H6AA	2.28	0.74
1:C:116:CYS:SG	3:C:902:GFB:H2A	2.28	0.73
1:H:25:LYS:O	1:H:29:ASP:HB2	1.90	0.71
1:K:16:SER:OG	2:K:901:NAP:O3X	2.07	0.71
1:K:131:ILE:HG23	1:K:132:HIS:CD2	2.26	0.70
1:D:116:CYS:SG	3:D:902:GFB:H2A	2.31	0.70
1:J:115:THR:HG21	1:J:171:THR:HG22	1.74	0.69
1:G:116:CYS:SG	3:G:902:GFB:C2A	2.83	0.67
1:A:58:PHE:O	1:A:61:VAL:O	2.13	0.66
1:L:164:THR:O	1:L:164:THR:HG22	1.94	0.66
1:C:195:VAL:HG22	1:C:205:LEU:HD22	1.78	0.65
1:F:58:PHE:O	1:F:61:VAL:O	2.16	0.64
1:D:113:LEU:O	2:D:901:NAP:H6N	1.97	0.64
1:C:131:ILE:HG23	1:C:132:HIS:CD2	2.33	0.64
1:C:193:HIS:CE1	1:C:321:LYS:HB2	2.33	0.64
1:B:116:CYS:SG	3:B:902:GFB:H2A	2.37	0.63
1:A:131:ILE:HG23	1:A:132:HIS:CD2	2.33	0.63
1:E:173:VAL:HG23	2:E:901:NAP:C4N	2.29	0.62
1:G:131:ILE:HG23	1:G:132:HIS:CD2	2.35	0.62
1:L:287:SER:O	1:L:291:THR:HG23	2.00	0.62
1:G:18:LEU:HB2	1:G:178:ASP:HA	1.81	0.62
1:A:281:LYS:NZ	5:A:2009:HOH:O	2.22	0.62
1:D:47:ASP:N	1:D:53:GLN:OE1	2.33	0.61
1:K:158:PHE:CD2	1:K:237:VAL:HG21	2.35	0.60
1:B:145:TYR:O	1:B:149:MET:HG2	2.01	0.60
1:H:236:GLU:OE2	1:H:292:TYR:OH	2.20	0.60
1:D:58:PHE:O	1:D:61:VAL:O	2.20	0.59
1:J:131:ILE:HG23	1:J:132:HIS:CD2	2.37	0.59
1:G:116:CYS:SG	3:G:902:GFB:C3	2.91	0.59
1:A:15:GLY:HA2	1:A:20:GLY:HA3	1.85	0.59
1:L:114:SER:HB3	1:L:117:ILE:HD12	1.85	0.58
1:L:118:PHE:CD1	1:L:131:ILE:HA	2.39	0.58
1:B:-6:ASN:O	1:B:-5:LEU:O	2.21	0.58
1:D:234:TYR:CZ	1:D:236:GLU:HB2	2.39	0.57
1:B:117:ILE:HG22	1:B:144:SER:HA	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ASP:OD1	1:F:179:ASN:N	2.37	0.57
1:A:287:SER:O	1:A:291:THR:HG23	2.05	0.57
1:K:88:ARG:NH1	1:L:95:ASP:OD1	2.39	0.56
1:F:187:VAL:HG23	3:F:902:GFB:C4	2.36	0.56
1:J:118:PHE:CD2	1:J:126:ILE:CG2	2.89	0.56
1:I:113:LEU:O	1:I:170:PRO:HD2	2.06	0.56
1:B:115:THR:HG21	1:B:171:THR:HG22	1.88	0.55
1:I:131:ILE:HG23	1:I:132:HIS:CD2	2.42	0.55
1:K:158:PHE:CG	1:K:237:VAL:HG21	2.42	0.55
1:L:288:LYS:O	1:L:291:THR:OG1	2.24	0.55
1:I:113:LEU:O	2:I:901:NAP:H6N	2.07	0.55
1:K:113:LEU:O	2:K:901:NAP:H6N	2.06	0.55
1:A:115:THR:HG21	1:A:171:THR:HG22	1.89	0.54
1:L:117:ILE:HD13	1:L:147:LYS:HB2	1.89	0.54
1:G:82:TYR:O	1:G:86:PHE:HD2	1.91	0.54
1:F:234:TYR:CZ	1:F:236:GLU:HB2	2.43	0.54
1:I:115:THR:HG21	1:I:171:THR:HG22	1.90	0.54
1:D:93:MET:O	1:D:97:VAL:HG23	2.08	0.54
1:G:113:LEU:O	1:G:170:PRO:HD2	2.07	0.54
1:I:240:ILE:HD11	1:I:289:LEU:HA	1.89	0.54
1:F:116:CYS:SG	3:F:902:GFB:H2A	2.49	0.53
1:F:187:VAL:HG23	3:F:902:GFB:C5	2.39	0.53
1:B:95:ASP:OD2	1:D:92:HIS:NE2	2.37	0.53
1:H:75:GLY:HA2	1:H:186:HIS:CD2	2.44	0.53
1:I:118:PHE:CD2	1:I:126:ILE:CG2	2.90	0.53
1:E:48:LEU:O	1:E:93:MET:HA	2.08	0.53
1:E:297:ARG:H	1:E:297:ARG:NE	2.06	0.53
1:C:265:PHE:CZ	1:C:267:GLY:HA3	2.44	0.53
1:L:212:ASN:N	1:L:213:PRO:CD	2.72	0.53
1:A:116:CYS:SG	3:A:902:GFB:H2A	2.49	0.52
1:B:26:VAL:HG12	1:B:31:ALA:HB3	1.90	0.52
1:G:116:CYS:HG	3:G:902:GFB:C3	2.22	0.52
1:B:64:THR:OG1	1:B:65:HIS:ND1	2.37	0.52
1:G:115:THR:HG21	1:G:171:THR:HG22	1.92	0.52
1:E:109:VAL:HG23	1:E:165:PHE:CE1	2.44	0.52
1:A:299:THR:O	1:A:300:PRO:C	2.52	0.51
1:D:187:VAL:O	1:D:191:LEU:HG	2.10	0.51
1:J:58:PHE:O	1:J:61:VAL:O	2.27	0.51
1:D:299:THR:O	1:D:300:PRO:C	2.52	0.51
1:A:212:ASN:N	1:A:213:PRO:CD	2.73	0.51
1:I:249:GLU:OE1	1:I:283:THR:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:THR:HG21	1:L:171:THR:HG22	1.92	0.51
1:B:234:TYR:CZ	1:B:236:GLU:HB2	2.46	0.51
3:J:902:GFB:H5'A	3:J:902:GFB:N3	2.26	0.51
1:G:147:LYS:O	1:G:150:ILE:HB	2.11	0.51
1:C:234:TYR:CZ	1:C:236:GLU:HB2	2.46	0.51
3:C:902:GFB:N3	3:C:902:GFB:H5'A	2.26	0.51
1:E:118:PHE:CD2	1:E:126:ILE:CG2	2.94	0.51
3:L:902:GFB:H5'A	3:L:902:GFB:N3	2.26	0.50
1:F:145:TYR:O	1:F:149:MET:HG2	2.10	0.50
1:L:117:ILE:HD13	1:L:147:LYS:CB	2.42	0.50
1:G:76:LEU:O	1:G:80:ILE:HG13	2.10	0.50
1:C:115:THR:HG21	1:C:171:THR:HG22	1.93	0.50
1:L:115:THR:C	1:L:117:ILE:H	2.20	0.50
1:G:158:PHE:CG	1:G:237:VAL:HG21	2.47	0.50
1:G:212:ASN:N	1:G:213:PRO:CD	2.75	0.50
1:H:172:ASN:ND2	3:H:902:GFB:H6AB	2.27	0.50
1:I:128:GLU:HG2	1:I:239:PRO:O	2.12	0.49
1:L:94:ASN:ND2	1:L:150:ILE:HD11	2.27	0.49
1:J:212:ASN:N	1:J:213:PRO:CD	2.75	0.49
1:L:13:THR:OG1	1:L:68:HIS:HA	2.11	0.49
1:E:115:THR:HG21	1:E:171:THR:HG22	1.94	0.49
3:A:902:GFB:N3	3:A:902:GFB:H5'A	2.28	0.49
1:C:84:LEU:HB2	1:F:156:ALA:HB1	1.94	0.49
1:C:175:GLY:HA2	1:C:308:THR:OG1	2.13	0.49
1:C:117:ILE:HG22	1:C:144:SER:HA	1.93	0.49
1:A:138:ASN:OD1	1:A:138:ASN:N	2.44	0.49
1:C:79:ASN:HA	1:C:86:PHE:CE2	2.48	0.49
1:F:113:LEU:O	2:F:901:NAP:H6N	2.13	0.49
1:E:13:THR:O	1:E:69:LEU:HB2	2.13	0.49
1:E:187:VAL:HG23	3:E:902:GFB:C4	2.43	0.49
1:L:130:MET:HA	1:L:133:ASN:ND2	2.27	0.49
3:F:902:GFB:N3	3:F:902:GFB:H5'A	2.28	0.48
1:B:67:ILE:HG23	1:B:227:PHE:CE1	2.49	0.48
1:H:26:VAL:HG12	1:H:31:ALA:HB3	1.94	0.48
1:I:116:CYS:SG	3:I:902:GFB:H2A	2.52	0.48
1:K:116:CYS:SG	3:K:902:GFB:H2A	2.52	0.48
1:A:145:TYR:O	1:A:149:MET:HG2	2.14	0.48
1:H:158:PHE:CG	1:H:237:VAL:HG21	2.49	0.48
3:K:902:GFB:H5'A	3:K:902:GFB:N3	2.28	0.48
1:D:131:ILE:HG23	1:D:132:HIS:CD2	2.49	0.48
1:G:113:LEU:O	2:G:901:NAP:H6N	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:NE2	3:A:902:GFB:H4A	2.29	0.47
1:J:174:PHE:CE1	1:J:217:PHE:HB3	2.49	0.47
1:C:116:CYS:SG	3:C:902:GFB:C2A	3.01	0.47
1:H:195:VAL:HG22	1:H:205:LEU:HD22	1.95	0.47
1:E:250:VAL:HG12	1:E:251:SER:O	2.13	0.47
3:E:902:GFB:H5'A	3:E:902:GFB:N3	2.29	0.47
1:K:212:ASN:O	1:K:213:PRO:C	2.54	0.47
1:D:108:LYS:NZ	1:D:234:TYR:O	2.47	0.47
1:D:116:CYS:SG	3:D:902:GFB:C2A	3.03	0.47
3:G:902:GFB:H5'A	3:G:902:GFB:N3	2.30	0.47
1:H:164:THR:HG22	1:H:164:THR:O	2.14	0.47
1:B:113:LEU:O	1:B:170:PRO:HD2	2.15	0.47
1:G:127:ASP:HA	1:G:241:ILE:CD1	2.45	0.47
3:B:902:GFB:H5'A	3:B:902:GFB:N3	2.30	0.47
1:B:116:CYS:SG	3:B:902:GFB:C2A	3.03	0.46
1:H:45:ASP:O	1:H:46:ALA:HB2	2.15	0.46
1:H:186:HIS:NE2	3:H:902:GFB:H4A	2.30	0.46
1:L:26:VAL:HG12	1:L:31:ALA:HB3	1.96	0.46
1:A:118:PHE:CD1	1:A:131:ILE:HA	2.49	0.46
1:D:226:LEU:O	1:D:230:VAL:HG23	2.15	0.46
1:G:128:GLU:HG2	1:G:239:PRO:O	2.16	0.46
1:H:118:PHE:CD2	1:H:126:ILE:HG21	2.50	0.46
1:H:175:GLY:O	1:H:178:ASP:HB2	2.15	0.46
1:H:117:ILE:HG22	1:H:144:SER:HA	1.97	0.46
1:K:240:ILE:HG23	1:K:240:ILE:O	2.15	0.46
1:A:79:ASN:HA	1:A:86:PHE:CE2	2.51	0.46
1:L:164:THR:O	1:L:164:THR:CG2	2.63	0.46
1:C:186:HIS:NE2	3:C:902:GFB:H4A	2.30	0.46
1:H:173:VAL:HG12	1:H:174:PHE:N	2.30	0.46
1:I:116:CYS:SG	3:I:902:GFB:H6AA	2.56	0.46
1:F:15:GLY:O	1:F:24:GLN:NE2	2.49	0.46
1:J:188:LEU:HD12	1:J:217:PHE:CD1	2.51	0.46
3:D:902:GFB:H5'A	3:D:902:GFB:N3	2.31	0.46
1:G:117:ILE:HG22	1:G:144:SER:HA	1.97	0.46
1:G:168:VAL:HG11	1:G:242:LEU:HD11	1.97	0.45
1:E:116:CYS:SG	3:E:902:GFB:C6A	3.02	0.45
1:G:116:CYS:SG	3:G:902:GFB:C4A	3.04	0.45
1:C:68:HIS:CE1	1:C:97:VAL:HG21	2.52	0.45
1:F:115:THR:OG1	1:F:171:THR:HA	2.17	0.45
1:J:187:VAL:HG23	3:J:902:GFB:C5	2.46	0.45
1:L:272:ASP:OD1	1:L:274:THR:OG1	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:TRP:CZ2	1:G:91:VAL:HG21	2.50	0.45
1:D:124:TYR:CD2	1:D:281:LYS:HE3	2.51	0.45
1:F:290:ARG:HD3	1:F:290:ARG:HA	1.83	0.45
1:K:147:LYS:NZ	2:K:901:NAP:O3D	2.50	0.45
1:E:95:ASP:HA	1:E:153:GLN:HE22	1.81	0.45
1:C:212:ASN:N	1:C:213:PRO:CD	2.80	0.45
1:E:58:PHE:O	1:E:61:VAL:O	2.35	0.45
1:I:16:SER:OG	2:I:901:NAP:O3X	2.35	0.45
1:E:158:PHE:CG	1:E:237:VAL:HG21	2.52	0.45
1:F:113:LEU:HD11	1:F:150:ILE:HB	1.98	0.45
1:H:223:LEU:O	1:H:224:ALA:C	2.60	0.45
1:J:16:SER:OG	2:J:901:NAP:O3X	2.31	0.45
1:H:118:PHE:CD2	1:H:126:ILE:CG2	3.00	0.45
1:K:187:VAL:HG23	3:K:902:GFB:C5	2.46	0.45
3:H:902:GFB:N3	3:H:902:GFB:H5'A	2.32	0.44
1:E:187:VAL:HG21	1:E:252:ILE:HD12	2.00	0.44
1:F:131:ILE:HG23	1:F:132:HIS:CD2	2.52	0.44
1:B:127:ASP:OD1	1:B:129:THR:HB	2.18	0.44
1:E:168:VAL:O	1:E:170:PRO:HD3	2.18	0.44
3:I:902:GFB:H5'A	3:I:902:GFB:N3	2.32	0.44
1:D:45:ASP:O	1:D:46:ALA:HB2	2.18	0.44
1:H:171:THR:HG23	1:H:243:SER:CB	2.48	0.44
1:A:76:LEU:O	1:A:80:ILE:HG13	2.17	0.44
1:B:214:ARG:O	1:B:215:ARG:HD3	2.17	0.44
1:I:67:ILE:HG23	1:I:227:PHE:CE1	2.53	0.44
1:J:118:PHE:CD2	1:J:126:ILE:HG21	2.51	0.44
1:K:117:ILE:HG22	1:K:144:SER:HA	1.98	0.44
1:D:26:VAL:HG12	1:D:31:ALA:HB3	1.99	0.44
1:B:118:PHE:CD2	1:B:126:ILE:CG2	3.00	0.44
1:C:75:GLY:HA2	1:C:186:HIS:CD2	2.53	0.44
1:E:145:TYR:O	1:E:149:MET:HG2	2.18	0.44
1:H:226:LEU:O	1:H:230:VAL:HG23	2.18	0.44
1:I:118:PHE:CD2	1:I:126:ILE:HG21	2.53	0.44
1:G:305:VAL:O	1:G:309:CYS:SG	2.75	0.43
1:J:17:GLY:HA3	2:J:901:NAP:O5B	2.18	0.43
1:L:272:ASP:OD1	1:L:272:ASP:C	2.61	0.43
1:C:118:PHE:CD2	1:C:126:ILE:HG23	2.53	0.43
1:F:79:ASN:HA	1:F:86:PHE:CE2	2.53	0.43
1:F:211:GLY:HA2	1:F:252:ILE:HB	2.01	0.43
1:H:63:PRO:HD2	1:H:104:VAL:HG11	1.99	0.43
1:F:207:VAL:O	1:F:271:PHE:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:ILE:HG23	1:L:132:HIS:CD2	2.53	0.43
1:B:158:PHE:CD1	1:B:237:VAL:HG21	2.54	0.43
1:F:19:VAL:HG22	1:F:223:LEU:HD23	2.00	0.43
1:I:117:ILE:HG22	1:I:144:SER:HA	2.01	0.43
1:C:158:PHE:CD1	1:C:237:VAL:HG21	2.53	0.43
1:E:250:VAL:HG13	1:E:254:GLU:HB2	1.99	0.43
1:I:10:ILE:HG12	1:I:65:HIS:HB2	1.99	0.43
1:C:125:PRO:HB2	1:C:285:SER:HB2	2.00	0.43
1:D:163:CYS:HB3	1:D:165:PHE:CE1	2.54	0.43
1:F:108:LYS:NZ	1:F:231:LEU:O	2.37	0.43
1:J:240:ILE:HD11	1:J:289:LEU:HA	2.00	0.43
1:A:113:LEU:O	1:A:170:PRO:HD2	2.19	0.43
1:A:212:ASN:N	1:A:213:PRO:HD2	2.34	0.42
1:C:10:ILE:HG21	1:C:38:TRP:CZ3	2.54	0.42
1:L:118:PHE:HB3	1:L:119:PRO:HD2	2.01	0.42
1:L:187:VAL:HA	3:L:902:GFB:C2	2.49	0.42
1:C:314:ASP:C	1:C:315:ASN:HD22	2.27	0.42
1:E:207:VAL:O	1:E:271:PHE:HA	2.19	0.42
1:E:226:LEU:O	1:E:230:VAL:HG23	2.19	0.42
1:G:116:CYS:SG	3:G:902:GFB:O3	2.72	0.42
1:G:301:PHE:O	1:G:305:VAL:HG23	2.20	0.42
1:A:87:TRP:CZ2	1:A:91:VAL:HG21	2.54	0.42
1:A:192:ILE:HG12	1:A:309:CYS:SG	2.60	0.42
1:G:116:CYS:HG	3:G:902:GFB:H2A	1.81	0.42
1:L:187:VAL:HG23	3:L:902:GFB:C4	2.49	0.42
1:B:113:LEU:O	2:B:901:NAP:H6N	2.20	0.42
1:E:272:ASP:OD1	1:E:272:ASP:C	2.63	0.42
1:E:272:ASP:OD1	1:E:274:THR:OG1	2.21	0.42
1:I:58:PHE:O	1:I:61:VAL:O	2.37	0.42
1:J:116:CYS:SG	3:J:902:GFB:H6AA	2.60	0.42
1:K:171:THR:HG23	1:K:243:SER:CB	2.50	0.42
1:A:113:LEU:HA	1:A:147:LYS:HD2	2.01	0.42
1:B:116:CYS:SG	3:B:902:GFB:C3	3.08	0.42
1:F:118:PHE:CD2	1:F:126:ILE:HG21	2.54	0.42
1:I:158:PHE:CG	1:I:237:VAL:HG21	2.55	0.42
1:L:48:LEU:O	1:L:93:MET:HA	2.20	0.42
1:L:187:VAL:HG23	3:L:902:GFB:C5	2.50	0.42
1:C:198:ALA:O	1:C:199:LYS:C	2.63	0.42
1:D:116:CYS:SG	3:D:902:GFB:H6AA	2.60	0.42
1:E:240:ILE:HD11	1:E:289:LEU:HA	2.02	0.42
1:J:113:LEU:HD13	1:J:167:ALA:HB1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:PHE:CG	1:L:237:VAL:HG21	2.54	0.42
1:A:96:ASN:O	1:A:100:SER:OG	2.32	0.42
1:B:87:TRP:CH2	1:B:91:VAL:HG21	2.55	0.42
1:C:201:SER:C	1:C:203:SER:H	2.27	0.42
1:K:13:THR:OG1	1:K:68:HIS:HA	2.20	0.42
1:E:188:LEU:HD12	1:E:217:PHE:CD1	2.55	0.41
1:F:99:HIS:O	1:F:102:PHE:HB3	2.19	0.41
1:K:145:TYR:O	1:K:149:MET:HG2	2.20	0.41
1:F:117:ILE:HG22	1:F:144:SER:HA	2.02	0.41
1:I:118:PHE:CG	1:I:126:ILE:HG21	2.55	0.41
1:A:301:PHE:O	1:A:305:VAL:HG23	2.20	0.41
1:J:181:ASN:O	1:J:185:GLY:N	2.53	0.41
1:K:315:ASN:O	1:K:316:TYR:C	2.64	0.41
1:A:13:THR:O	1:A:69:LEU:HB2	2.19	0.41
1:A:127:ASP:OD1	1:A:129:THR:HB	2.21	0.41
1:C:247:GLU:CD	1:C:247:GLU:H	2.28	0.41
1:F:212:ASN:N	1:F:213:PRO:CD	2.83	0.41
1:K:186:HIS:NE2	3:K:902:GFB:H4A	2.34	0.41
1:C:124:TYR:CD2	1:C:281:LYS:HE3	2.56	0.41
1:K:66:VAL:HB	1:K:109:VAL:HG22	2.02	0.41
1:H:166:THR:OG1	1:H:167:ALA:N	2.54	0.41
1:C:113:LEU:HD11	1:C:150:ILE:HB	2.02	0.41
1:E:79:ASN:HA	1:E:86:PHE:CE2	2.56	0.41
1:E:153:GLN:O	1:E:154:ASN:C	2.63	0.41
1:G:93:MET:O	1:G:97:VAL:HG23	2.21	0.41
1:I:45:ASP:O	1:I:46:ALA:HB2	2.21	0.41
1:K:168:VAL:HG11	1:K:242:LEU:HD11	2.03	0.41
1:C:223:LEU:O	1:C:224:ALA:C	2.62	0.41
1:C:288:LYS:O	1:C:291:THR:OG1	2.30	0.41
1:F:47:ASP:OD1	1:F:47:ASP:C	2.63	0.41
1:G:223:LEU:O	1:G:224:ALA:C	2.64	0.41
1:J:87:TRP:O	1:J:91:VAL:HG23	2.21	0.41
1:D:186:HIS:CD2	3:D:902:GFB:H5A	2.56	0.41
1:E:212:ASN:N	1:E:213:PRO:CD	2.84	0.41
1:F:187:VAL:O	1:F:191:LEU:HG	2.20	0.41
1:L:114:SER:OG	1:L:115:THR:N	2.54	0.41
1:C:127:ASP:OD1	1:C:127:ASP:C	2.64	0.41
1:C:229:TRP:O	1:C:230:VAL:C	2.64	0.41
1:C:229:TRP:CD2	1:C:293:LEU:HD11	2.56	0.41
1:L:38:TRP:HB3	1:L:40:PHE:CE2	2.56	0.41
1:A:12:VAL:HG22	1:A:67:ILE:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD13	1:C:38:TRP:CZ2	2.56	0.40
1:H:250:VAL:HG13	1:H:254:GLU:HB2	2.02	0.40
1:J:86:PHE:O	1:J:90:ASN:HB2	2.21	0.40
1:L:67:ILE:HG23	1:L:227:PHE:CE1	2.55	0.40
1:A:290:ARG:HA	1:A:290:ARG:HD3	1.88	0.40
1:D:158:PHE:CG	1:D:237:VAL:HG21	2.56	0.40
1:H:75:GLY:HA2	1:H:186:HIS:HD2	1.85	0.40
1:I:212:ASN:N	1:I:213:PRO:CD	2.84	0.40
1:D:286:ASN:OD1	1:D:286:ASN:C	2.63	0.40
1:E:290:ARG:HA	1:E:290:ARG:HD3	1.87	0.40
1:F:71:ALA:HB3	2:F:901:NAP:H3D	2.04	0.40
1:F:86:PHE:O	1:F:90:ASN:HB2	2.22	0.40
1:H:66:VAL:HB	1:H:109:VAL:HG22	2.03	0.40
1:H:261:GLU:O	1:H:262:ALA:C	2.63	0.40
1:A:158:PHE:CG	1:A:237:VAL:HG21	2.57	0.40
1:B:117:ILE:CG2	1:B:144:SER:HA	2.50	0.40
1:C:9:ARG:HB3	1:C:63:PRO:HA	2.04	0.40
1:E:116:CYS:SG	3:E:902:GFB:C4A	3.10	0.40
1:G:179:ASN:HB2	1:G:320:ARG:NH2	2.37	0.40

