



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:15 PM UTC

PDB ID : 5BP4 / pdb_00005bp4
Title : Modifying region (DH-ER-KR) of a mycocerosic acid synthase-like (MAS-like) PKS
Authors : Herbst, D.A.; Jakob, P.R.; Zaehring, F.; Maier, T.
Deposited on : 2015-05-27
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

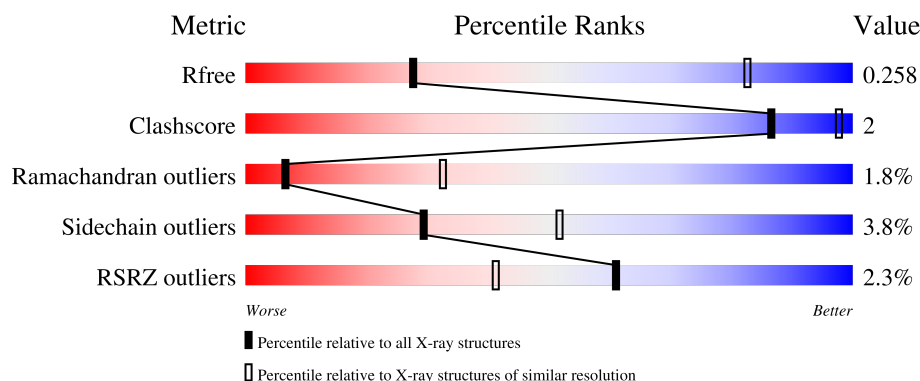
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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.



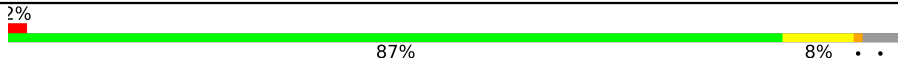
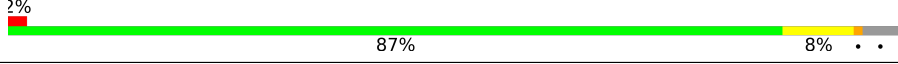
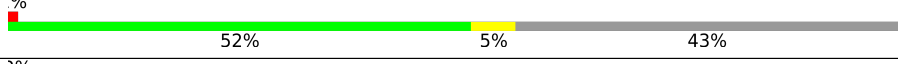
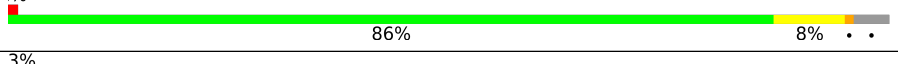
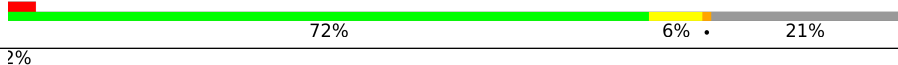
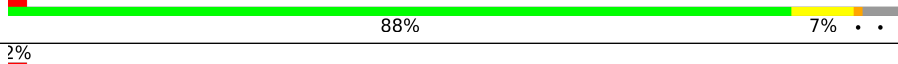
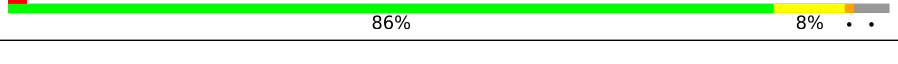
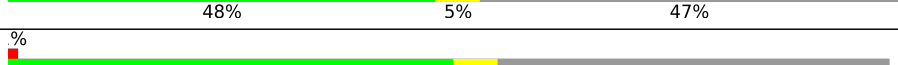
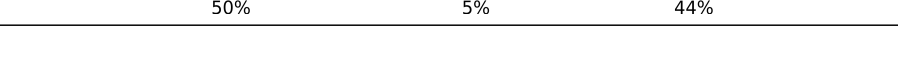
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	1140	2% 85% 10% ..
1	B	1140	2% 87% 9% ..
1	C	1140	3% 88% 8% ..
1	D	1140	2% 87% 8% ..
1	E	1140	3% 87% 8% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1140	
1	G	1140	
1	H	1140	
1	I	1140	
1	J	1140	
1	K	1140	
1	L	1140	
1	M	1140	
1	N	1140	
1	O	1140	
1	P	1140	
1	Q	1140	
1	R	1140	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 262498 atoms, of which 129384 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 Mycocerosic acid synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	B	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	C	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	D	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	E	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	F	1093	Total	C	H	N	O	S	0	0	0
			16142	5122	7965	1467	1564	24			
1	G	1088	Total	C	H	N	O	S	0	0	0
			16079	5102	7939	1462	1552	24			
1	H	1097	Total	C	H	N	O	S	0	0	0
			16195	5138	7991	1471	1571	24			
1	I	655	Total	C	H	N	O	S	0	0	0
			9680	3057	4801	872	935	15			
1	J	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	K	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	L	897	Total	C	H	N	O	S	0	0	0
			13209	4199	6535	1183	1272	20			
1	M	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	N	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	O	633	Total	C	H	N	O	S	0	0	0
			9327	2950	4625	839	898	15			
1	P	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	608	Total	C	H	N	O	S	0	0	0
			8979	2846	4455	804	859	15			
1	R	637	Total	C	H	N	O	S	0	0	0
			9417	2980	4669	844	909	15			

There are 54 discrepancies between the modelled and reference sequences:

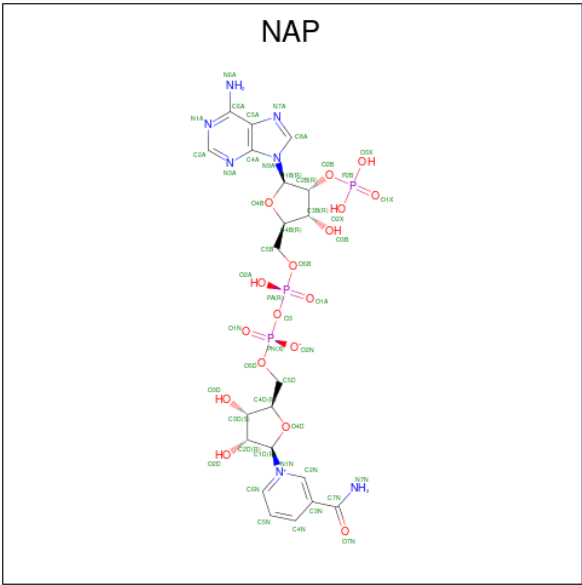
Chain	Residue	Modelled	Actual	Comment	Reference
A	882	SER	-	expression tag	UNP A0R1E8
A	883	MET	-	expression tag	UNP A0R1E8
A	2021	GLN	-	expression tag	UNP A0R1E8
B	882	SER	-	expression tag	UNP A0R1E8
B	883	MET	-	expression tag	UNP A0R1E8
B	2021	GLN	-	expression tag	UNP A0R1E8
C	882	SER	-	expression tag	UNP A0R1E8
C	883	MET	-	expression tag	UNP A0R1E8
C	2021	GLN	-	expression tag	UNP A0R1E8
D	882	SER	-	expression tag	UNP A0R1E8
D	883	MET	-	expression tag	UNP A0R1E8
D	2021	GLN	-	expression tag	UNP A0R1E8
E	882	SER	-	expression tag	UNP A0R1E8
E	883	