All (1) 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:C:-2:GLN:O	1:K:297:ARG:NH1[1_565]	2.17	0.03

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	312/336 (93%)	295 (95%)	16 (5%)	1 (0%)	36 58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	318/336 (95%)	299 (94%)	17 (5%)	2 (1%)	21	42
1	C	319/336 (95%)	308 (97%)	11 (3%)	0	100	100
1	D	313/336 (93%)	302 (96%)	8 (3%)	3 (1%)	12	28
1	E	318/336 (95%)	304 (96%)	12 (4%)	2 (1%)	21	42
1	F	311/336 (93%)	296 (95%)	14 (4%)	1 (0%)	36	58
1	G	318/336 (95%)	301 (95%)	16 (5%)	1 (0%)	36	58
1	H	313/336 (93%)	296 (95%)	17 (5%)	0	100	100
1	I	319/336 (95%)	307 (96%)	11 (3%)	1 (0%)	36	58
1	J	311/336 (93%)	292 (94%)	18 (6%)	1 (0%)	36	58
1	K	311/336 (93%)	292 (94%)	18 (6%)	1 (0%)	36	58
1	L	318/336 (95%)	300 (94%)	16 (5%)	2 (1%)	21	42
All	All	3781/4032 (94%)	3592 (95%)	174 (5%)	15 (0%)	30	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-5	LEU
1	D	320	ARG
1	G	60	LYS
1	L	116	CYS
1	B	46	ALA
1	J	46	ALA
1	D	46	ALA
1	E	-1	SER
1	E	46	ALA
1	I	46	ALA
1	A	46	ALA
1	D	131	ILE
1	K	30	GLY
1	L	60	LYS
1	F	176	PRO

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	240/288 (83%)	232 (97%)	8 (3%)	33	61
1	B	233/288 (81%)	231 (99%)	2 (1%)	70	87
1	C	242/288 (84%)	234 (97%)	8 (3%)	33	61
1	D	235/288 (82%)	230 (98%)	5 (2%)	47	73
1	E	241/288 (84%)	237 (98%)	4 (2%)	53	78
1	F	235/288 (82%)	228 (97%)	7 (3%)	36	64
1	G	233/288 (81%)	230 (99%)	3 (1%)	61	82
1	H	236/288 (82%)	232 (98%)	4 (2%)	53	78
1	I	241/288 (84%)	236 (98%)	5 (2%)	47	73
1	J	230/288 (80%)	229 (100%)	1 (0%)	84	93
1	K	231/288 (80%)	228 (99%)	3 (1%)	61	82
1	L	232/288 (81%)	226 (97%)	6 (3%)	40	68
All	All	2829/3456 (82%)	2773 (98%)	56 (2%)	48	74

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	84	LEU
1	A	138	ASN
1	A	238	GLU
1	A	260	VAL
1	A	281	LYS
1	A	313	THR
1	A	318	GLN
1	B	113	LEU
1	B	270	THR
1	C	107	ARG
1	C	112	CYS
1	C	123	THR
1	C	227	PHE
1	C	281	LYS
1	C	297	ARG
1	C	315	ASN
1	C	318	GLN
1	D	84	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	113	LEU
1	D	123	THR
1	D	138	ASN
1	D	227	PHE
1	E	84	LEU
1	E	227	PHE
1	E	297	ARG
1	E	318	GLN
1	F	59	GLU
1	F	112	CYS
1	F	113	LEU
1	F	138	ASN
1	F	227	PHE
1	F	250	VAL
1	F	281	LYS
1	G	-2	GLN
1	G	112	CYS
1	G	283	THR
1	H	138	ASN
1	H	163	CYS
1	H	227	PHE
1	H	313	THR
1	I	59	GLU
1	I	123	THR
1	I	138	ASN
1	I	227	PHE
1	I	297	ARG
1	J	227	PHE
1	K	129	THR
1	K	227	PHE
1	K	250	VAL
1	L	59	GLU
1	L	113	LEU
1	L	117	ILE
1	L	227	PHE
1	L	246	GLU
1	L	313	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	GLN
1	A	266	HIS
1	B	24	GLN
1	C	24	GLN
1	C	79	ASN
1	C	196	HIS
1	C	225	GLN
1	C	279	GLN
1	C	315	ASN
1	D	225	GLN
1	D	235	ASN
1	D	315	ASN
1	E	24	GLN
1	E	79	ASN
1	E	153	GLN
1	E	159	GLN
1	E	177	HIS
1	E	225	GLN
1	E	235	ASN
1	F	212	ASN
1	G	24	GLN
1	G	177	HIS
1	G	225	GLN
1	G	315	ASN
1	H	24	GLN
1	H	79	ASN
1	H	140	ASN
1	H	172	ASN
1	I	132	HIS
1	I	133	ASN
1	I	177	HIS
1	I	235	ASN
1	J	79	ASN
1	J	212	ASN
1	J	266	HIS
1	J	315	ASN
1	K	24	GLN
1	K	133	ASN
1	K	225	GLN
1	K	315	ASN
1	L	79	ASN
1	L	132	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	901	-	50,52,52	1.20	6 (12%)	71,80,80	1.55	9 (12%)
2	NAP	G	901	-	50,52,52	1.21	5 (10%)	71,80,80	1.57	11 (15%)
2	NAP	D	901	-	50,52,52	1.17	4 (8%)	71,80,80	1.64	11 (15%)
3	GFB	F	902	-	40,41,41	1.25	5 (12%)	61,64,64	1.95	14 (22%)
3	GFB	D	902	-	40,41,41	1.39	5 (12%)	61,64,64	1.74	14 (22%)
3	GFB	C	902	-	40,41,41	1.40	8 (20%)	61,64,64	1.70	11 (18%)
2	NAP	F	901	-	50,52,52	1.19	6 (12%)	71,80,80	1.65	14 (19%)
2	NAP	L	901	-	50,52,52	1.23	6 (12%)	71,80,80	1.58	11 (15%)
3	GFB	A	902	-	40,41,41	1.38	5 (12%)	61,64,64	1.67	14 (22%)
2	NAP	E	901	-	50,52,52	1.19	7 (14%)	71,80,80	1.50	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	I	901	-	50,52,52	1.37	8 (16%)	71,80,80	1.62	10 (14%)
3	GFB	E	902	-	40,41,41	1.35	5 (12%)	61,64,64	1.76	13 (21%)
2	NAP	K	901	-	50,52,52	1.15	6 (12%)	71,80,80	1.57	10 (14%)
3	GFB	H	902	-	40,41,41	1.30	3 (7%)	61,64,64	1.78	12 (19%)
3	GFB	L	902	-	40,41,41	1.36	6 (15%)	61,64,64	1.66	12 (19%)
2	NAP	J	901	-	50,52,52	1.18	6 (12%)	71,80,80	1.62	11 (15%)
2	NAP	C	901	-	50,52,52	1.23	7 (14%)	71,80,80	1.63	14 (19%)
3	GFB	B	902	-	40,41,41	1.42	7 (17%)	61,64,64	1.64	12 (19%)
3	GFB	I	902	-	40,41,41	1.37	7 (17%)	61,64,64	1.72	11 (18%)
3	GFB	G	902	-	40,41,41	1.42	7 (17%)	61,64,64	1.67	15 (24%)
3	GFB	J	902	-	40,41,41	1.45	8 (20%)	61,64,64	1.68	14 (22%)
4	EDO	F	1321	-	3,3,3	0.55	0	2,2,2	0.21	0
2	NAP	B	901	-	50,52,52	1.19	8 (16%)	71,80,80	1.67	10 (14%)
2	NAP	H	901	-	50,52,52	1.13	6 (12%)	71,80,80	1.60	11 (15%)
3	GFB	K	902	-	40,41,41	1.36	6 (15%)	61,64,64	1.82	14 (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	A	901	-	-	7/35/67/67	0/5/5/5
2	NAP	G	901	-	-	7/35/67/67	0/5/5/5
2	NAP	D	901	-	-	7/35/67/67	0/5/5/5
3	GFB	F	902	-	-	8/21/57/57	0/4/4/4
3	GFB	D	902	-	-	7/21/57/57	0/4/4/4
3	GFB	C	902	-	-	7/21/57/57	0/4/4/4
2	NAP	F	901	-	-	7/35/67/67	0/5/5/5
2	NAP	L	901	-	-	7/35/67/67	0/5/5/5
3	GFB	A	902	-	-	9/21/57/57	0/4/4/4
2	NAP	E	901	-	-	7/35/67/67	0/5/5/5
2	NAP	I	901	-	-	7/35/67/67	0/5/5/5
3	GFB	E	902	-	-	7/21/57/57	0/4/4/4
2	NAP	K	901	-	-	8/35/67/67	0/5/5/5
3	GFB	H	902	-	-	9/21/57/57	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GFB	L	902	-	-	6/21/57/57	0/4/4/4
2	NAP	J	901	-	-	7/35/67/67	0/5/5/5
2	NAP	C	901	-	-	7/35/67/67	0/5/5/5
3	GFB	B	902	-	-	7/21/57/57	0/4/4/4
3	GFB	I	902	-	-	7/21/57/57	0/4/4/4
3	GFB	G	902	-	-	8/21/57/57	0/4/4/4
3	GFB	J	902	-	-	8/21/57/57	0/4/4/4
4	EDO	F	1321	-	-	1/1/1/1	-
2	NAP	B	901	-	-	6/35/67/67	0/5/5/5
2	NAP	H	901	-	-	7/35/67/67	0/5/5/5
3	GFB	K	902	-	-	7/21/57/57	0/4/4/4

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	901	NAP	C5A-C4A	4.64	1.47	1.39
2	E	901	NAP	C5A-C4A	4.56	1.47	1.39
2	J	901	NAP	C5A-C4A	4.50	1.47	1.39
2	L	901	NAP	C5A-C4A	4.44	1.47	1.39
2	I	901	NAP	C5A-C4A	4.41	1.47	1.39
2	A	901	NAP	C5A-C4A	4.23	1.46	1.39
2	K	901	NAP	C5A-C4A	4.18	1.46	1.39
2	C	901	NAP	C5A-C4A	4.10	1.46	1.39
2	D	901	NAP	C5A-C4A	3.92	1.46	1.39
2	F	901	NAP	C5A-C4A	3.81	1.45	1.39
3	A	902	GFB	C4A-C3	3.66	1.61	1.52
2	B	901	NAP	C5A-C4A	3.65	1.45	1.39
2	I	901	NAP	PN-O3	3.65	1.63	1.59
3	K	902	GFB	P-O2P	3.61	1.63	1.59
2	H	901	NAP	C5A-C4A	3.61	1.45	1.39
3	J	902	GFB	P1-O2P	3.57	1.63	1.59
3	E	902	GFB	C5-C6	-3.53	1.31	1.44
2	D	901	NAP	PA-O3	3.46	1.63	1.59
3	J	902	GFB	C5-N7	-3.44	1.32	1.39
2	F	901	NAP	PA-O3	3.43	1.63	1.59
3	D	902	GFB	C5-C6	-3.26	1.32	1.44
3	B	902	GFB	C5-C6	-3.20	1.32	1.44
3	A	902	GFB	C5-C6	-3.17	1.32	1.44
3	C	902	GFB	C5-C6	-3.17	1.32	1.44
3	B	902	GFB	C4A-C3	3.14	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	GFB	C4A-C5A	3.14	1.59	1.52
3	K	902	GFB	O4'-C1'	3.10	1.49	1.42
3	K	902	GFB	C5-C6	-3.09	1.33	1.44
3	E	902	GFB	C4A-C5A	3.08	1.59	1.52
3	C	902	GFB	C5-N7	-3.05	1.32	1.39
3	L	902	GFB	P1-O2P	3.03	1.62	1.59
3	J	902	GFB	C5-C6	-3.03	1.33	1.44
3	L	902	GFB	C5-C6	-2.98	1.33	1.44
3	G	902	GFB	C5-C6	-2.97	1.33	1.44
3	L	902	GFB	C4A-C5A	2.97	1.59	1.52
2	A	901	NAP	C5A-C6A	2.96	1.49	1.41
3	I	902	GFB	C5-C6	-2.95	1.33	1.44
3	C	902	GFB	P-O2P	-2.93	1.56	1.59
2	C	901	NAP	PA-O3	2.91	1.62	1.59
3	H	902	GFB	C5-N7	-2.89	1.33	1.39
3	I	902	GFB	C4A-C5A	2.89	1.59	1.52
3	E	902	GFB	O4'-C1'	2.87	1.48	1.42
3	D	902	GFB	C4A-C3	2.86	1.59	1.52
3	A	902	GFB	C5-N7	-2.85	1.33	1.39
3	B	902	GFB	C5-N7	-2.84	1.33	1.39
3	I	902	GFB	O4'-C1'	2.84	1.48	1.42
2	I	901	NAP	PA-O3	2.81	1.62	1.59
3	G	902	GFB	C4A-C5A	2.78	1.59	1.52
2	I	901	NAP	O4D-C1D	2.78	1.44	1.40
3	E	902	GFB	C5-N7	-2.78	1.33	1.39
3	H	902	GFB	C5-C6	-2.77	1.34	1.44
3	F	902	GFB	C5-C6	-2.75	1.34	1.44
3	I	902	GFB	C5-N7	-2.73	1.33	1.39
3	B	902	GFB	P-O2P	2.71	1.62	1.59
3	C	902	GFB	C4A-C3	2.71	1.59	1.52
2	C	901	NAP	C5A-C6A	2.71	1.48	1.41
2	G	901	NAP	C5A-C6A	2.71	1.48	1.41
2	B	901	NAP	C8A-N7A	2.69	1.36	1.31
3	D	902	GFB	C5-N7	-2.68	1.33	1.39
3	F	902	GFB	C5-N7	-2.67	1.33	1.39
2	L	901	NAP	PN-O3	2.65	1.62	1.59
3	G	902	GFB	C4A-C3	2.64	1.59	1.52
2	K	901	NAP	PA-O3	2.62	1.62	1.59
2	H	901	NAP	C5A-N7A	-2.62	1.34	1.39
2	J	901	NAP	C5A-C6A	2.61	1.48	1.41
2	E	901	NAP	C8A-N7A	2.60	1.36	1.31
2	D	901	NAP	C8A-N7A	2.60	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	GFB	C4A-C5A	2.59	1.58	1.52
2	H	901	NAP	C4A-N9A	-2.59	1.32	1.37
3	K	902	GFB	C4A-C5A	2.58	1.58	1.52
3	L	902	GFB	C5-N7	-2.57	1.33	1.39
2	I	901	NAP	C5A-C6A	2.56	1.48	1.41
3	F	902	GFB	C4A-C3	2.54	1.58	1.52
3	G	902	GFB	C4-N9	-2.54	1.31	1.38
2	L	901	NAP	PA-O3	2.54	1.62	1.59
3	G	902	GFB	C5-N7	-2.52	1.34	1.39
2	G	901	NAP	C4A-N9A	-2.51	1.32	1.37
2	E	901	NAP	PA-O3	2.51	1.62	1.59
2	H	901	NAP	PA-O3	2.50	1.62	1.59
2	A	901	NAP	C5A-N7A	-2.50	1.34	1.39
2	F	901	NAP	C5A-C6A	2.50	1.47	1.41
2	C	901	NAP	C5A-N7A	-2.50	1.34	1.39
3	E	902	GFB	C4A-C3	2.48	1.58	1.52
2	F	901	NAP	C5A-N7A	-2.48	1.34	1.39
2	I	901	NAP	C5A-N7A	-2.47	1.34	1.39
2	E	901	NAP	C5A-N7A	-2.46	1.34	1.39
3	J	902	GFB	C8-N9	-2.45	1.32	1.37
2	H	901	NAP	C5A-C6A	2.45	1.47	1.41
2	K	901	NAP	C5A-C6A	2.44	1.47	1.41
2	L	901	NAP	C8A-N7A	2.44	1.36	1.31
2	B	901	NAP	PN-O3	2.41	1.62	1.59
3	J	902	GFB	C4A-C3	2.41	1.58	1.52
3	I	902	GFB	C4A-C3	2.40	1.58	1.52
2	G	901	NAP	C8A-N7A	2.39	1.36	1.31
2	L	901	NAP	C5A-C6A	2.38	1.47	1.41
3	H	902	GFB	C4A-C3	2.37	1.58	1.52
3	G	902	GFB	P1-O2P	2.37	1.62	1.59
2	B	901	NAP	PA-O3	2.36	1.62	1.59
3	D	902	GFB	P1-O2P	2.35	1.62	1.59
2	A	901	NAP	C8A-N7A	2.34	1.36	1.31
2	B	901	NAP	C5A-N7A	-2.34	1.34	1.39
2	B	901	NAP	C5A-C6A	2.34	1.47	1.41
2	L	901	NAP	C5A-N7A	-2.33	1.34	1.39
2	K	901	NAP	C4A-N9A	-2.33	1.32	1.37
2	I	901	NAP	C4A-N9A	-2.32	1.32	1.37
2	I	901	NAP	C8A-N7A	2.31	1.36	1.31
2	J	901	NAP	C8A-N7A	2.30	1.36	1.31
2	C	901	NAP	PN-O3	2.30	1.62	1.59
2	A	901	NAP	C4A-N9A	-2.29	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	NAP	C4A-N9A	-2.28	1.33	1.37
3	C	902	GFB	C4A-C5A	2.28	1.57	1.52
2	H	901	NAP	C8A-N7A	2.27	1.36	1.31
3	J	902	GFB	C4-N9	-2.27	1.32	1.38
3	L	902	GFB	C4A-C3	2.25	1.58	1.52
2	F	901	NAP	C8A-N7A	2.25	1.36	1.31
3	J	902	GFB	P1-O2X	-2.25	1.44	1.55
3	A	902	GFB	C4A-C5A	2.24	1.57	1.52
3	J	902	GFB	O4'-C1'	2.24	1.47	1.42
2	J	901	NAP	C5A-N7A	-2.22	1.35	1.39
2	J	901	NAP	C4A-N9A	-2.22	1.33	1.37
2	J	901	NAP	PA-O3	2.21	1.61	1.59
3	K	902	GFB	C4A-C3	2.20	1.58	1.52
2	B	901	NAP	C4A-N9A	-2.20	1.33	1.37
2	F	901	NAP	C4A-N9A	-2.20	1.33	1.37
3	C	902	GFB	P1-O2P	2.19	1.61	1.59
2	K	901	NAP	C8A-N7A	2.18	1.35	1.31
2	E	901	NAP	O4D-C1D	2.17	1.43	1.40
2	B	901	NAP	P2B-O2B	2.17	1.63	1.59
2	K	901	NAP	C5A-N7A	-2.17	1.35	1.39
3	B	902	GFB	C1-C2A	-2.16	1.46	1.52
3	I	902	GFB	P1-O2P	2.14	1.61	1.59
3	C	902	GFB	O2'-C2'	2.14	1.48	1.43
3	G	902	GFB	O4'-C1'	2.13	1.46	1.42
3	K	902	GFB	C5-N7	-2.11	1.34	1.39
2	G	901	NAP	C5A-N7A	-2.09	1.35	1.39
2	E	901	NAP	C4A-N9A	-2.09	1.33	1.37
3	F	902	GFB	C4-N9	-2.08	1.32	1.38
3	B	902	GFB	C4-N9	-2.07	1.32	1.38
2	A	901	NAP	O4D-C1D	2.07	1.43	1.40
3	L	902	GFB	C4-N9	-2.06	1.32	1.38
2	C	901	NAP	C8A-N7A	2.06	1.35	1.31
3	C	902	GFB	O4'-C1'	2.06	1.46	1.42
3	I	902	GFB	C4-N9	-2.06	1.32	1.38
2	D	901	NAP	C5A-C6A	2.04	1.46	1.41
3	F	902	GFB	C4A-C5A	2.03	1.57	1.52
2	E	901	NAP	PN-O3	2.02	1.61	1.59
3	A	902	GFB	O4'-C1'	2.01	1.46	1.42

All (288) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	902	GFB	O5-C1-O1	-6.61	102.72	111.36
3	K	902	GFB	O5-C1-O1	-6.48	102.89	111.36
3	H	902	GFB	C2-N3-C4	5.78	122.26	112.30
3	E	902	GFB	C2-N3-C4	5.70	122.11	112.30
3	I	902	GFB	C2-N3-C4	5.49	121.75	112.30
3	F	902	GFB	C2-N3-C4	5.44	121.67	112.30
3	D	902	GFB	C2-N3-C4	5.43	121.65	112.30
2	B	901	NAP	C5A-C4A-N3A	-5.38	119.31	126.72
3	C	902	GFB	O5-C1-O1	-5.22	104.55	111.36
3	B	902	GFB	C2-N3-C4	5.19	121.24	112.30
2	A	901	NAP	C5A-C4A-N3A	-5.18	119.59	126.72
3	A	902	GFB	C2-N3-C4	5.17	121.20	112.30
3	J	902	GFB	C2-N3-C4	5.15	121.18	112.30
3	H	902	GFB	C5-C4-N3	-5.13	120.22	128.39
2	I	901	NAP	C5A-C4A-N3A	-5.09	119.71	126.72
2	F	901	NAP	C5A-C4A-N3A	-5.08	119.72	126.72
3	L	902	GFB	C2-N3-C4	5.04	120.99	112.30
2	G	901	NAP	C5A-C4A-N3A	-5.03	119.79	126.72
2	H	901	NAP	C5A-C4A-N3A	-4.95	119.91	126.72
2	K	901	NAP	C5A-C4A-N3A	-4.94	119.92	126.72
2	L	901	NAP	C5A-C4A-N3A	-4.92	119.94	126.72
2	C	901	NAP	C5A-C4A-N3A	-4.88	119.99	126.72
3	K	902	GFB	C2-N3-C4	4.88	120.70	112.30
3	F	902	GFB	C5-C4-N3	-4.84	120.69	128.39
2	D	901	NAP	C5A-C4A-N3A	-4.80	120.11	126.72
2	J	901	NAP	C5A-C4A-N3A	-4.74	120.19	126.72
3	E	902	GFB	C5-C4-N3	-4.68	120.94	128.39
3	G	902	GFB	C2-N3-C4	4.62	120.26	112.30
3	I	902	GFB	C5-C4-N3	-4.60	121.07	128.39
3	C	902	GFB	C2-N3-C4	4.60	120.22	112.30
2	H	901	NAP	N3A-C2A-N1A	-4.60	121.62	128.58
3	J	902	GFB	C5-C4-N3	-4.55	121.14	128.39
3	D	902	GFB	C5-C4-N3	-4.52	121.19	128.39
2	B	901	NAP	N3A-C2A-N1A	-4.52	121.74	128.58
3	C	902	GFB	C5-C4-N3	-4.46	121.29	128.39
3	A	902	GFB	C3-C4A-C5A	4.44	116.56	109.81
3	K	902	GFB	C3-C4A-C5A	4.41	116.52	109.81
2	J	901	NAP	C4A-N9A-C8A	4.39	110.34	105.74
2	J	901	NAP	N3A-C4A-N9A	4.39	134.63	127.17
3	D	902	GFB	C3-C4A-C5A	4.38	116.47	109.81
2	E	901	NAP	C5A-C4A-N3A	-4.37	120.71	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	GFB	C5-C4-N3	-4.35	121.47	128.39
2	I	901	NAP	N3A-C4A-N9A	4.32	134.51	127.17
3	F	902	GFB	C2-N1-C6	-4.31	117.29	125.11
2	F	901	NAP	N3A-C2A-N1A	-4.28	122.10	128.58
2	B	901	NAP	N3A-C4A-N9A	4.25	134.39	127.17
2	D	901	NAP	C4A-N9A-C8A	4.24	110.19	105.74
3	F	902	GFB	C3-C4A-C5A	4.22	116.23	109.81
2	A	901	NAP	N3A-C4A-N9A	4.19	134.30	127.17
2	D	901	NAP	N3A-C2A-N1A	-4.19	122.23	128.58
2	F	901	NAP	N3A-C4A-N9A	4.19	134.30	127.17
2	C	901	NAP	N3A-C4A-N9A	4.19	134.29	127.17
2	B	901	NAP	C2A-N3A-C4A	4.19	122.05	111.83
2	K	901	NAP	N3A-C4A-N9A	4.17	134.26	127.17
2	L	901	NAP	N3A-C4A-N9A	4.16	134.25	127.17
3	I	902	GFB	C3-C4A-C5A	4.16	116.13	109.81
2	H	901	NAP	N3A-C4A-N9A	4.06	134.08	127.17
2	G	901	NAP	N3A-C4A-N9A	4.06	134.07	127.17
3	K	902	GFB	C5-C4-N3	-4.05	121.94	128.39
3	A	902	GFB	C5-C4-N3	-4.04	121.96	128.39
2	J	901	NAP	N3A-C2A-N1A	-4.04	122.47	128.58
3	E	902	GFB	C3-C4A-C5A	4.02	115.92	109.81
3	H	902	GFB	C3-C4A-C5A	4.01	115.91	109.81
3	I	902	GFB	O5-C1-O1	-4.01	106.12	111.36
2	D	901	NAP	N3A-C4A-N9A	4.01	133.99	127.17
2	E	901	NAP	N3A-C2A-N1A	-4.00	122.52	128.58
2	H	901	NAP	C2A-N3A-C4A	3.98	121.54	111.83
3	L	902	GFB	C3-C4A-C5A	3.97	115.85	109.81
3	L	902	GFB	O5-C1-O1	-3.96	106.19	111.36
3	L	902	GFB	C5-C4-N3	-3.96	122.09	128.39
2	E	901	NAP	N3A-C4A-N9A	3.94	133.87	127.17
2	C	901	NAP	C4A-N9A-C8A	3.94	109.87	105.74
2	F	901	NAP	C2A-N3A-C4A	3.93	121.44	111.83
3	D	902	GFB	O5-C1-O1	-3.91	106.25	111.36
3	G	902	GFB	C3-C4A-C5A	3.91	115.75	109.81
2	E	901	NAP	C4A-N9A-C8A	3.90	109.83	105.74
3	B	902	GFB	C3-C4A-C5A	3.90	115.74	109.81
2	B	901	NAP	C4A-N9A-C8A	3.90	109.83	105.74
2	A	901	NAP	C2A-N3A-C4A	3.89	121.32	111.83
3	G	902	GFB	C5-C4-N3	-3.88	122.21	128.39
2	I	901	NAP	C4A-N9A-C8A	3.86	109.79	105.74
3	G	902	GFB	C2-N1-C6	-3.85	118.12	125.11
2	L	901	NAP	N3A-C2A-N1A	-3.85	122.75	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	901	NAP	C4A-N9A-C8A	3.83	109.76	105.74
2	L	901	NAP	C4A-N9A-C8A	3.82	109.75	105.74
2	H	901	NAP	C4A-N9A-C8A	3.81	109.73	105.74
2	I	901	NAP	N3A-C2A-N1A	-3.80	122.83	128.58
3	C	902	GFB	C3-C4A-C5A	3.79	115.58	109.81
2	I	901	NAP	C2A-N3A-C4A	3.74	120.97	111.83
2	D	901	NAP	C4A-C5A-N7A	-3.73	106.32	110.58
2	K	901	NAP	C4A-N9A-C8A	3.72	109.64	105.74
2	K	901	NAP	N3A-C2A-N1A	-3.71	122.97	128.58
2	A	901	NAP	N3A-C2A-N1A	-3.71	122.97	128.58
2	F	901	NAP	C4A-N9A-C8A	3.71	109.63	105.74
2	K	901	NAP	C2A-N3A-C4A	3.69	120.85	111.83
3	E	902	GFB	O5-C1-O1	-3.68	106.56	111.36
2	G	901	NAP	C4A-C5A-N7A	-3.67	106.38	110.58
2	J	901	NAP	C2A-N3A-C4A	3.65	120.74	111.83
2	D	901	NAP	N9A-C8A-N7A	-3.64	108.77	113.94
2	D	901	NAP	C2A-N3A-C4A	3.63	120.69	111.83
2	L	901	NAP	C4A-C5A-N7A	-3.62	106.44	110.58
2	C	901	NAP	N3A-C2A-N1A	-3.55	123.21	128.58
3	J	902	GFB	C3-C4A-C5A	3.54	115.20	109.81
2	B	901	NAP	C4A-C5A-N7A	-3.52	106.56	110.58
2	C	901	NAP	C2A-N3A-C4A	3.52	120.42	111.83
3	H	902	GFB	O5-C1-O1	-3.48	106.81	111.36
2	L	901	NAP	C2A-N3A-C4A	3.48	120.32	111.83
3	J	902	GFB	C2-N1-C6	-3.47	118.81	125.11
2	I	901	NAP	C4A-C5A-N7A	-3.47	106.62	110.58
2	A	901	NAP	C4A-C5A-N7A	-3.46	106.62	110.58
3	J	902	GFB	O5-C1-O1	-3.46	106.84	111.36
2	G	901	NAP	C2A-N3A-C4A	3.45	120.27	111.83
2	F	901	NAP	C4A-C5A-N7A	-3.45	106.64	110.58
2	C	901	NAP	C4A-C5A-N7A	-3.44	106.65	110.58
2	B	901	NAP	N9A-C8A-N7A	-3.44	109.06	113.94
2	A	901	NAP	C4A-N9A-C8A	3.43	109.34	105.74
2	G	901	NAP	N3A-C2A-N1A	-3.42	123.40	128.58
2	D	901	NAP	C5A-N7A-C8A	3.42	108.82	103.45
3	E	902	GFB	C2-N1-C6	-3.38	118.98	125.11
3	H	902	GFB	C2-N1-C6	-3.34	119.06	125.11
3	J	902	GFB	C4A-C3-C2A	3.34	116.69	110.83
2	K	901	NAP	C4A-C5A-N7A	-3.28	106.84	110.58
2	H	901	NAP	N9A-C8A-N7A	-3.22	109.36	113.94
3	C	902	GFB	C2-N1-C6	-3.22	119.27	125.11
3	A	902	GFB	C2-N1-C6	-3.22	119.27	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	GFB	C2-N1-C6	-3.20	119.31	125.11
3	D	902	GFB	C2-N1-C6	-3.20	119.31	125.11
2	E	901	NAP	C2A-N3A-C4A	3.19	119.62	111.83
3	G	902	GFB	O2X-P1-O2P	3.18	115.87	107.27
2	C	901	NAP	N9A-C8A-N7A	-3.14	109.48	113.94
3	L	902	GFB	C2-N1-C6	-3.12	119.45	125.11
2	J	901	NAP	C4A-C5A-N7A	-3.11	107.03	110.58
2	H	901	NAP	C4A-C5A-N7A	-3.10	107.04	110.58
3	E	902	GFB	C4A-C3-C2A	3.07	116.22	110.83
2	C	901	NAP	C5A-N7A-C8A	3.07	108.28	103.45
3	I	902	GFB	C2-N1-C6	-3.07	119.55	125.11
2	B	901	NAP	C5A-N7A-C8A	3.06	108.26	103.45
2	G	901	NAP	N9A-C8A-N7A	-3.03	109.64	113.94
2	J	901	NAP	N9A-C8A-N7A	-3.01	109.67	113.94
2	L	901	NAP	C5A-N7A-C8A	3.01	108.17	103.45
3	E	902	GFB	N1-C2-N3	-3.00	117.83	123.32
3	B	902	GFB	C4A-C3-C2A	3.00	116.09	110.83
3	L	902	GFB	C4A-C3-C2A	2.99	116.09	110.83
3	H	902	GFB	C4A-C3-C2A	2.97	116.05	110.83
3	F	902	GFB	C4A-C3-C2A	2.97	116.04	110.83
2	E	901	NAP	C2A-N1A-C6A	2.97	123.61	118.73
2	G	901	NAP	C5A-N7A-C8A	2.94	108.08	103.45
2	F	901	NAP	N9A-C8A-N7A	-2.93	109.78	113.94
3	C	902	GFB	C4A-C3-C2A	2.93	115.97	110.83
3	L	902	GFB	N1-C2-N3	-2.92	117.97	123.32
2	E	901	NAP	C4A-C5A-N7A	-2.91	107.26	110.58
3	A	902	GFB	C4A-C3-C2A	2.90	115.92	110.83
3	K	902	GFB	N9-C8-N7	-2.89	108.04	113.40
2	L	901	NAP	N9A-C8A-N7A	-2.89	109.84	113.94
3	E	902	GFB	N9-C8-N7	-2.88	108.06	113.40
3	I	902	GFB	C4A-C3-C2A	2.88	115.89	110.83
2	I	901	NAP	N9A-C8A-N7A	-2.88	109.86	113.94
2	F	901	NAP	C5A-N7A-C8A	2.87	107.97	103.45
2	I	901	NAP	C5A-N7A-C8A	2.87	107.95	103.45
2	E	901	NAP	N9A-C8A-N7A	-2.86	109.87	113.94
3	K	902	GFB	C2-N1-C6	-2.86	119.93	125.11
3	F	902	GFB	N9-C8-N7	-2.86	108.10	113.40
3	A	902	GFB	N1-C2-N3	-2.83	118.15	123.32
3	I	902	GFB	N1-C2-N3	-2.82	118.17	123.32
3	G	902	GFB	N9-C8-N7	-2.81	108.19	113.40
2	H	901	NAP	C5A-N7A-C8A	2.80	107.84	103.45
3	D	902	GFB	N1-C2-N3	-2.79	118.22	123.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	902	GFB	O6-C6-C5	-2.79	119.17	126.53
3	B	902	GFB	N1-C2-N3	-2.79	118.22	123.32
3	A	902	GFB	N9-C8-N7	-2.79	108.23	113.40
3	G	902	GFB	O5-C1-O1	-2.78	107.73	111.36
2	L	901	NAP	C3N-C7N-N7N	2.78	121.16	117.74
3	D	902	GFB	N9-C8-N7	-2.75	108.30	113.40
2	J	901	NAP	C5A-N7A-C8A	2.75	107.78	103.45
3	K	902	GFB	C4A-C3-C2A	2.75	115.66	110.83
3	G	902	GFB	C4A-C3-C2A	2.73	115.62	110.83
2	F	901	NAP	C6A-C5A-N7A	2.72	137.34	132.09
2	A	901	NAP	C5A-N7A-C8A	2.72	107.73	103.45
2	I	901	NAP	C3N-C7N-N7N	2.71	121.08	117.74
3	L	902	GFB	N9-C8-N7	-2.70	108.39	113.40
3	I	902	GFB	N9-C8-N7	-2.70	108.39	113.40
3	H	902	GFB	O5-C1-C2A	-2.70	104.82	110.37
3	K	902	GFB	N1-C2-N3	-2.69	118.40	123.32
3	B	902	GFB	O5-C1-O1	-2.66	107.89	111.36
3	F	902	GFB	C5-C6-N1	2.65	119.99	113.25
2	E	901	NAP	C5A-N7A-C8A	2.65	107.61	103.45
2	K	901	NAP	N9A-C8A-N7A	-2.64	110.19	113.94
2	A	901	NAP	N9A-C8A-N7A	-2.64	110.19	113.94
2	B	901	NAP	C6A-C5A-N7A	2.63	137.16	132.09
2	J	901	NAP	C3N-C7N-N7N	2.61	120.96	117.74
3	H	902	GFB	N1-C2-N3	-2.61	118.54	123.32
2	A	901	NAP	C6A-C5A-N7A	2.60	137.11	132.09
2	I	901	NAP	C6A-C5A-N7A	2.60	137.11	132.09
3	E	902	GFB	N9-C4-N3	2.60	131.15	125.95
2	C	901	NAP	C6A-C5A-N7A	2.60	137.09	132.09
2	K	901	NAP	C6A-C5A-N7A	2.59	137.09	132.09
2	K	901	NAP	C5A-N7A-C8A	2.59	107.51	103.45
3	E	902	GFB	C5-C6-N1	2.58	119.82	113.25
2	D	901	NAP	C6A-C5A-N7A	2.58	137.06	132.09
2	J	901	NAP	C6A-C5A-N7A	2.57	137.04	132.09
3	J	902	GFB	O5-C1-C2A	-2.55	105.12	110.37
3	A	902	GFB	O5-C1-O1	-2.54	108.04	111.36
2	L	901	NAP	C6A-C5A-N7A	2.54	136.99	132.09
3	E	902	GFB	N2-C2-N1	2.53	122.11	116.76
2	K	901	NAP	C3N-C7N-N7N	2.52	120.85	117.74
2	H	901	NAP	C6A-C5A-N7A	2.51	136.92	132.09
3	B	902	GFB	C5-C6-N1	2.50	119.62	113.25
3	F	902	GFB	N9-C4-N3	2.50	130.95	125.95
3	H	902	GFB	N9-C8-N7	-2.49	108.78	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	GFB	N9-C8-N7	-2.48	108.80	113.40
3	J	902	GFB	N9-C8-N7	-2.47	108.81	113.40
2	G	901	NAP	O7N-C7N-N7N	-2.47	119.04	122.62
3	J	902	GFB	N1-C2-N3	-2.47	118.80	123.32
2	F	901	NAP	C3N-C7N-N7N	2.47	120.78	117.74
3	D	902	GFB	N9-C4-N3	2.46	130.88	125.95
3	D	902	GFB	N2-C2-N1	2.46	121.94	116.76
3	L	902	GFB	N9-C4-N3	2.43	130.82	125.95
2	G	901	NAP	C6A-C5A-N7A	2.43	136.78	132.09
3	D	902	GFB	O6-C6-C5	-2.41	120.16	126.53
3	H	902	GFB	N9-C4-N3	2.41	130.78	125.95
3	D	902	GFB	O2X-P1-O2P	2.41	113.79	107.27
3	G	902	GFB	C5-C6-N1	2.40	119.37	113.25
2	B	901	NAP	C3N-C7N-N7N	2.39	120.68	117.74
3	F	902	GFB	O1-C1-C2A	2.39	112.75	108.38
3	I	902	GFB	N9-C4-N3	2.39	130.72	125.95
3	B	902	GFB	O2X-P1-O2P	2.37	113.69	107.27
2	H	901	NAP	C2A-N1A-C6A	2.36	122.61	118.73
3	G	902	GFB	O6-C6-C5	-2.36	120.29	126.53
3	K	902	GFB	N9-C4-N3	2.36	130.67	125.95
2	D	901	NAP	C2A-N1A-C6A	2.35	122.59	118.73
3	C	902	GFB	N9-C8-N7	-2.34	109.05	113.40
3	L	902	GFB	C5-C6-N1	2.34	119.20	113.25
3	F	902	GFB	O2X-P1-O2P	2.33	113.57	107.27
3	D	902	GFB	C4A-C3-C2A	2.33	114.92	110.83
3	L	902	GFB	O6-C6-C5	-2.33	120.39	126.53
2	C	901	NAP	O2A-PA-O1A	2.32	123.24	112.44
2	G	901	NAP	C3N-C7N-N7N	2.32	120.60	117.74
3	H	902	GFB	C5-C6-N1	2.29	119.07	113.25
3	J	902	GFB	N9-C4-N3	2.28	130.52	125.95
3	C	902	GFB	O6-C6-C5	-2.28	120.51	126.53
3	A	902	GFB	O5-C5A-C4A	2.28	113.66	109.55
3	G	902	GFB	N9-C4-N3	2.28	130.51	125.95
3	J	902	GFB	O6-C6-C5	-2.27	120.53	126.53
3	J	902	GFB	N2-C2-N1	2.27	121.56	116.76
3	D	902	GFB	C5-C6-N1	2.27	119.03	113.25
3	F	902	GFB	O6-C6-C5	-2.27	120.55	126.53
2	J	901	NAP	C2A-N1A-C6A	2.26	122.45	118.73
2	C	901	NAP	C3N-C7N-N7N	2.26	120.52	117.74
2	F	901	NAP	O2B-P2B-O1X	-2.25	101.30	109.33
3	J	902	GFB	O1-C1-C2A	2.24	112.48	108.38
3	A	902	GFB	N2-C2-N1	2.22	121.44	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	902	GFB	O2X-P1-O2P	2.21	113.25	107.27
2	F	901	NAP	O4B-C1B-N9A	2.21	112.34	108.09
3	J	902	GFB	C5-C6-N1	2.20	118.86	113.25
3	C	902	GFB	N2-C2-N1	2.20	121.41	116.76
3	G	902	GFB	O5-C1-C2A	-2.20	105.85	110.37
3	I	902	GFB	C5-C6-N1	2.20	118.84	113.25
3	L	902	GFB	N2-C2-N1	2.19	121.39	116.76
3	K	902	GFB	N2-C2-N1	2.19	121.38	116.76
3	C	902	GFB	N9-C4-N3	2.18	130.32	125.95
3	F	902	GFB	N1-C2-N3	-2.18	119.34	123.32
2	L	901	NAP	C2A-N1A-C6A	2.17	122.30	118.73
3	G	902	GFB	N1-C2-N3	-2.17	119.36	123.32
3	A	902	GFB	O6-C6-C5	-2.16	120.84	126.53
3	G	902	GFB	C1-O5-C5A	-2.16	109.96	113.63
2	H	901	NAP	C2B-C1B-N9A	-2.15	110.21	113.75
3	A	902	GFB	C8-N7-C5	2.15	108.08	104.26
3	A	902	GFB	C5-C6-N1	2.14	118.71	113.25
3	F	902	GFB	C8-N7-C5	2.14	108.08	104.26
2	F	901	NAP	O7N-C7N-N7N	-2.14	119.53	122.62
3	C	902	GFB	N1-C2-N3	-2.13	119.42	123.32
2	C	901	NAP	C5N-C4N-C3N	-2.12	118.28	120.36
3	A	902	GFB	N9-C4-N3	2.11	130.18	125.95
3	K	902	GFB	C8-N7-C5	2.11	108.01	104.26
2	D	901	NAP	C2B-C1B-N9A	-2.10	110.30	113.75
2	E	901	NAP	C6A-C5A-N7A	2.09	136.11	132.09
3	I	902	GFB	N2-C2-N1	2.08	121.16	116.76
3	D	902	GFB	C8-N7-C5	2.08	107.97	104.26
3	K	902	GFB	C5-C6-N1	2.08	118.54	113.25
3	B	902	GFB	N2-C2-N1	2.07	121.14	116.76
3	H	902	GFB	C4-C5-N7	-2.07	107.39	110.67
3	K	902	GFB	O6-C6-C5	-2.06	121.09	126.53
2	C	901	NAP	O7N-C7N-C3N	-2.05	117.09	119.60
3	G	902	GFB	N2-C2-N1	2.05	121.08	116.76
3	E	902	GFB	C8-N7-C5	2.03	107.87	104.26
2	C	901	NAP	P2B-O2B-C2B	-2.02	118.03	123.43
3	B	902	GFB	O5-C1-C2A	-2.02	106.22	110.37
2	F	901	NAP	C2A-N1A-C6A	2.02	122.04	118.73

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAP	C5D-O5D-PN-O3
2	A	901	NAP	C5D-O5D-PN-O1N
2	A	901	NAP	C5D-O5D-PN-O2N
2	A	901	NAP	O4D-C1D-N1N-C2N
2	B	901	NAP	C5D-O5D-PN-O3
2	B	901	NAP	C5D-O5D-PN-O2N
2	B	901	NAP	O4D-C1D-N1N-C2N
2	C	901	NAP	C5D-O5D-PN-O3
2	C	901	NAP	C5D-O5D-PN-O1N
2	C	901	NAP	C5D-O5D-PN-O2N
2	C	901	NAP	O4D-C1D-N1N-C2N
2	D	901	NAP	C5D-O5D-PN-O3
2	D	901	NAP	C5D-O5D-PN-O2N
2	D	901	NAP	O4D-C1D-N1N-C2N
2	E	901	NAP	C5D-O5D-PN-O3
2	E	901	NAP	C5D-O5D-PN-O1N
2	E	901	NAP	C5D-O5D-PN-O2N
2	E	901	NAP	O4D-C1D-N1N-C2N
2	F	901	NAP	C5D-O5D-PN-O3
2	F	901	NAP	C5D-O5D-PN-O1N
2	F	901	NAP	C5D-O5D-PN-O2N
2	F	901	NAP	O4D-C1D-N1N-C2N
2	G	901	NAP	C5D-O5D-PN-O3
2	G	901	NAP	C5D-O5D-PN-O1N
2	G	901	NAP	C5D-O5D-PN-O2N
2	G	901	NAP	O4D-C1D-N1N-C2N
2	H	901	NAP	C5D-O5D-PN-O3
2	H	901	NAP	C5D-O5D-PN-O1N
2	H	901	NAP	C5D-O5D-PN-O2N
2	H	901	NAP	O4D-C1D-N1N-C2N
2	I	901	NAP	C5D-O5D-PN-O3
2	I	901	NAP	C5D-O5D-PN-O2N
2	I	901	NAP	O4D-C1D-N1N-C2N
2	J	901	NAP	C5D-O5D-PN-O3
2	J	901	NAP	C5D-O5D-PN-O1N
2	J	901	NAP	C5D-O5D-PN-O2N
2	J	901	NAP	O4D-C1D-N1N-C2N
2	K	901	NAP	C5D-O5D-PN-O3
2	K	901	NAP	C5D-O5D-PN-O1N
2	K	901	NAP	C5D-O5D-PN-O2N
2	K	901	NAP	O4D-C1D-N1N-C2N
2	L	901	NAP	C5D-O5D-PN-O3
2	L	901	NAP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	901	NAP	C5D-O5D-PN-O2N
2	L	901	NAP	O4D-C1D-N1N-C2N
3	A	902	GFB	C5'-O5'-P-O3P
3	A	902	GFB	C1-O1-P1-O2P
3	B	902	GFB	P1-O2P-P-O5'
3	B	902	GFB	C5'-O5'-P-O3P
3	B	902	GFB	C5'-O5'-P-O2P
3	B	902	GFB	C1-O1-P1-O2P
3	C	902	GFB	P1-O2P-P-O5'
3	C	902	GFB	C5'-O5'-P-O3P
3	C	902	GFB	C5'-O5'-P-O2P
3	C	902	GFB	C1-O1-P1-O2P
3	D	902	GFB	P1-O2P-P-O5'
3	D	902	GFB	C5'-O5'-P-O3P
3	D	902	GFB	C5'-O5'-P-O2P
3	D	902	GFB	C1-O1-P1-O2P
3	E	902	GFB	P1-O2P-P-O5'
3	E	902	GFB	C5'-O5'-P-O3P
3	E	902	GFB	C1-O1-P1-O2P
3	F	902	GFB	C5'-O5'-P-O3P
3	F	902	GFB	C1-O1-P1-O2P
3	G	902	GFB	P1-O2P-P-O5'
3	G	902	GFB	C5'-O5'-P-O3P
3	G	902	GFB	C5'-O5'-P-O2P
3	G	902	GFB	C1-O1-P1-O2P
3	H	902	GFB	C5'-O5'-P-O3P
3	H	902	GFB	C5'-O5'-P-O2P
3	H	902	GFB	C1-O1-P1-O2P
3	I	902	GFB	P1-O2P-P-O5'
3	I	902	GFB	C5'-O5'-P-O3P
3	I	902	GFB	C5'-O5'-P-O2P
3	I	902	GFB	C1-O1-P1-O2P
3	J	902	GFB	P1-O2P-P-O5'
3	J	902	GFB	C5'-O5'-P-O3P
3	J	902	GFB	C5'-O5'-P-O2P
3	J	902	GFB	C1-O1-P1-O2P
3	K	902	GFB	P1-O2P-P-O5'
3	K	902	GFB	C5'-O5'-P-O3P
3	K	902	GFB	C5'-O5'-P-O2P
3	K	902	GFB	C1-O1-P1-O2P
3	L	902	GFB	P1-O2P-P-O5'
3	L	902	GFB	C5'-O5'-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L	902	GFB	C5'-O5'-P-O2P
3	L	902	GFB	C1-O1-P1-O2P
3	A	902	GFB	C2A-C1-O1-P1
3	B	902	GFB	C2A-C1-O1-P1
3	D	902	GFB	C2A-C1-O1-P1
3	E	902	GFB	C2A-C1-O1-P1
3	G	902	GFB	C2A-C1-O1-P1
3	H	902	GFB	C2A-C1-O1-P1
3	I	902	GFB	C2A-C1-O1-P1
3	L	902	GFB	C2A-C1-O1-P1
4	F	1321	EDO	O1-C1-C2-O2
3	C	902	GFB	C2A-C1-O1-P1
3	F	902	GFB	C2A-C1-O1-P1
3	J	902	GFB	C2A-C1-O1-P1
3	K	902	GFB	C2A-C1-O1-P1
3	A	902	GFB	P1-O2P-P-O5'
3	F	902	GFB	P1-O2P-P-O5'
3	H	902	GFB	P1-O2P-P-O5'
3	C	902	GFB	C3'-C4'-C5'-O5'
2	B	901	NAP	C5D-O5D-PN-O1N
2	D	901	NAP	C5D-O5D-PN-O1N
2	I	901	NAP	C5D-O5D-PN-O1N
3	A	902	GFB	C5'-O5'-P-O1P
3	A	902	GFB	C5'-O5'-P-O2P
3	B	902	GFB	C5'-O5'-P-O1P
3	C	902	GFB	C5'-O5'-P-O1P
3	D	902	GFB	C5'-O5'-P-O1P
3	E	902	GFB	C5'-O5'-P-O1P
3	E	902	GFB	C5'-O5'-P-O2P
3	F	902	GFB	C5'-O5'-P-O1P
3	F	902	GFB	C5'-O5'-P-O2P
3	G	902	GFB	C5'-O5'-P-O1P
3	H	902	GFB	C5'-O5'-P-O1P
3	I	902	GFB	C5'-O5'-P-O1P
3	J	902	GFB	C5'-O5'-P-O1P
3	K	902	GFB	C5'-O5'-P-O1P
3	L	902	GFB	C5'-O5'-P-O1P
2	A	901	NAP	O4D-C1D-N1N-C6N
2	B	901	NAP	O4D-C1D-N1N-C6N
2	C	901	NAP	O4D-C1D-N1N-C6N
2	D	901	NAP	O4D-C1D-N1N-C6N
2	E	901	NAP	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	901	NAP	O4D-C1D-N1N-C6N
2	G	901	NAP	O4D-C1D-N1N-C6N
2	H	901	NAP	O4D-C1D-N1N-C6N
2	I	901	NAP	O4D-C1D-N1N-C6N
2	J	901	NAP	O4D-C1D-N1N-C6N
2	K	901	NAP	O4D-C1D-N1N-C6N
2	L	901	NAP	O4D-C1D-N1N-C6N
2	A	901	NAP	C2B-O2B-P2B-O1X
2	B	901	NAP	C2B-O2B-P2B-O1X
2	C	901	NAP	C2B-O2B-P2B-O1X
2	D	901	NAP	C2B-O2B-P2B-O1X
2	E	901	NAP	C2B-O2B-P2B-O1X
2	F	901	NAP	C2B-O2B-P2B-O1X
2	G	901	NAP	C2B-O2B-P2B-O1X
2	I	901	NAP	C2B-O2B-P2B-O1X
2	J	901	NAP	C2B-O2B-P2B-O1X
2	K	901	NAP	C2B-O2B-P2B-O1X
3	I	902	GFB	C3'-C4'-C5'-O5'
3	A	902	GFB	C1-O1-P1-O1X
3	B	902	GFB	C1-O1-P1-O1X
3	G	902	GFB	C1-O1-P1-O1X
3	G	902	GFB	C1-O1-P1-O2X
3	H	902	GFB	C1-O1-P1-O1X
2	J	901	NAP	O4B-C4B-C5B-O5B
3	H	902	GFB	C3'-C4'-C5'-O5'
3	J	902	GFB	C3'-C4'-C5'-O5'
3	E	902	GFB	P1-O2P-P-O3P
3	F	902	GFB	P1-O2P-P-O3P
3	H	902	GFB	P1-O2P-P-O3P
3	J	902	GFB	P1-O2P-P-O3P
3	K	902	GFB	P1-O2P-P-O3P
2	D	901	NAP	O4B-C4B-C5B-O5B
2	E	901	NAP	O4B-C4B-C5B-O5B
2	G	901	NAP	O4B-C4B-C5B-O5B
2	H	901	NAP	O4B-C4B-C5B-O5B
2	I	901	NAP	O4B-C4B-C5B-O5B
2	K	901	NAP	O4B-C4B-C5B-O5B
2	L	901	NAP	O4B-C4B-C5B-O5B
3	A	902	GFB	C3'-C4'-C5'-O5'
2	C	901	NAP	C2B-O2B-P2B-O2X
2	K	901	NAP	C2B-O2B-P2B-O2X
3	F	902	GFB	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	901	NAP	C2B-O2B-P2B-O1X
2	L	901	NAP	C2B-O2B-P2B-O1X
3	A	902	GFB	P1-O2P-P-O3P
2	A	901	NAP	O4B-C4B-C5B-O5B
2	F	901	NAP	O4B-C4B-C5B-O5B
3	D	902	GFB	C3'-C4'-C5'-O5'

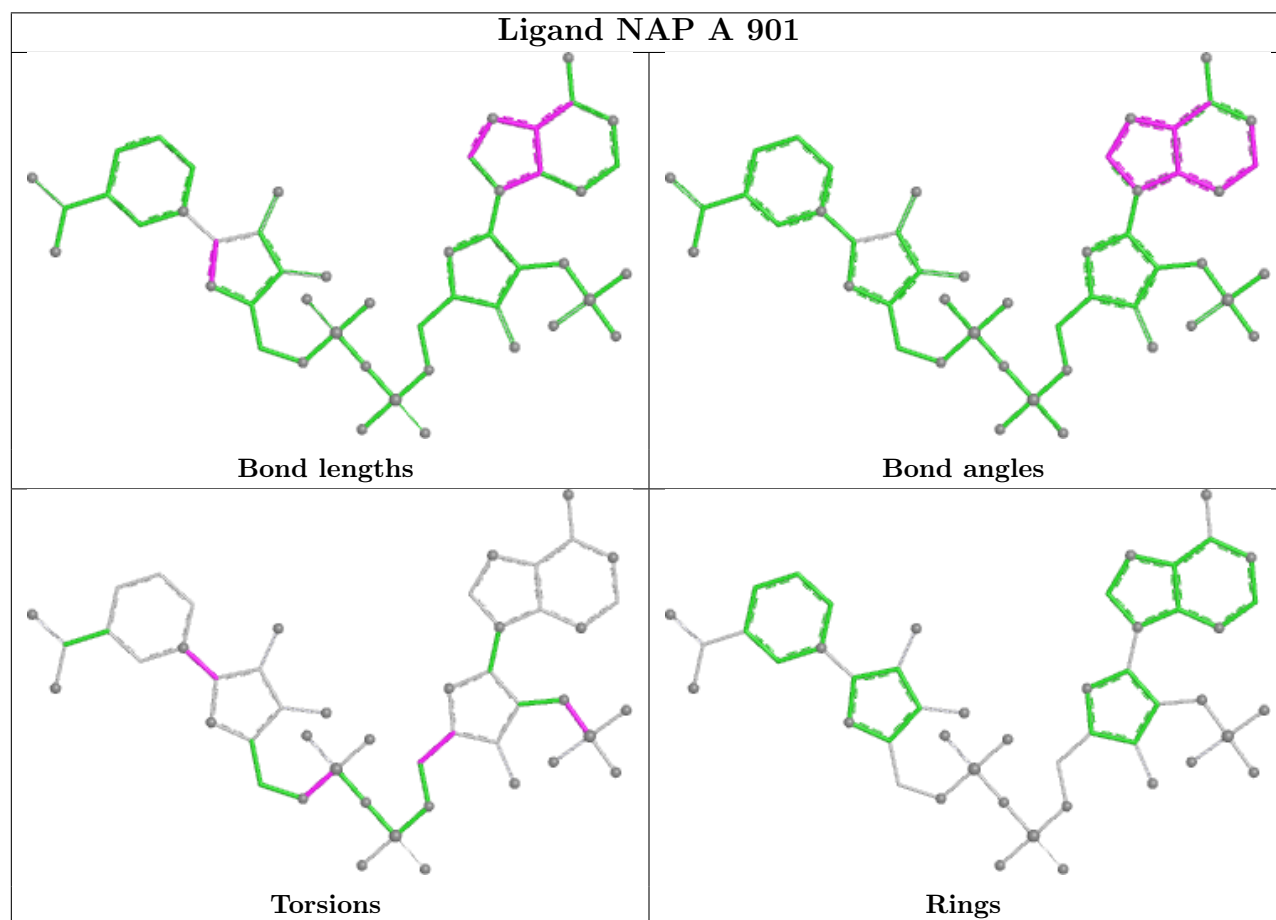
There are no ring outliers.

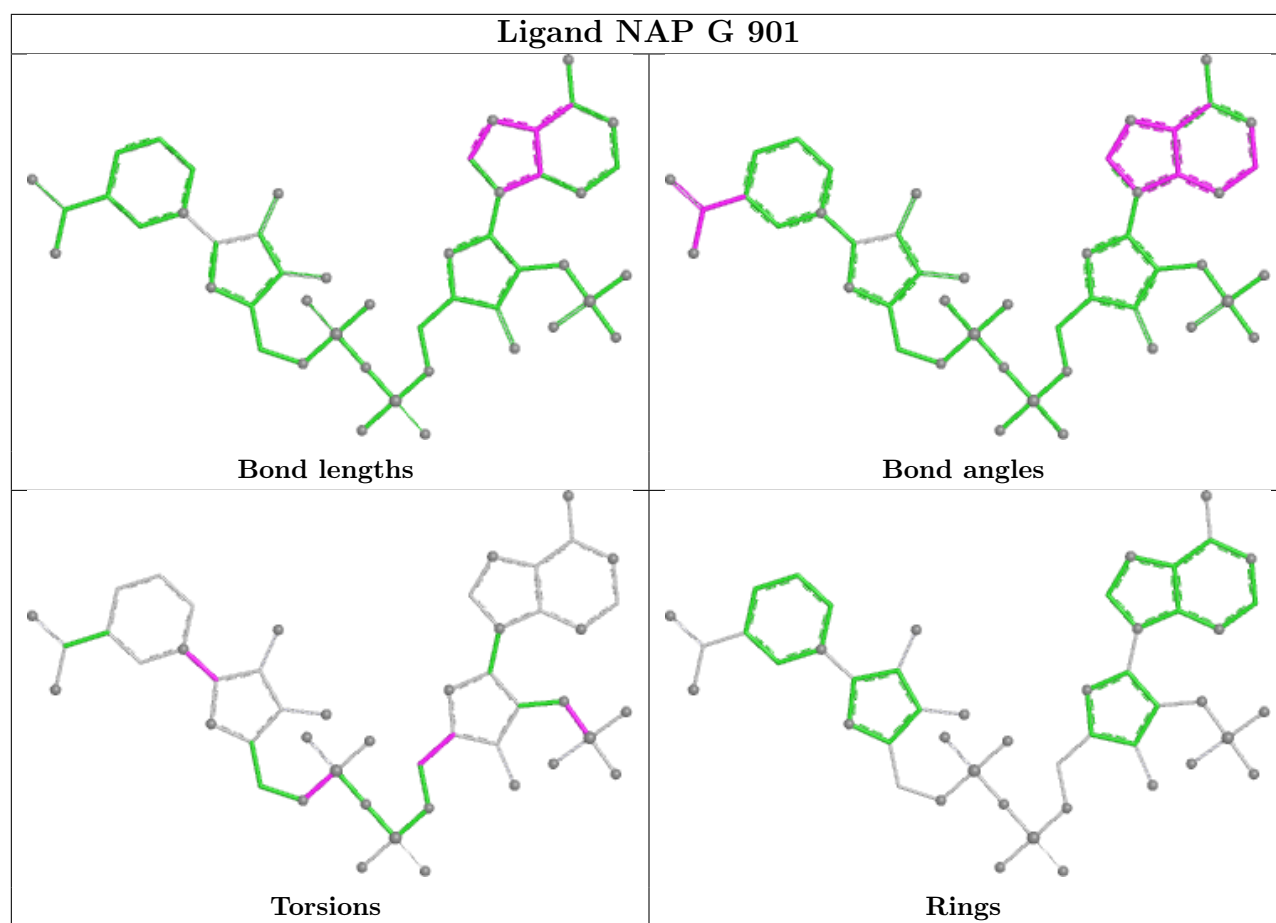
20 monomers are involved in 64 short contacts:

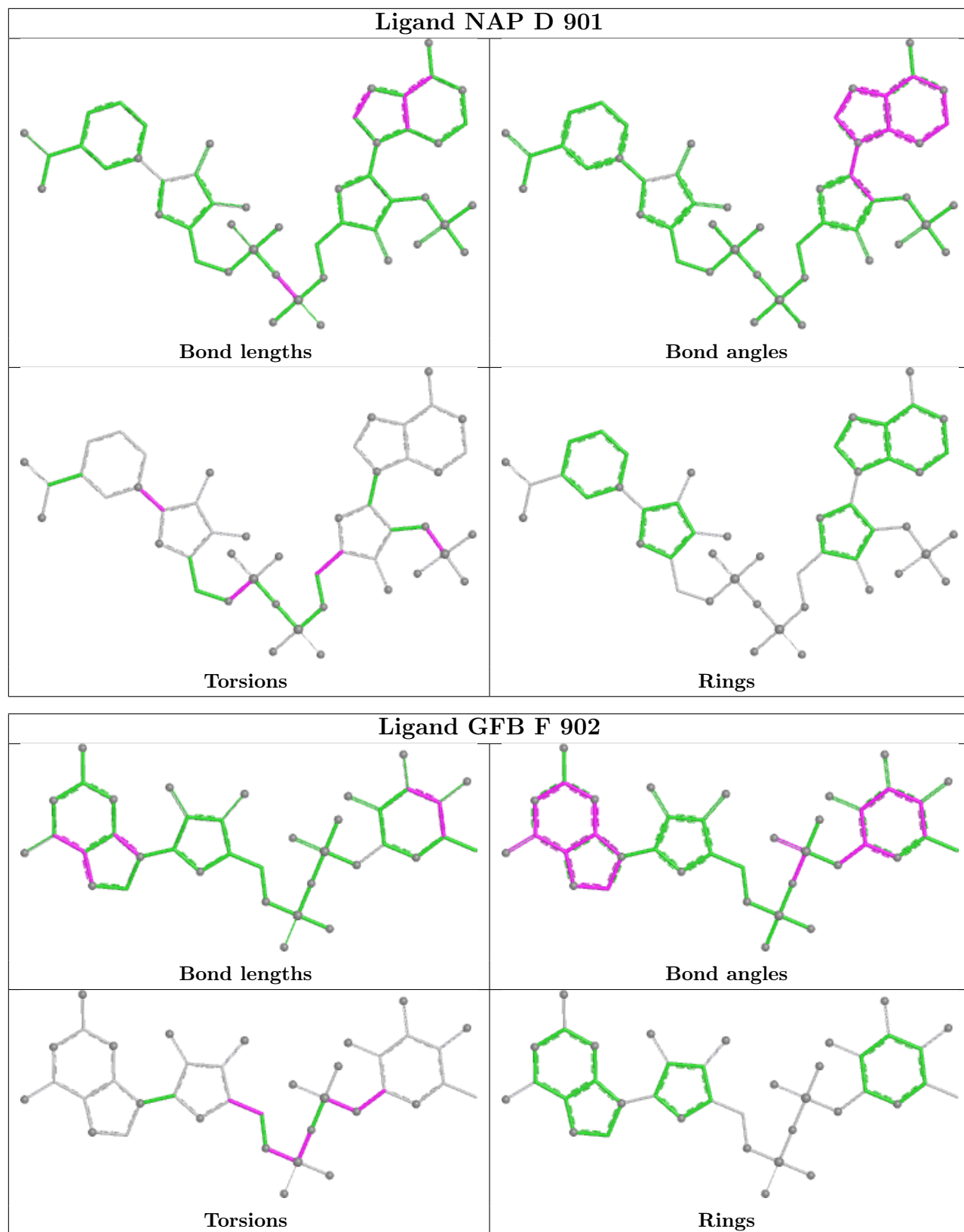
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	901	NAP	1	0
2	D	901	NAP	1	0
3	F	902	GFB	4	0
3	D	902	GFB	5	0
3	C	902	GFB	4	0
2	F	901	NAP	2	0
3	A	902	GFB	3	0
2	E	901	NAP	1	0
2	I	901	NAP	2	0
3	E	902	GFB	5	0
2	K	901	NAP	3	0
3	H	902	GFB	3	0
3	L	902	GFB	5	0
2	J	901	NAP	2	0
3	B	902	GFB	4	0
3	I	902	GFB	3	0
3	G	902	GFB	8	0
3	J	902	GFB	3	0
2	B	901	NAP	1	0
3	K	902	GFB	4	0

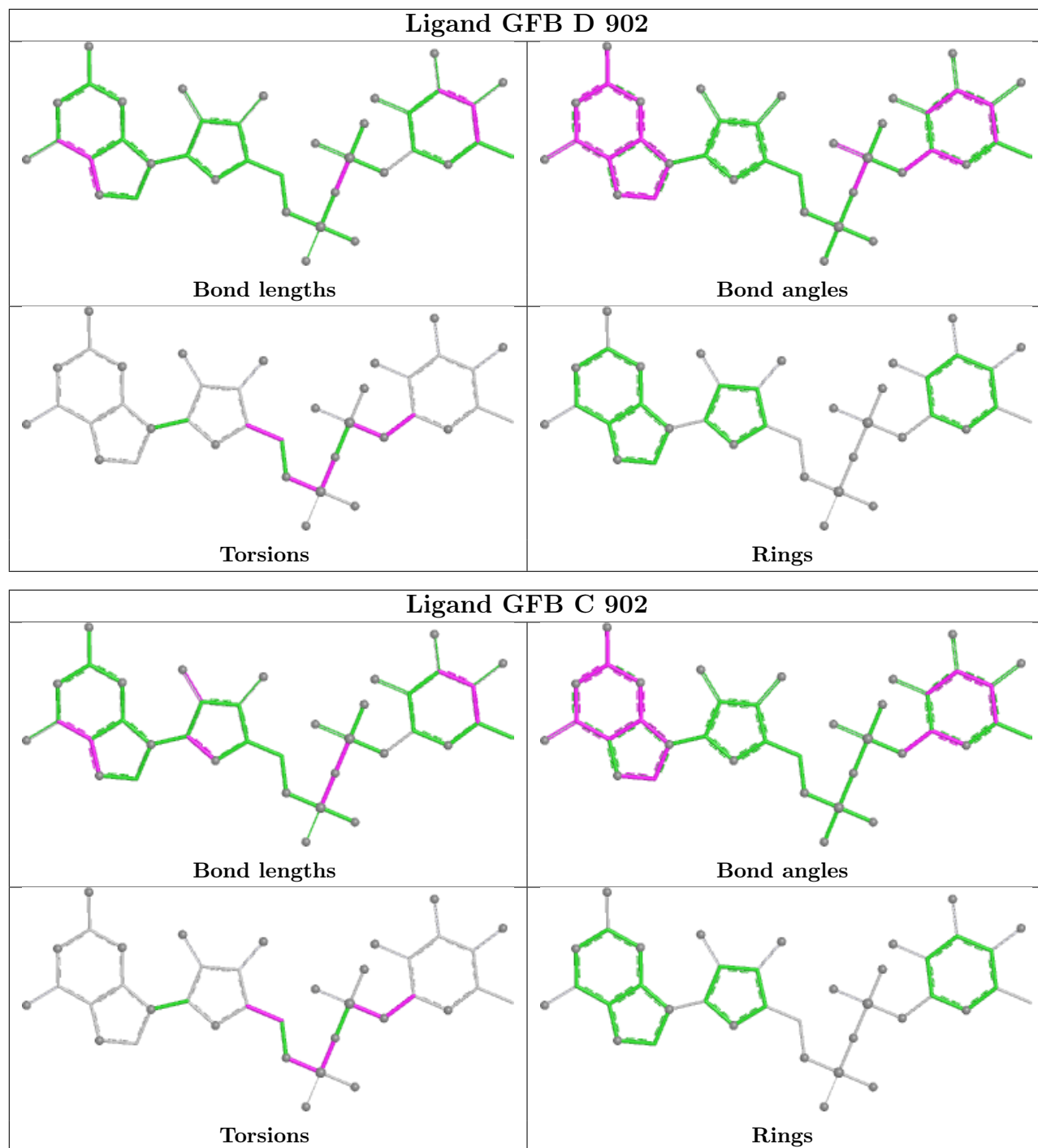
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

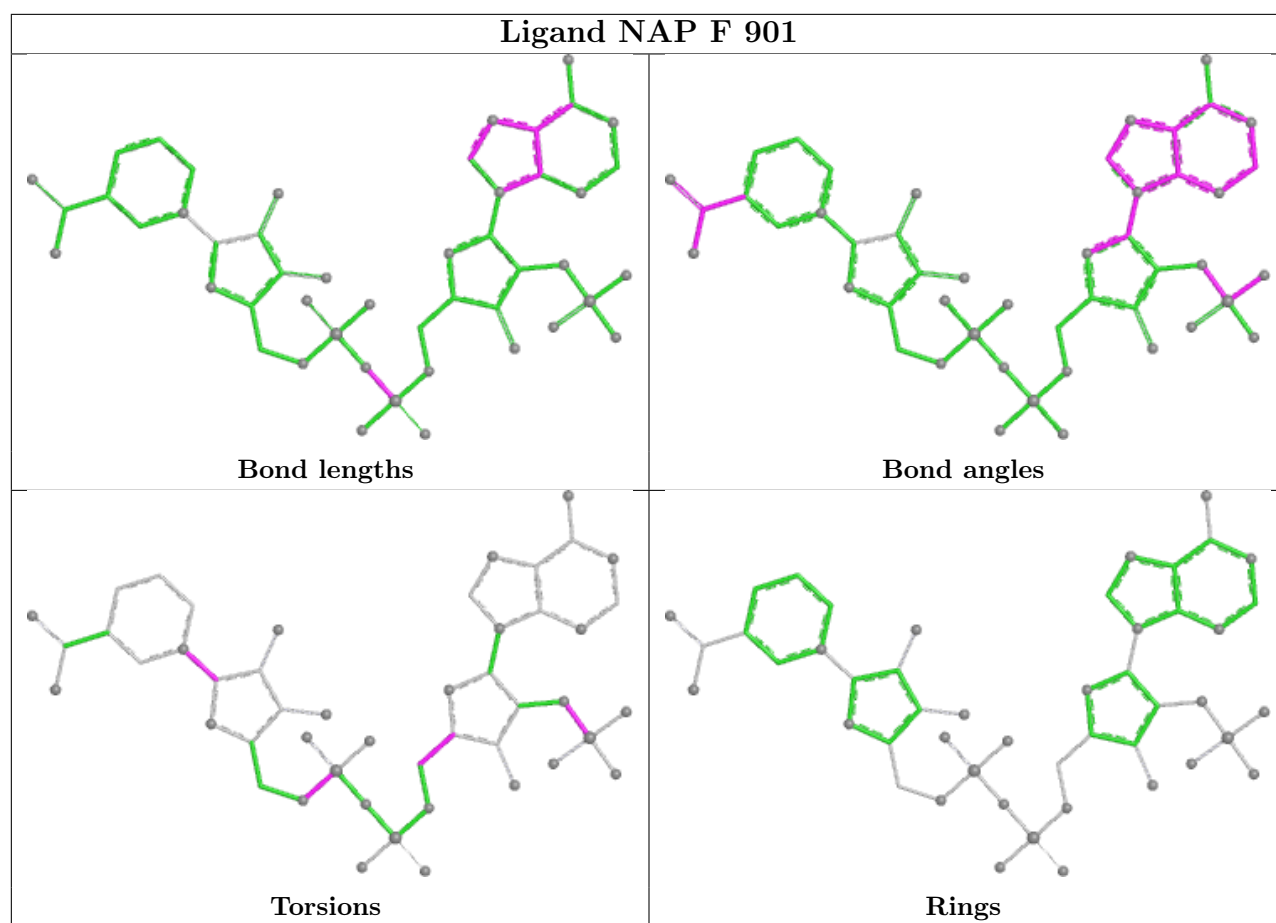
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



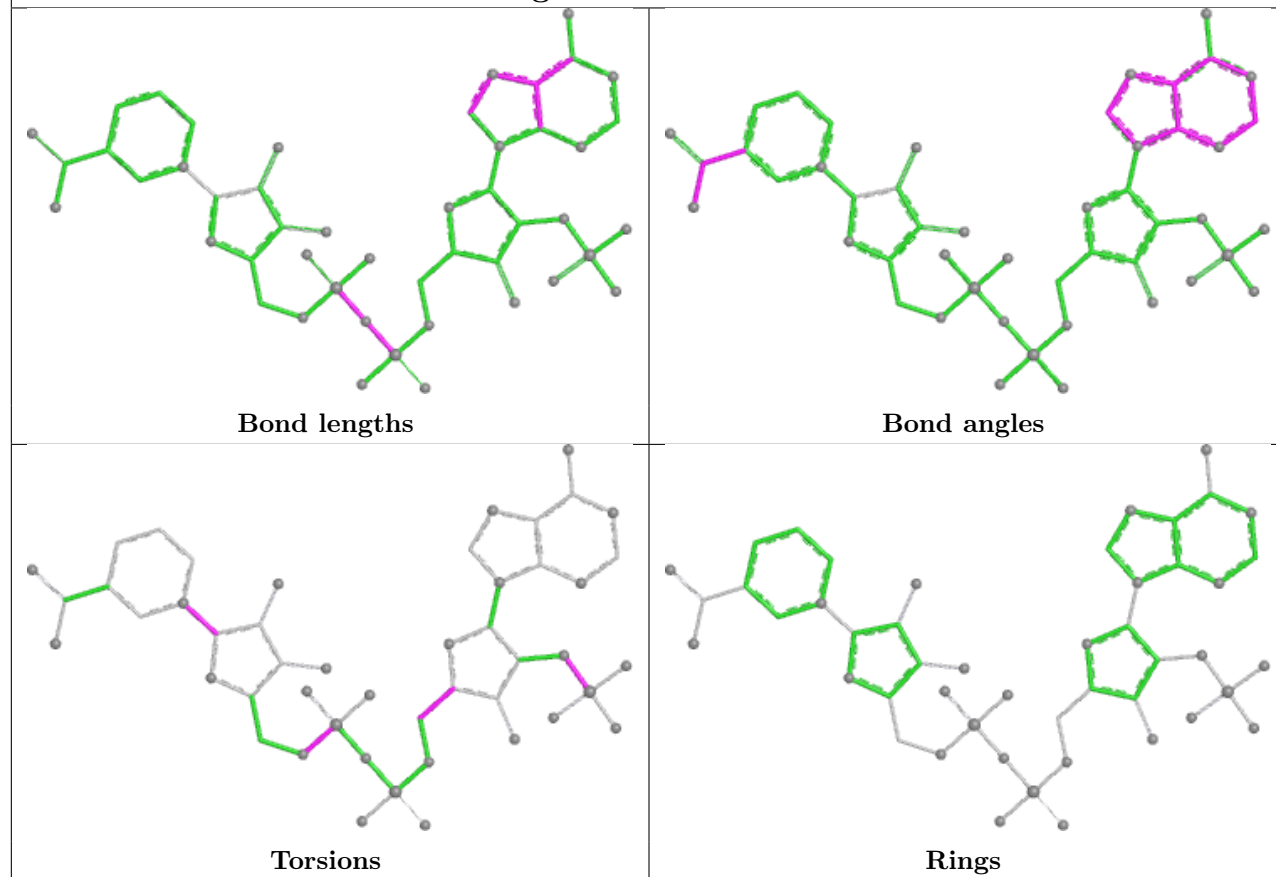




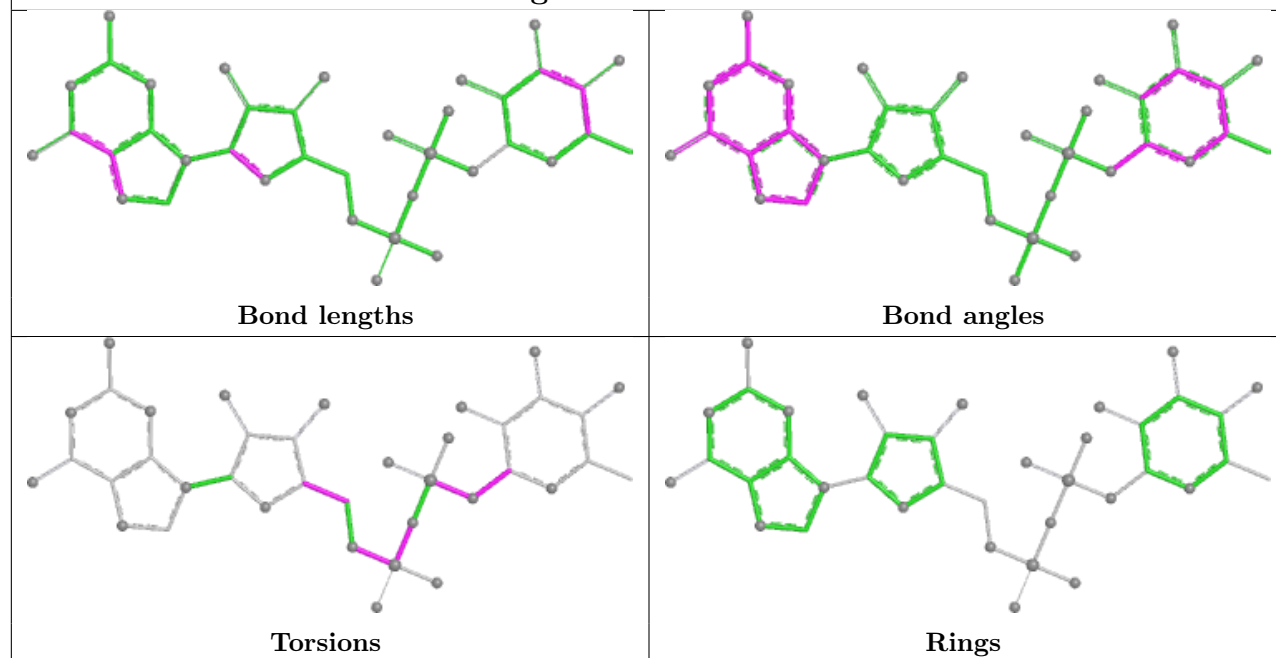


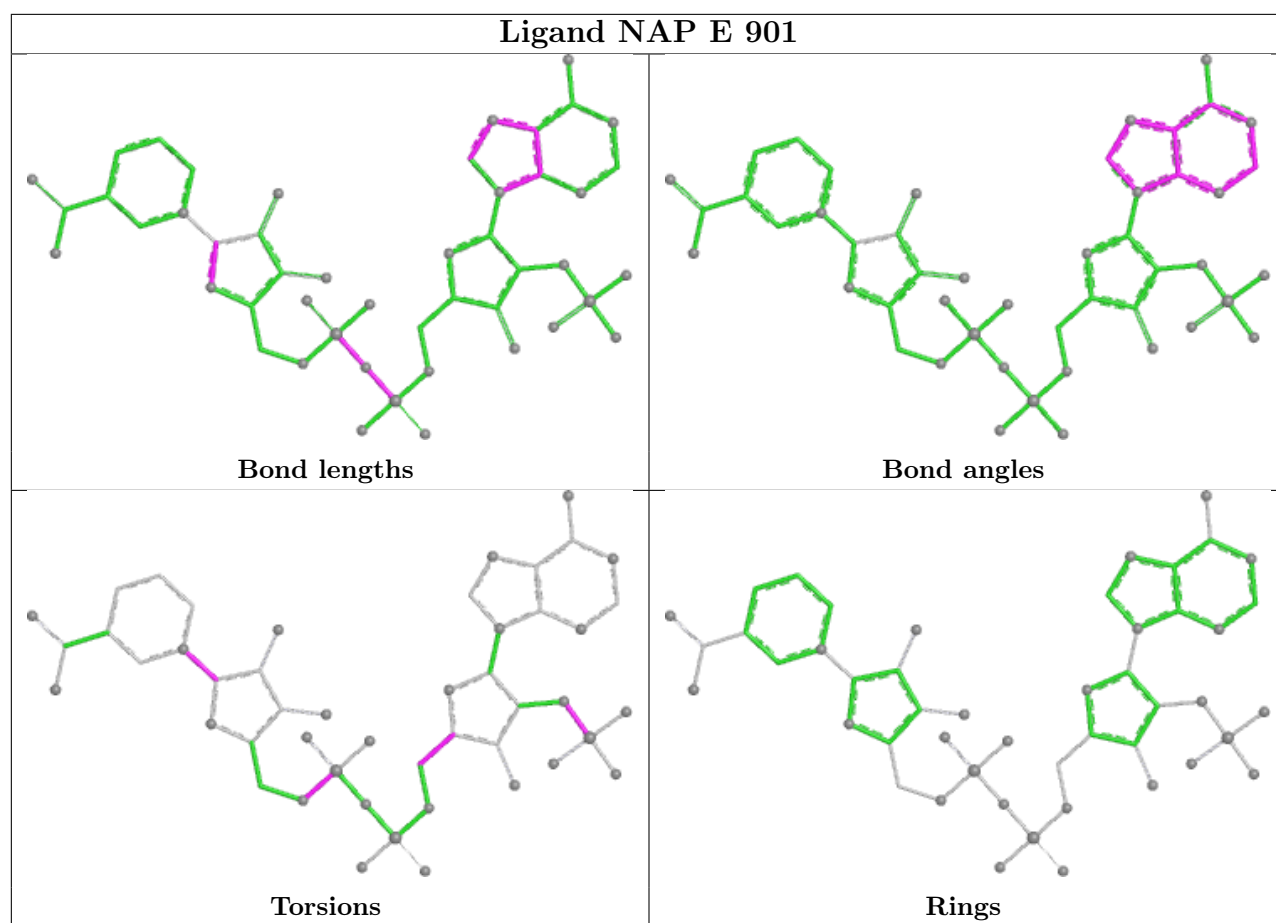


Ligand NAP L 901

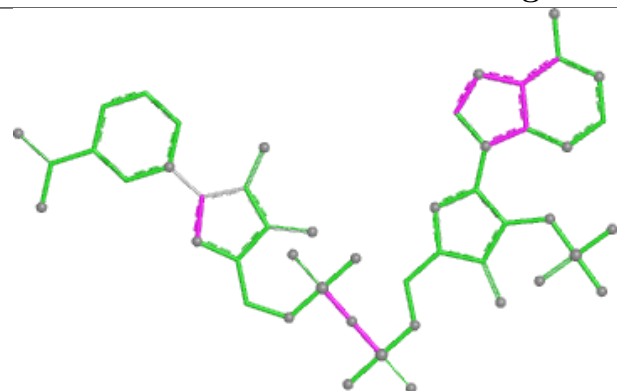


Ligand GFB A 902

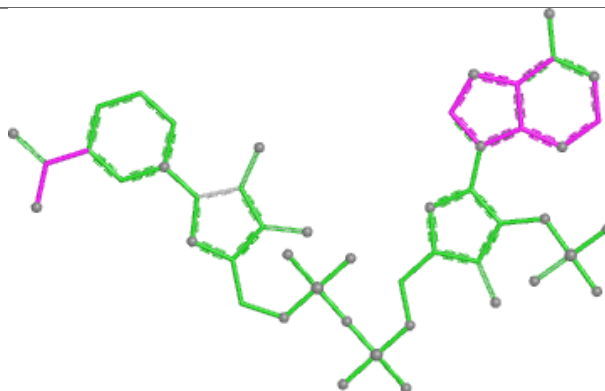




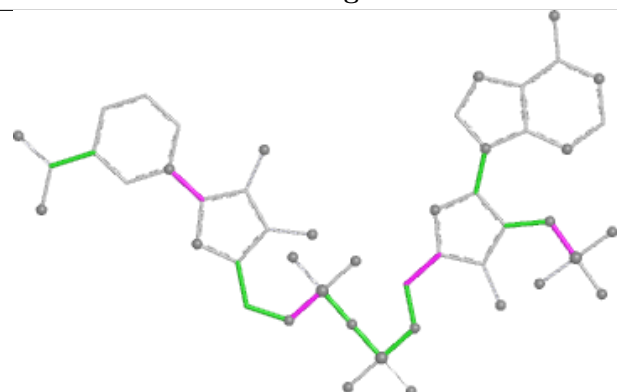
Ligand NAP I 901



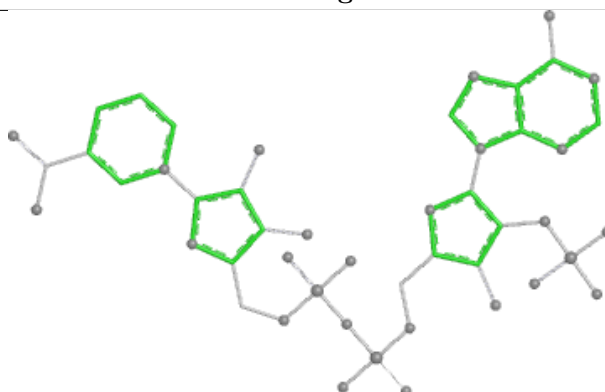
Bond lengths



Bond angles

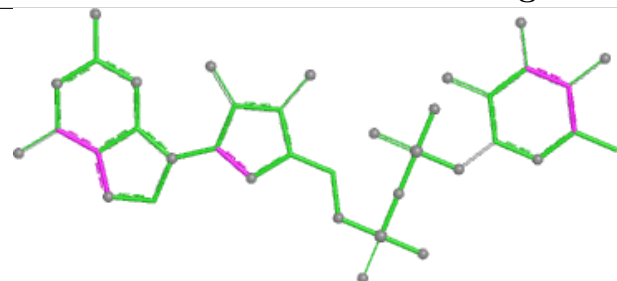


Torsions

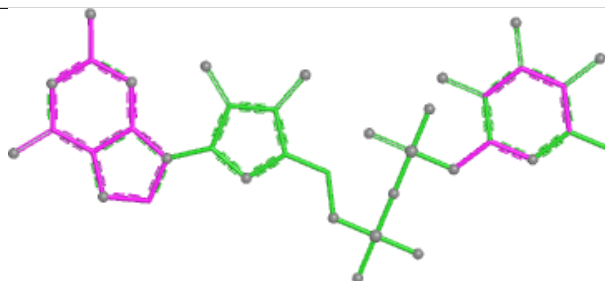


Rings

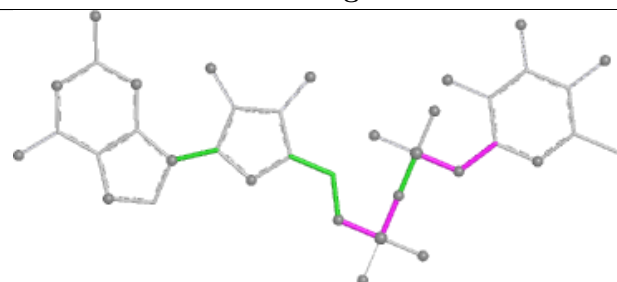
Ligand GFB E 902



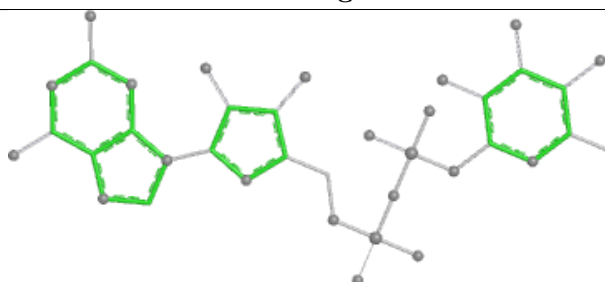
Bond lengths



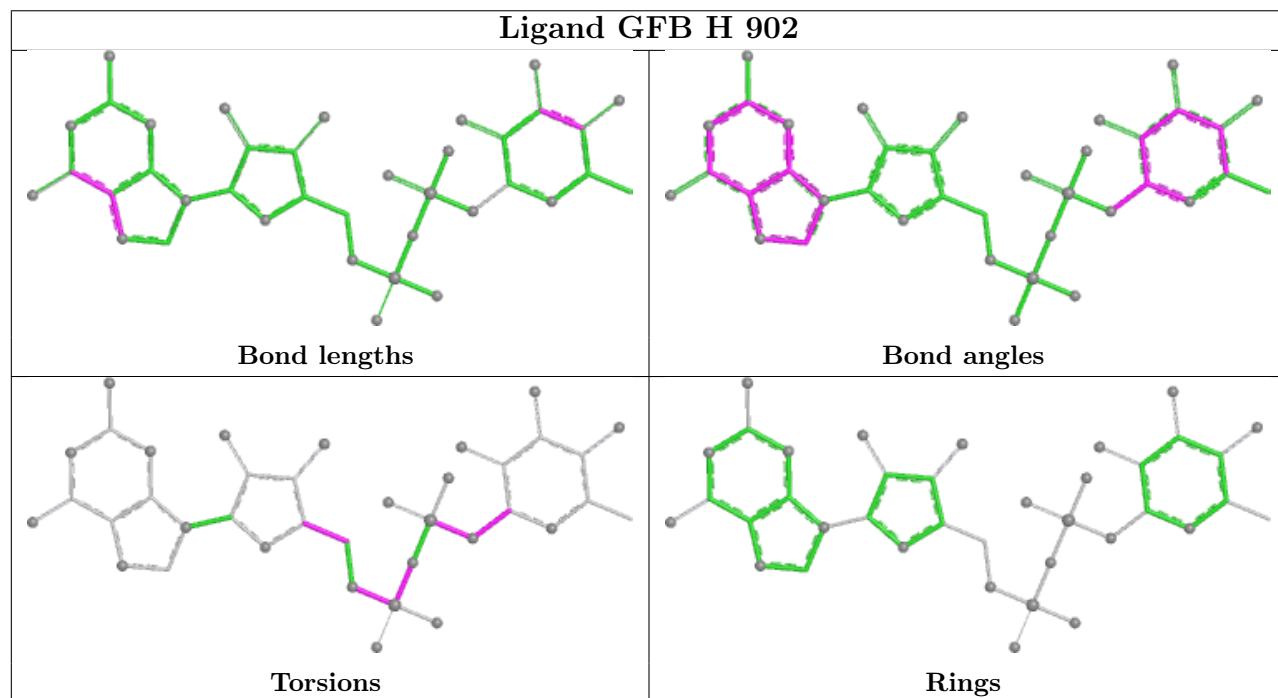
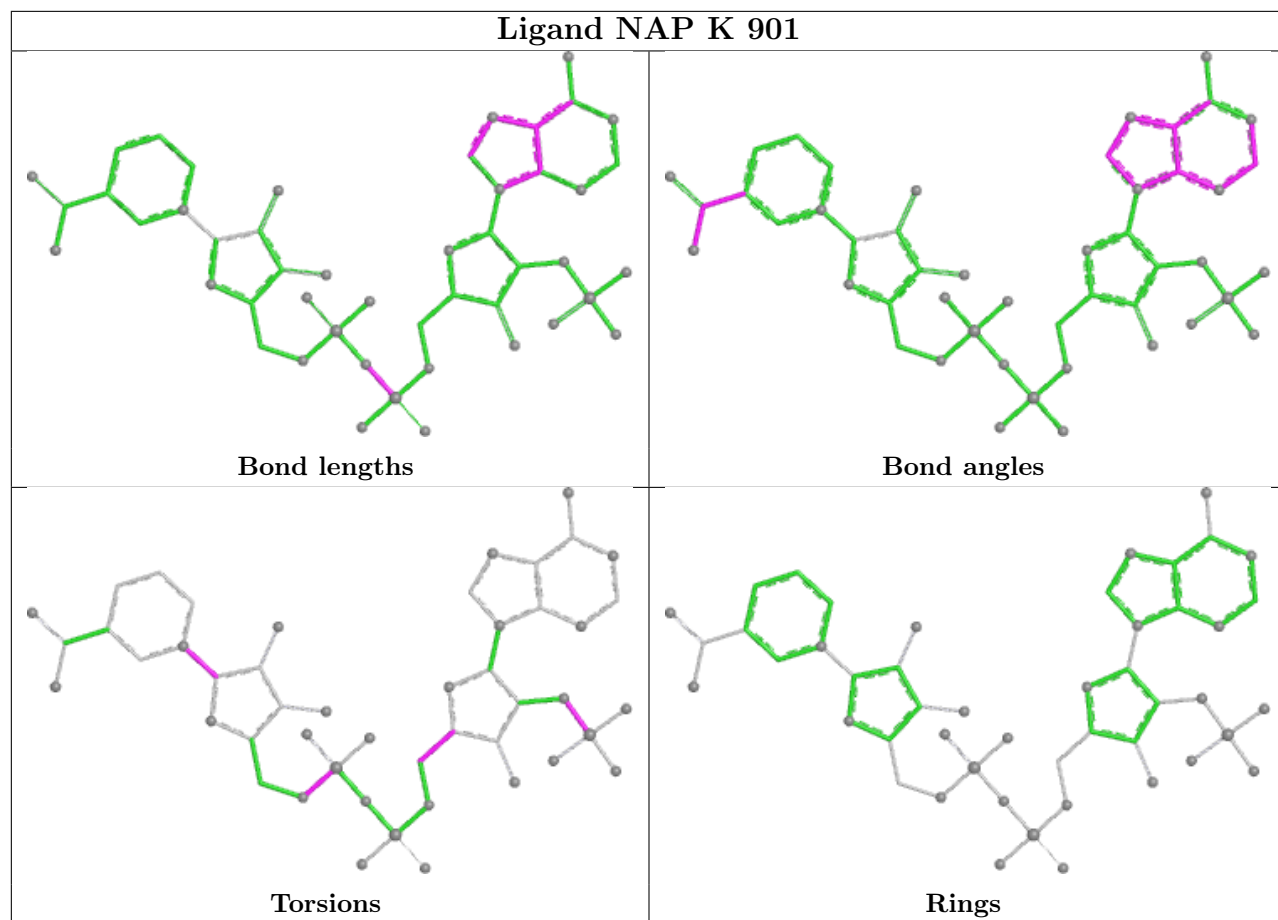
Bond angles



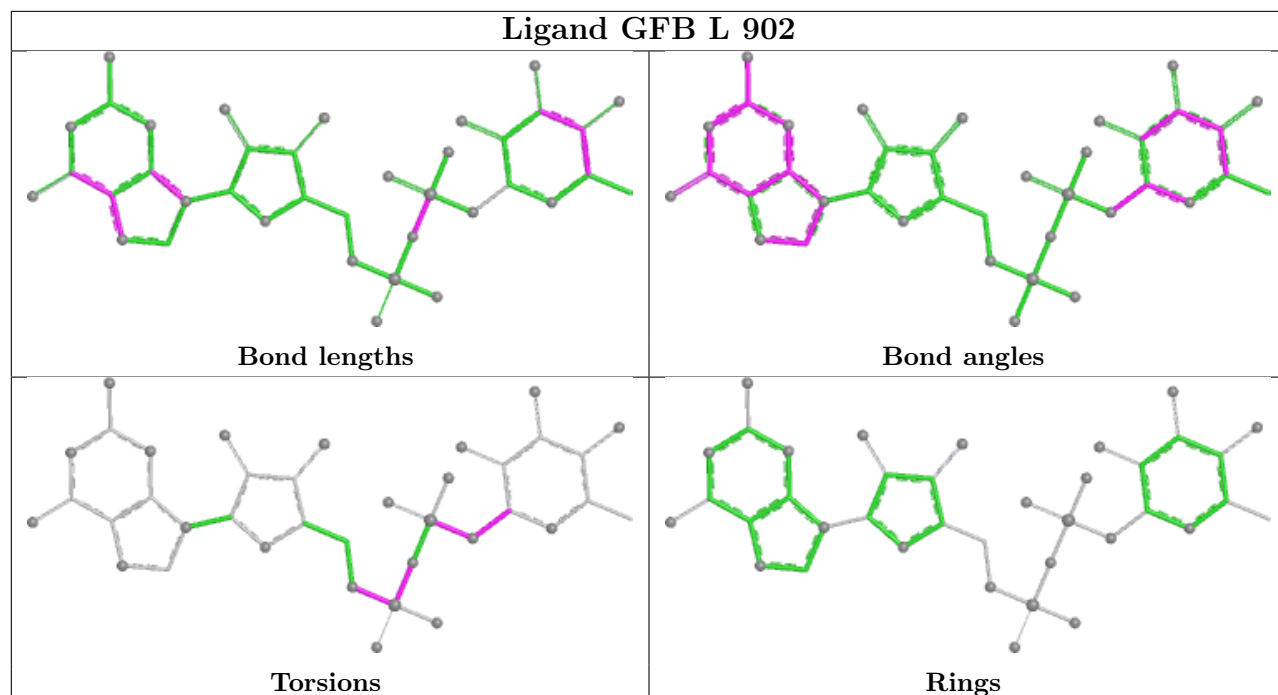
Torsions



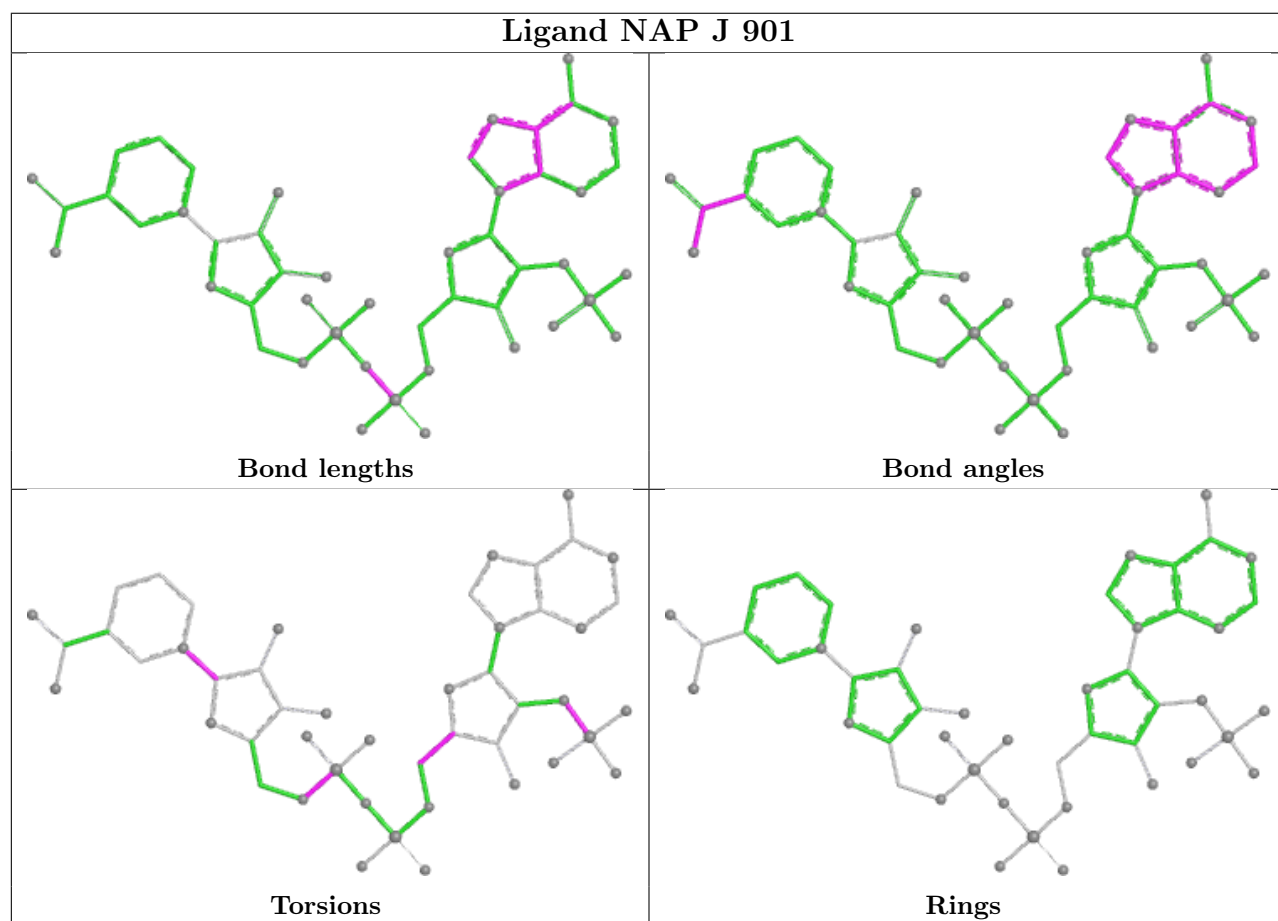
Rings

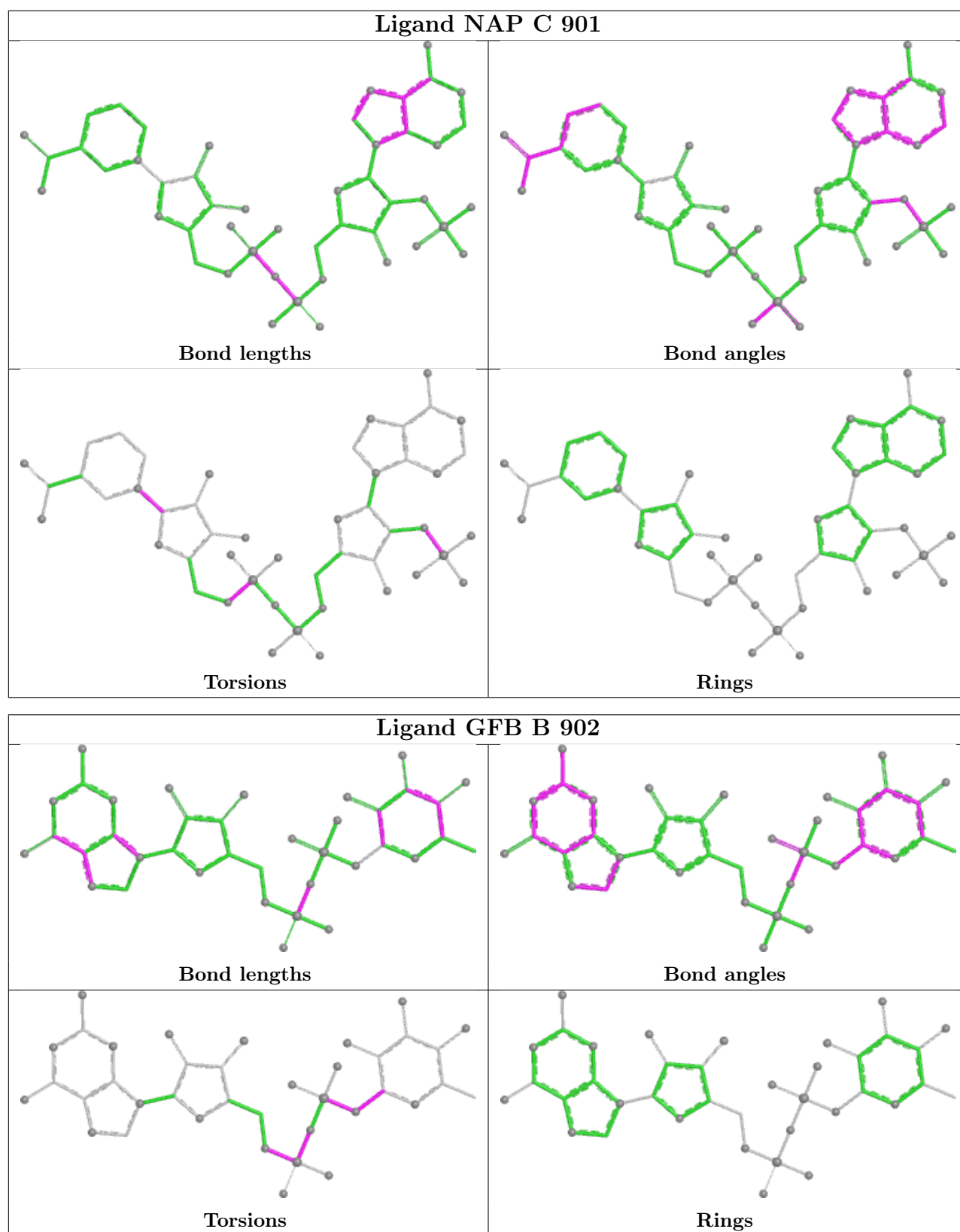


Ligand GFB L 902

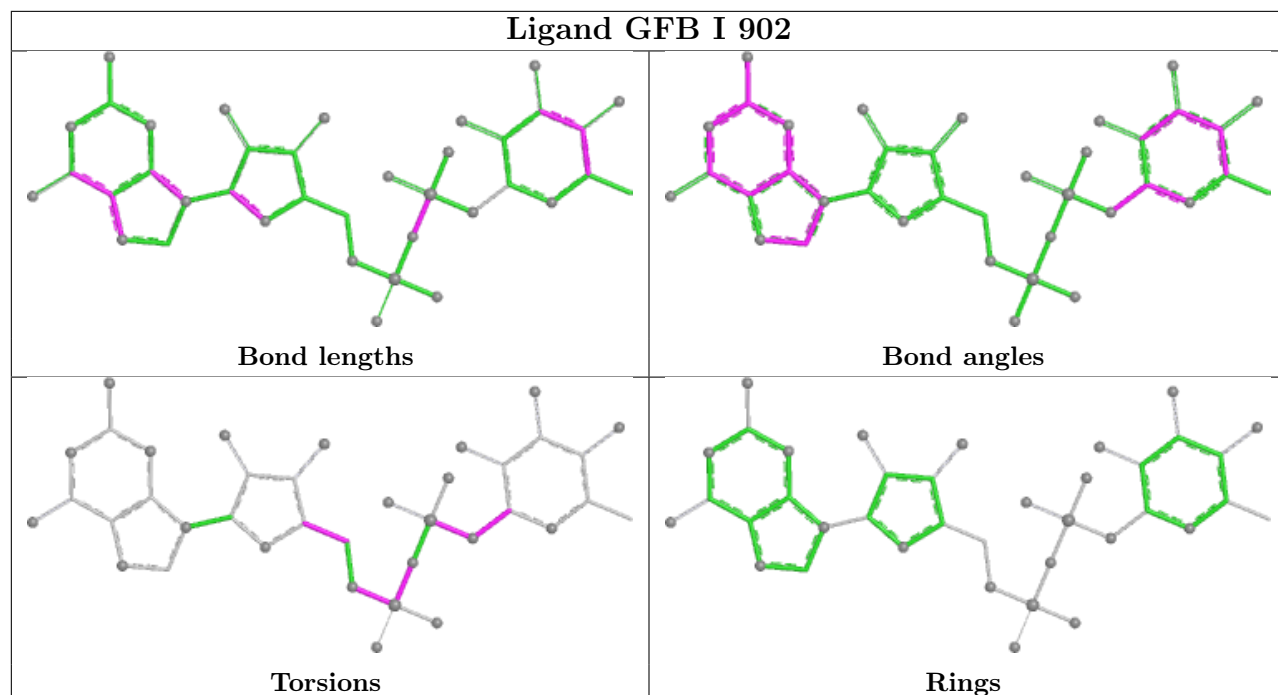


Ligand NAP J 901

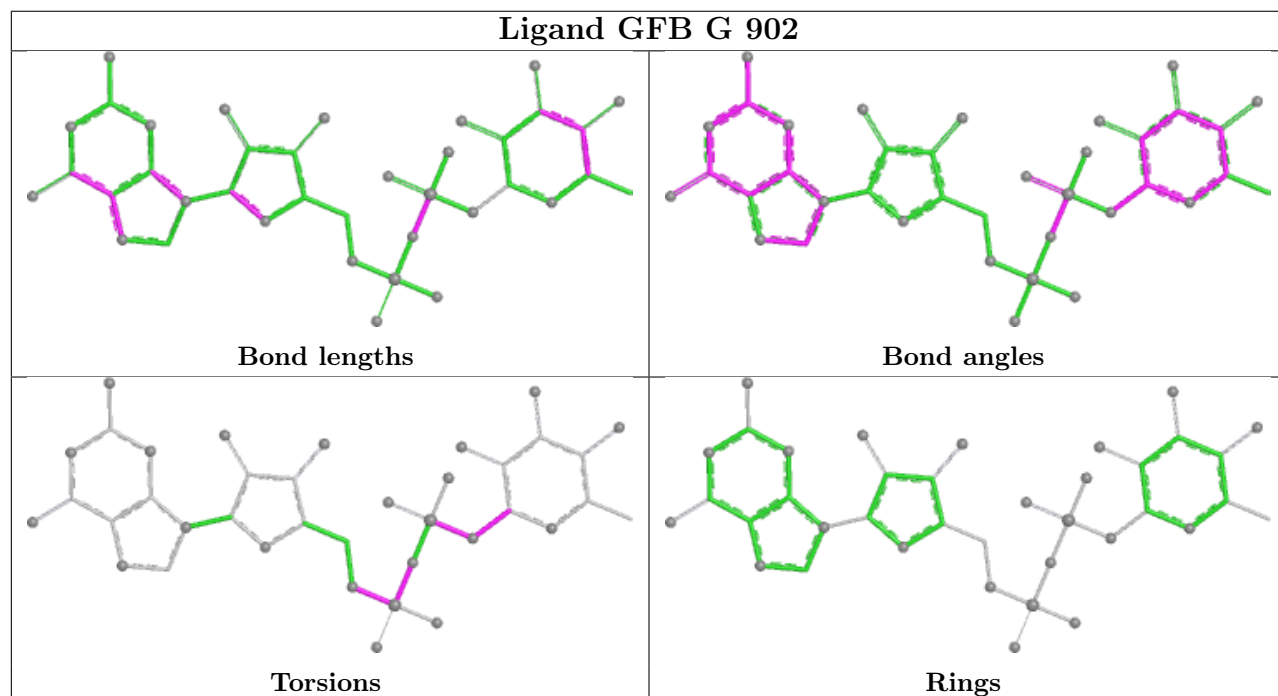




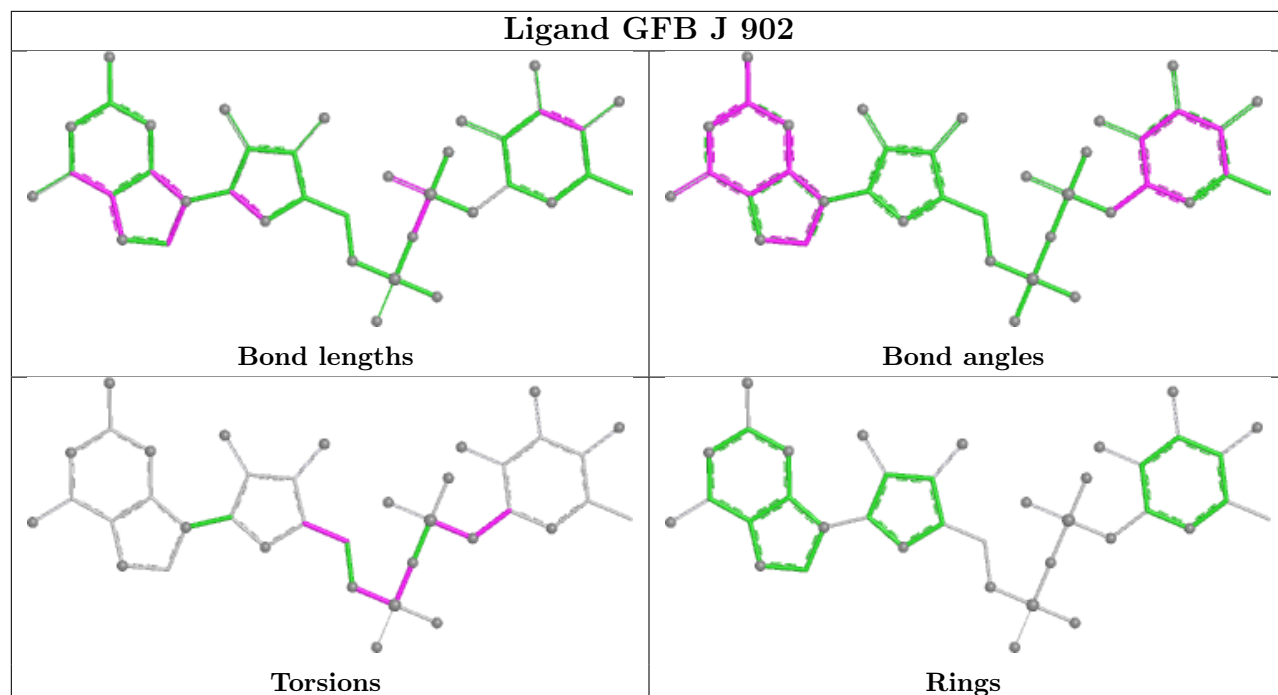
Ligand GFB I 902



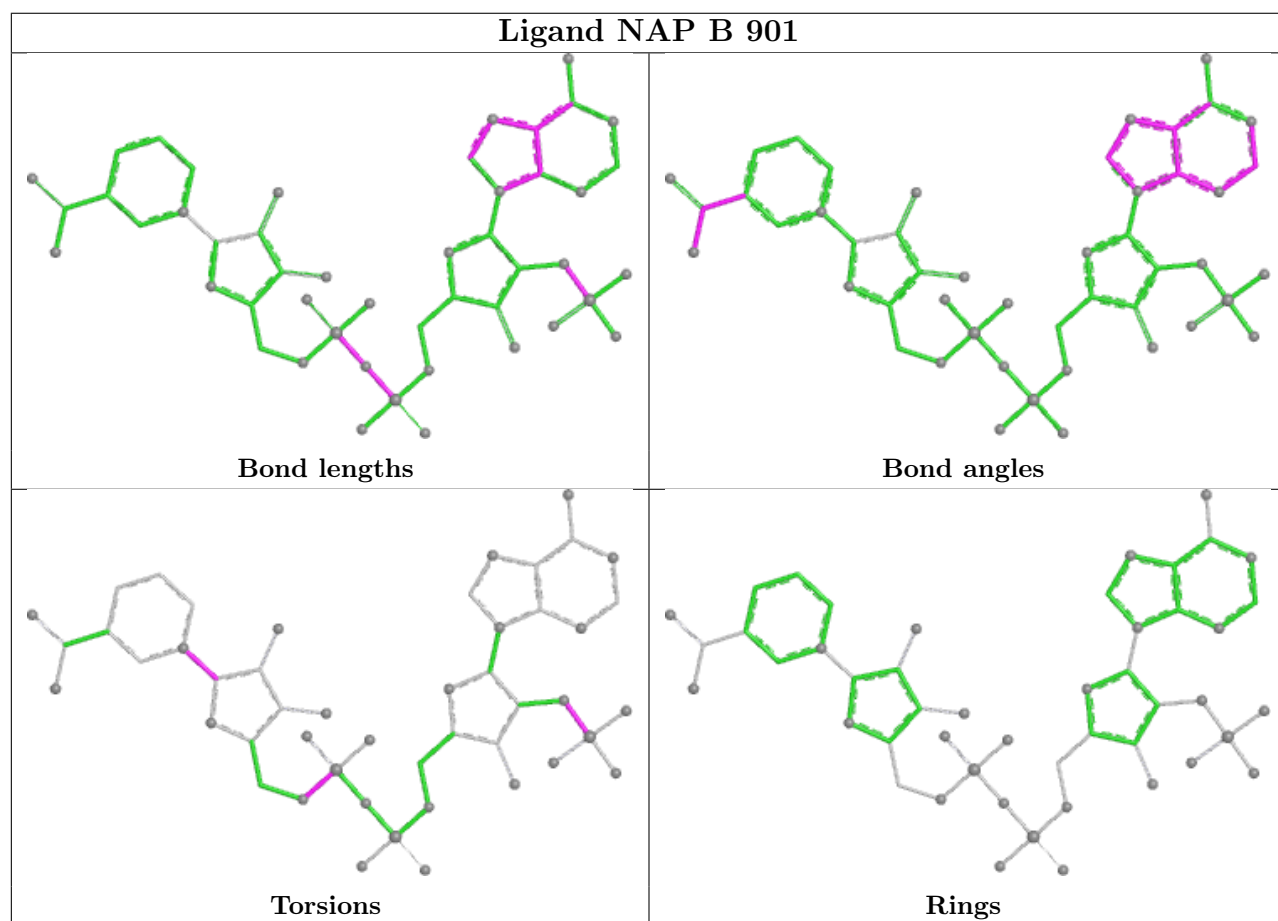
Ligand GFB G 902

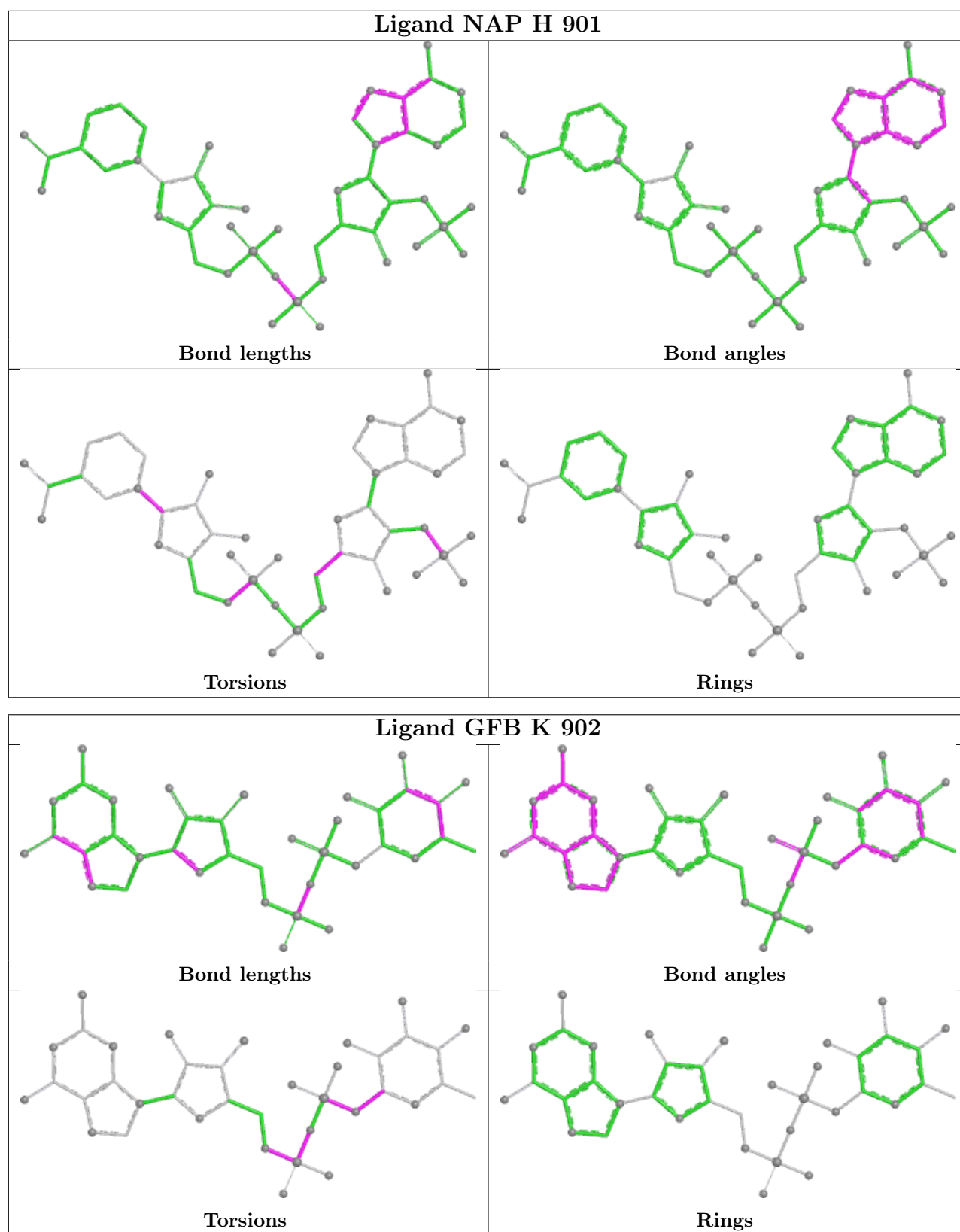


Ligand GFB J 902



Ligand NAP B 901





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/336 (93%)	-1.51	0 100 100	26, 41, 58, 75	0
1	B	320/336 (95%)	-1.52	0 100 100	27, 42, 66, 77	0
1	C	321/336 (95%)	-1.51	0 100 100	28, 41, 66, 93	0
1	D	315/336 (93%)	-1.51	0 100 100	25, 43, 61, 76	0
1	E	320/336 (95%)	-1.47	0 100 100	29, 46, 66, 79	0
1	F	313/336 (93%)	-1.48	0 100 100	27, 43, 63, 76	0
1	G	320/336 (95%)	-1.52	0 100 100	29, 45, 64, 81	0
1	H	315/336 (93%)	-1.47	0 100 100	32, 48, 68, 80	0
1	I	321/336 (95%)	-1.48	0 100 100	32, 48, 64, 77	0
1	J	313/336 (93%)	-1.47	0 100 100	32, 53, 75, 93	0
1	K	313/336 (93%)	-1.44	0 100 100	31, 53, 81, 106	0
1	L	320/336 (95%)	-1.41	0 100 100	35, 54, 79, 92	0
All	All	3805/4032 (94%)	-1.48	0 100 100	25, 46, 69, 106	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

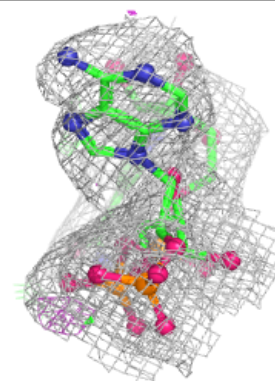
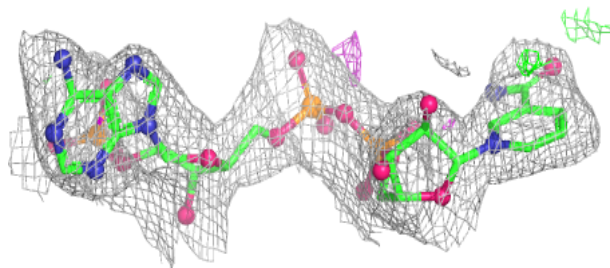
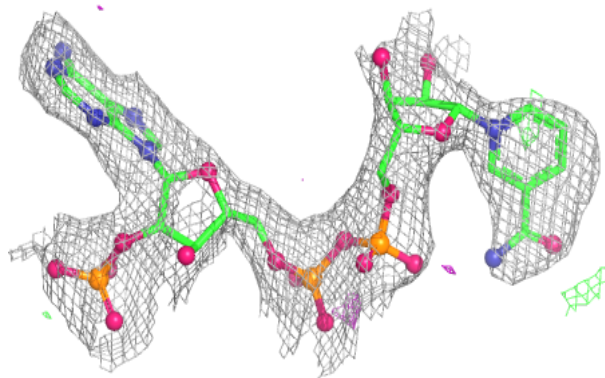
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	F	1321	4/4	0.95	0.08	44,49,49,49	0
2	NAP	B	901	48/48	0.99	0.03	35,38,40,41	0
2	NAP	C	901	48/48	0.99	0.03	29,32,36,37	0
2	NAP	D	901	48/48	0.99	0.03	33,37,43,47	0
2	NAP	E	901	48/48	0.99	0.03	37,40,45,47	0
2	NAP	F	901	48/48	0.99	0.03	37,45,54,56	0
2	NAP	G	901	48/48	0.99	0.03	37,42,49,53	0
2	NAP	H	901	48/48	0.99	0.03	36,41,48,55	0
2	NAP	I	901	48/48	0.99	0.03	33,43,47,50	0
2	NAP	J	901	48/48	0.99	0.03	46,56,61,62	0
2	NAP	K	901	48/48	0.99	0.04	47,53,57,60	0
2	NAP	L	901	48/48	0.99	0.03	38,47,56,56	0
3	GFB	A	902	38/38	0.99	0.04	27,31,42,43	0
3	GFB	B	902	38/38	0.99	0.03	29,33,41,43	0
3	GFB	C	902	38/38	0.99	0.03	29,30,42,47	0
3	GFB	D	902	38/38	0.99	0.03	26,28,38,42	0
3	GFB	E	902	38/38	0.99	0.03	37,43,61,61	0
3	GFB	F	902	38/38	0.99	0.03	29,37,47,49	0
3	GFB	G	902	38/38	0.99	0.03	29,33,44,47	0
3	GFB	H	902	38/38	0.99	0.03	29,35,40,41	0
3	GFB	I	902	38/38	0.99	0.04	35,38,47,48	0
3	GFB	K	902	38/38	0.99	0.03	29,37,45,50	0
3	GFB	L	902	38/38	0.99	0.03	39,44,57,61	0
2	NAP	A	901	48/48	0.99	0.04	31,36,42,45	0
3	GFB	J	902	38/38	1.00	0.03	40,47,53,54	0

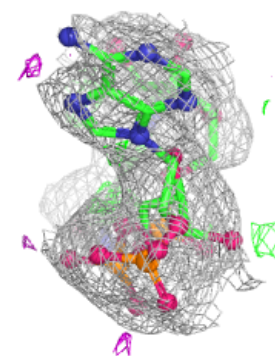
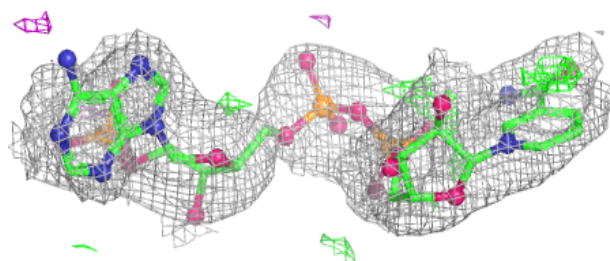
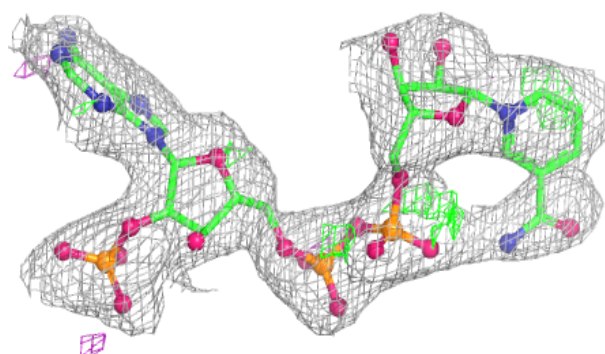
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 901:

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

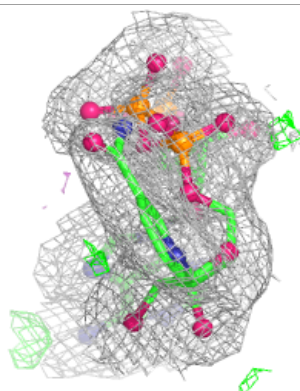
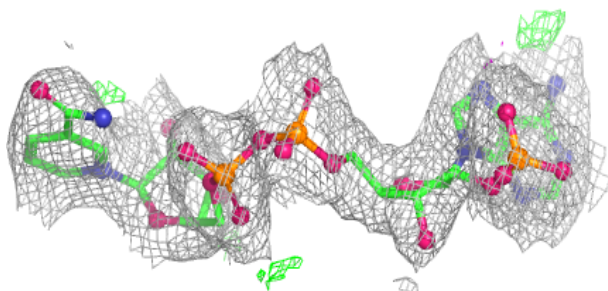
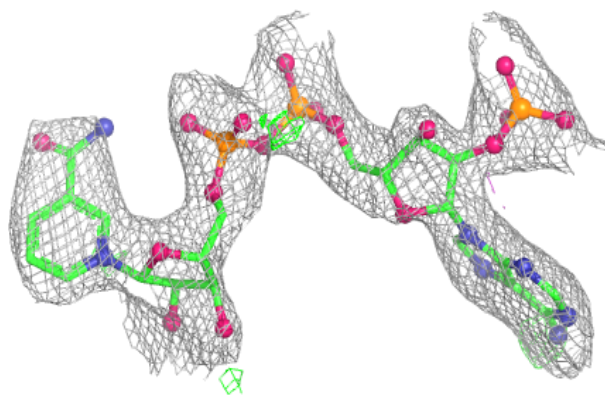
**Electron density around NAP C 901:**

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

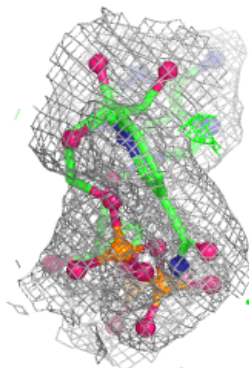
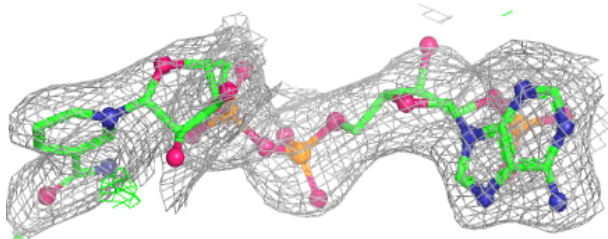
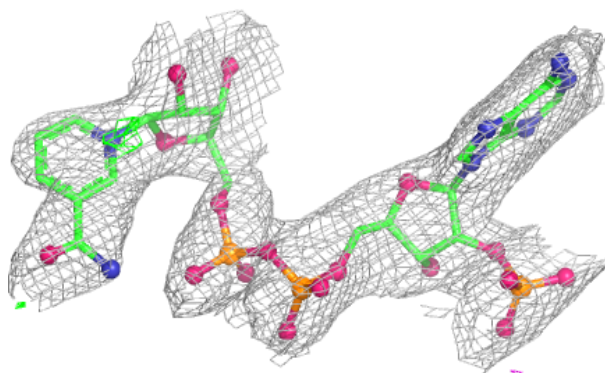


Electron density around NAP D 901:

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

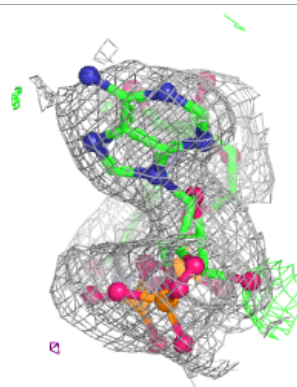
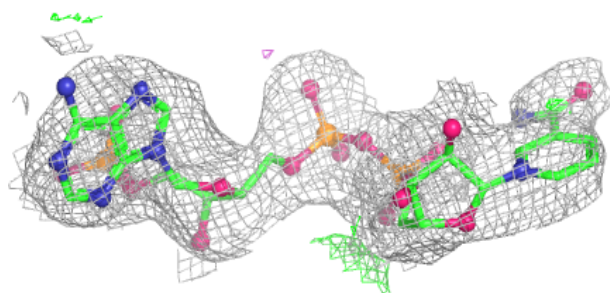
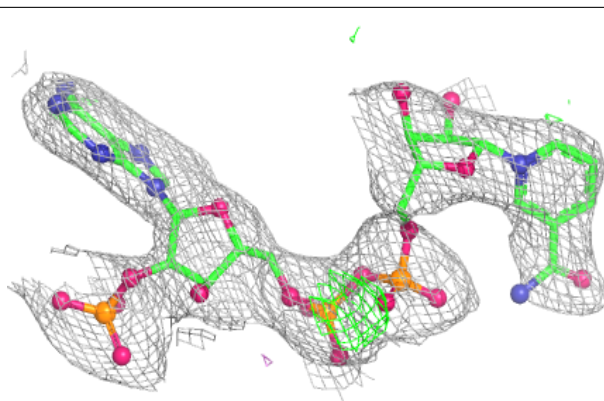
**Electron density around NAP E 901:**

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

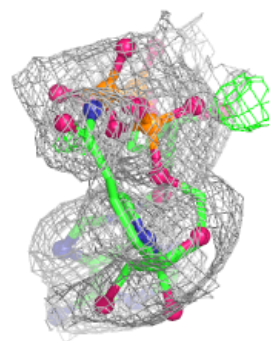
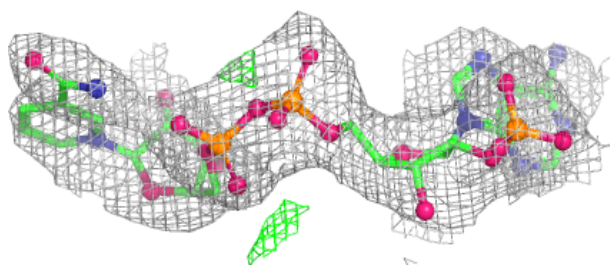
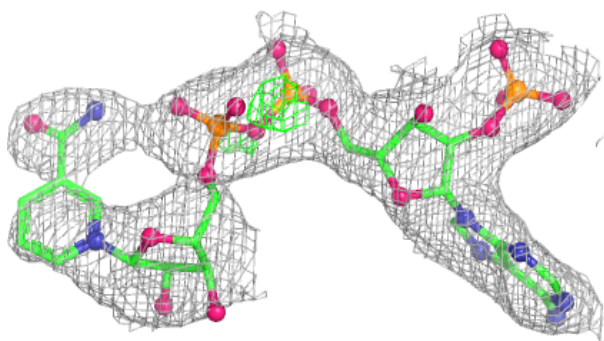


Electron density around NAP F 901:

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

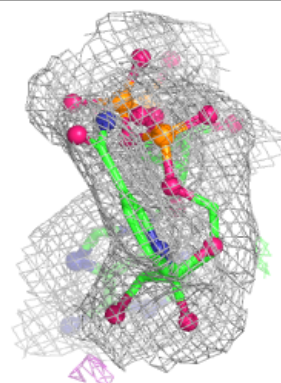
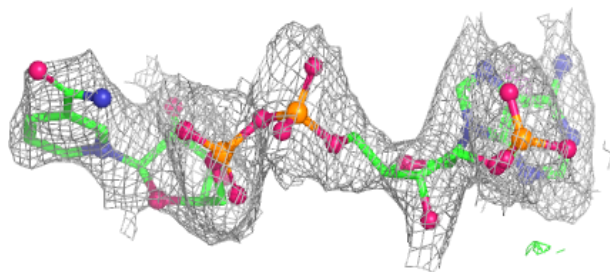
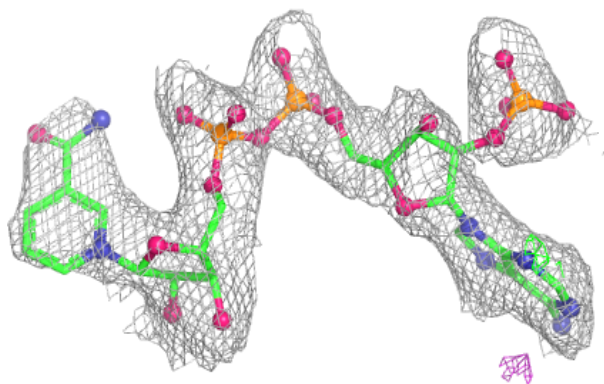
**Electron density around NAP G 901:**

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

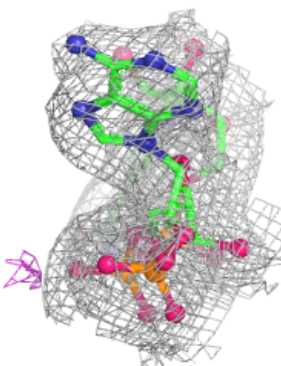
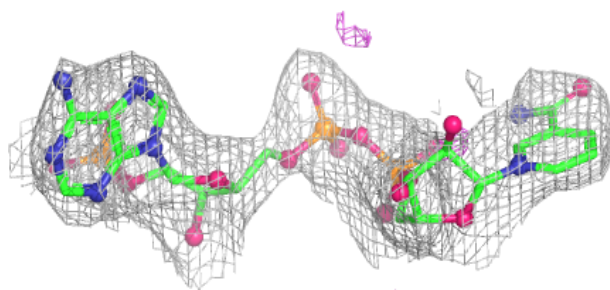
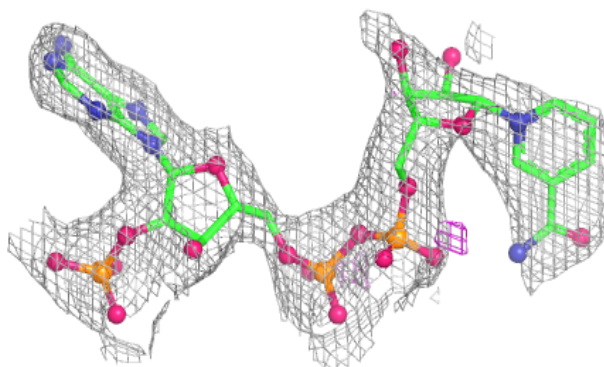


Electron density around NAP H 901:

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

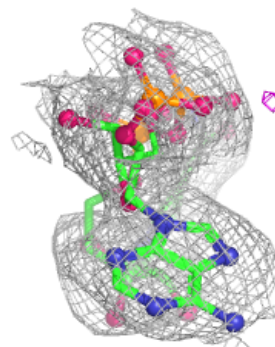
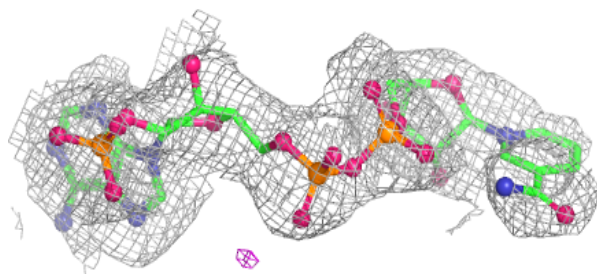
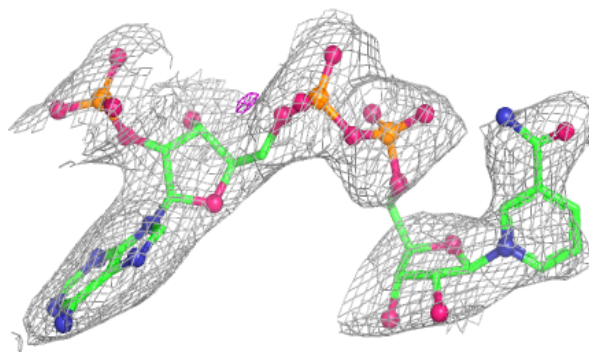
**Electron density around NAP I 901:**

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

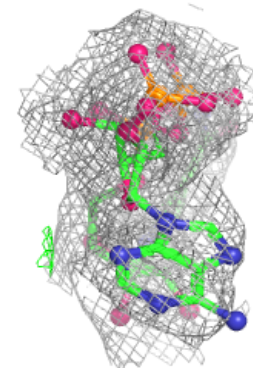
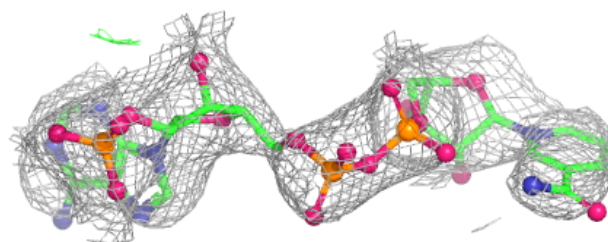
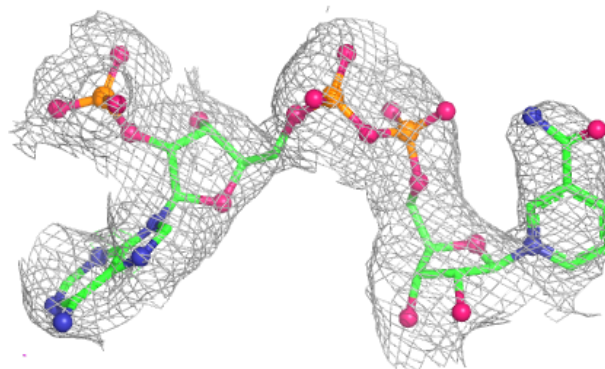


Electron density around NAP J 901:

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

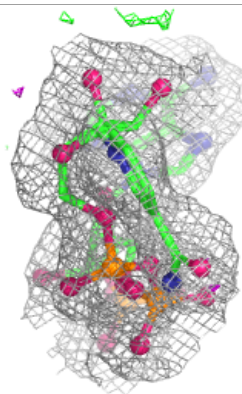
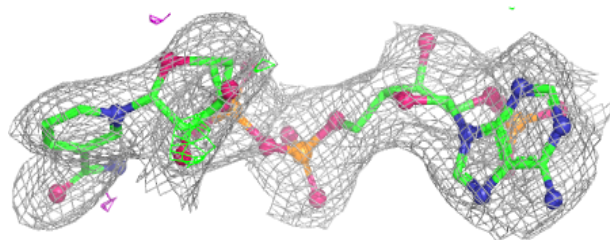
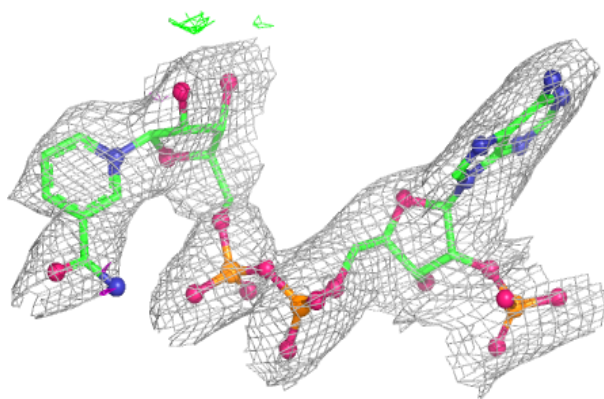
**Electron density around NAP K 901:**

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

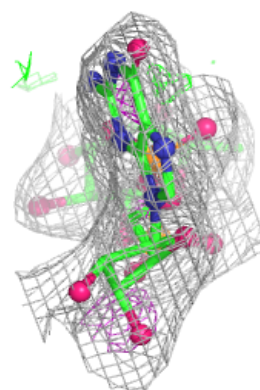
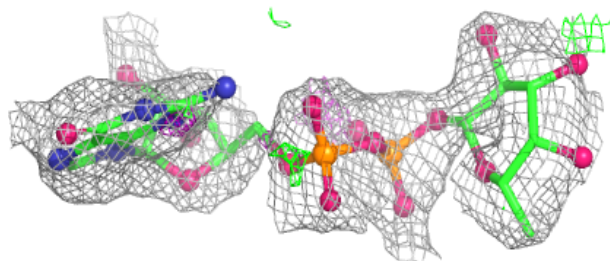
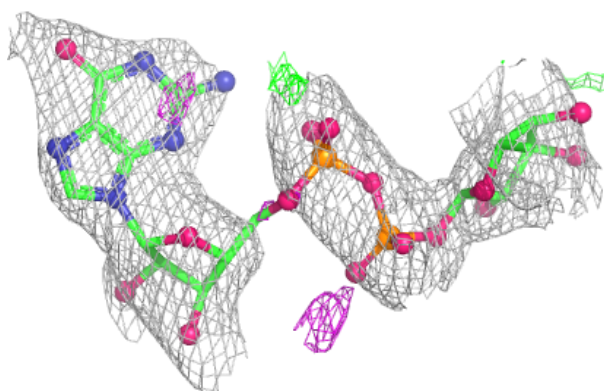


Electron density around NAP L 901:

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

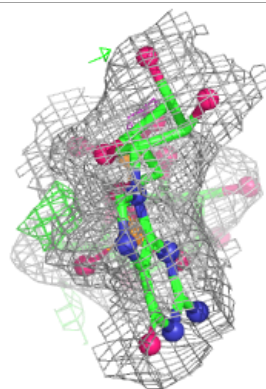
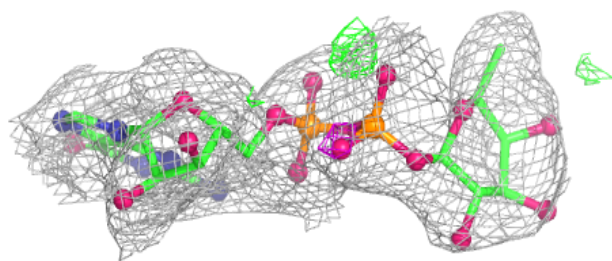
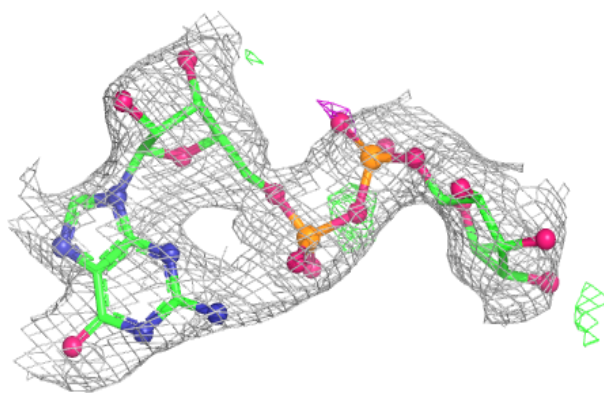
**Electron density around GFB A 902:**

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

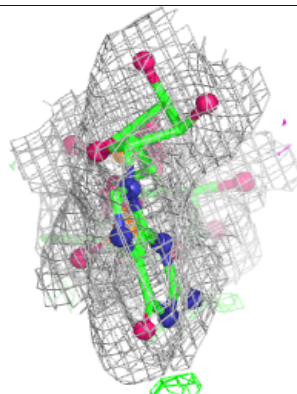
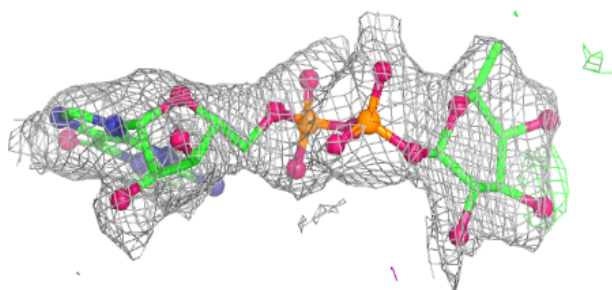
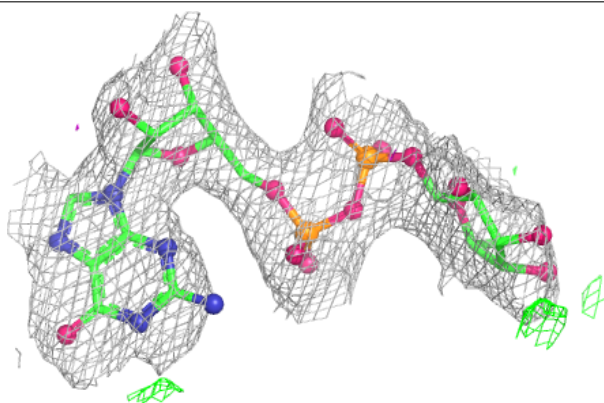


Electron density around GFB B 902:

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

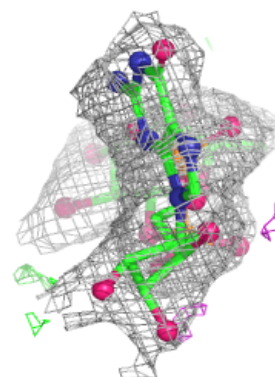
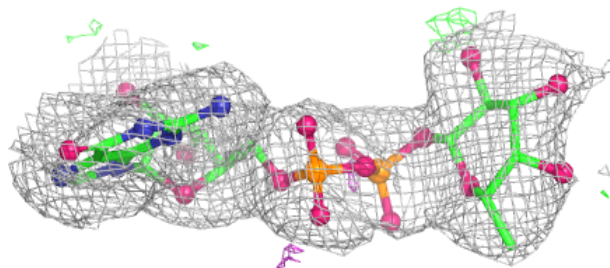
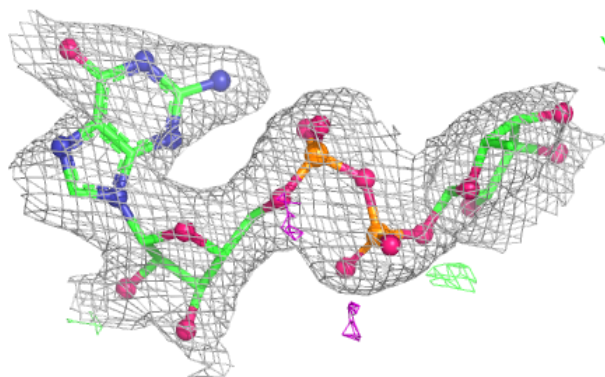
**Electron density around GFB C 902:**

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

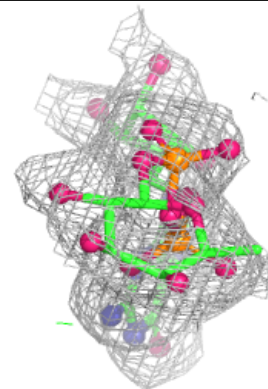
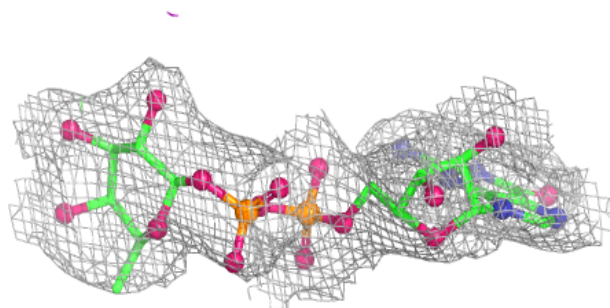
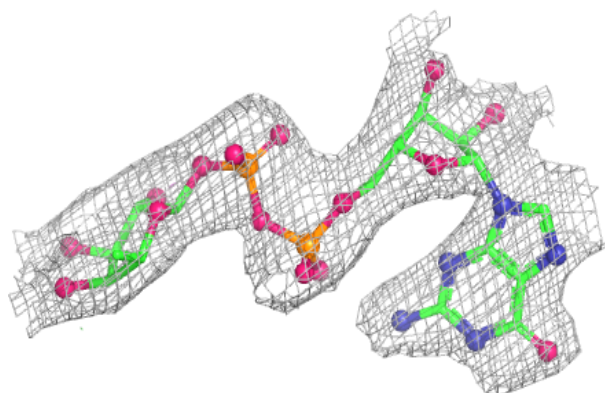


Electron density around GFB D 902:

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

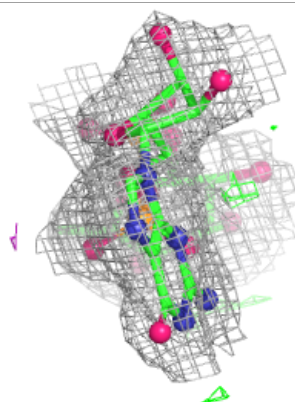
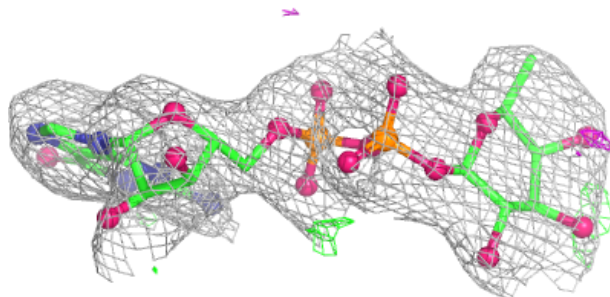
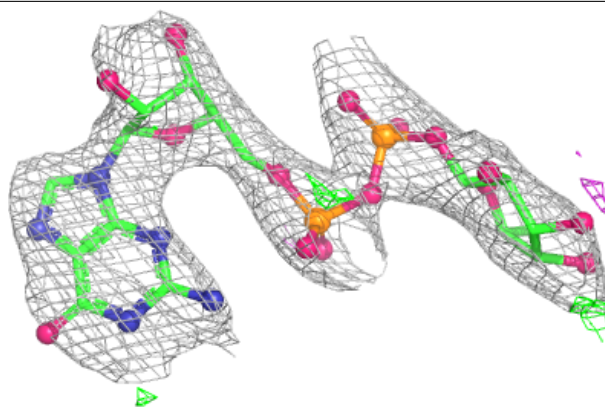
**Electron density around GFB E 902:**

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

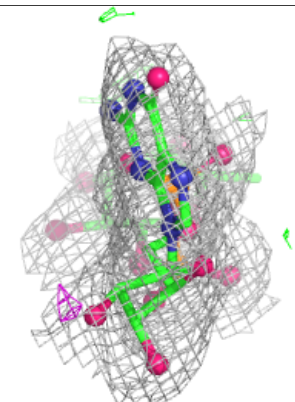
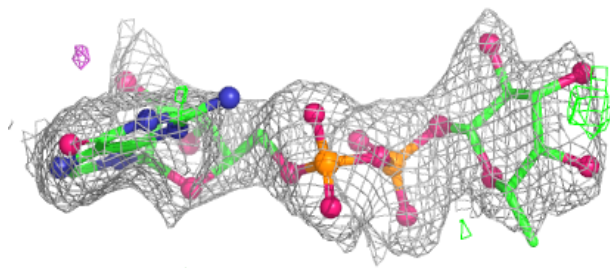
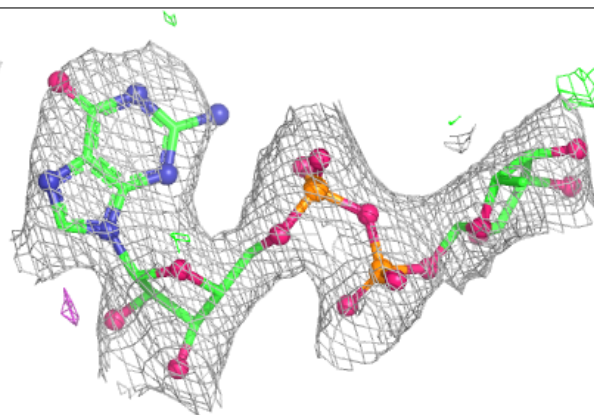


Electron density around GFB F 902:

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

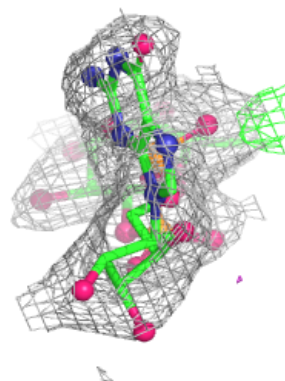
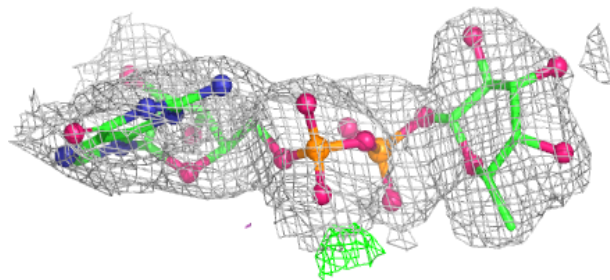
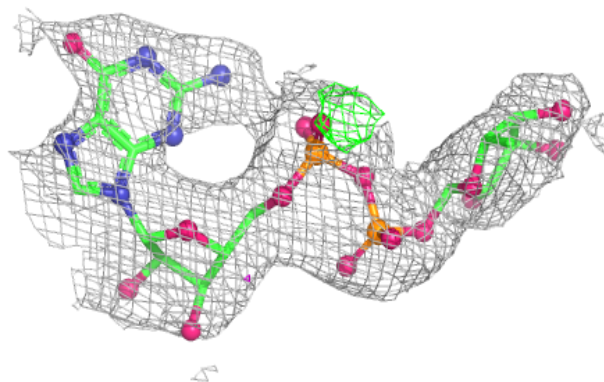
**Electron density around GFB G 902:**

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

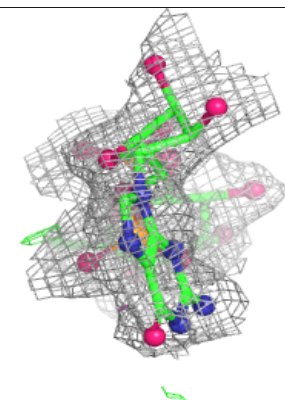
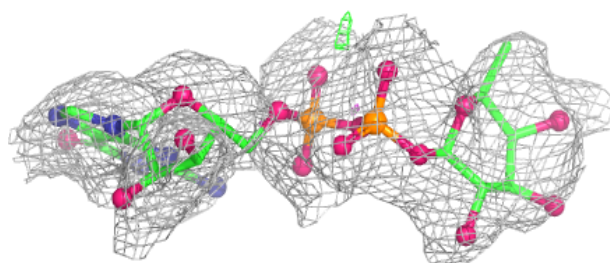
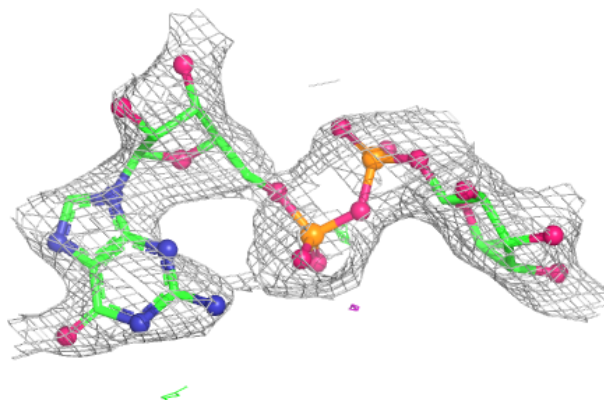


Electron density around GFB H 902:

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

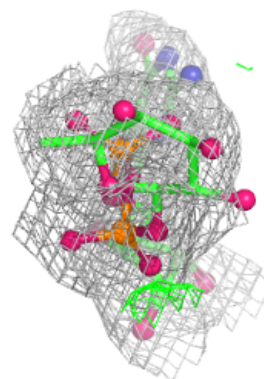
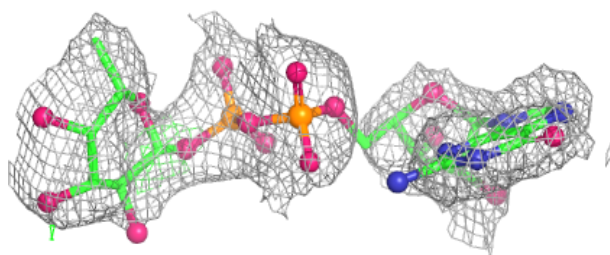
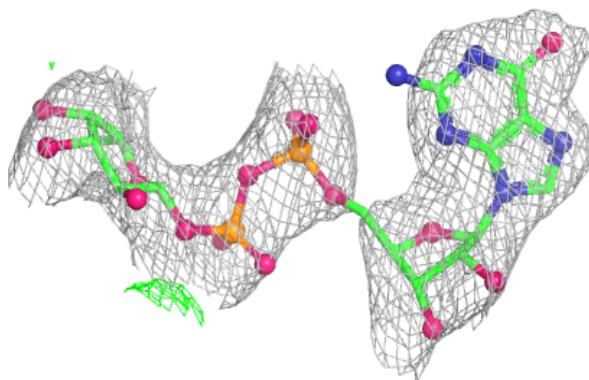
**Electron density around GFB I 902:**

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

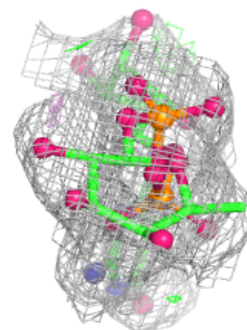
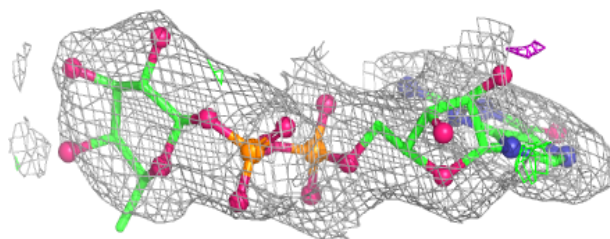
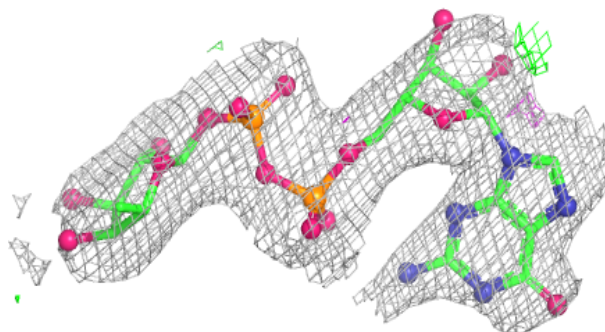


Electron density around GFB K 902:

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

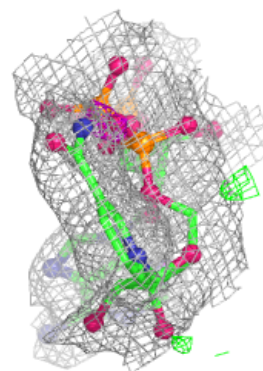
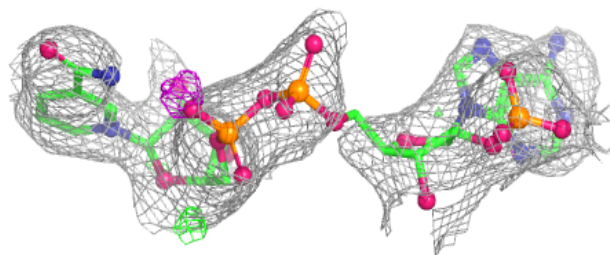
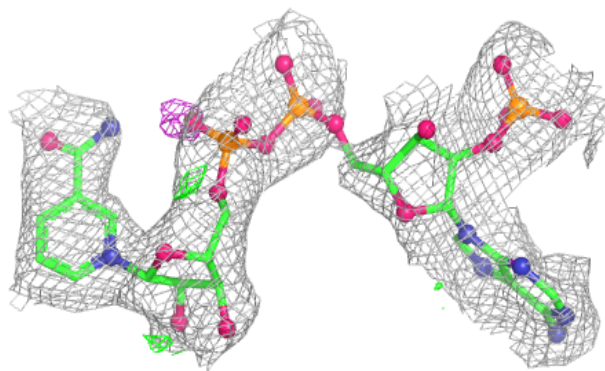
**Electron density around GFB L 902:**

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

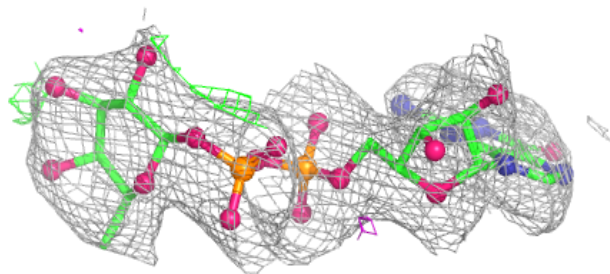
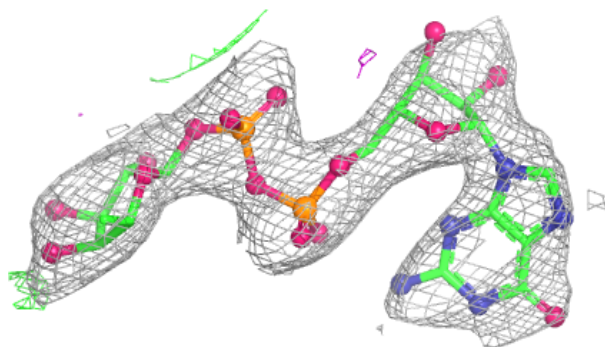


Electron density around NAP A 901:

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

**Electron density around GFB J 902:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.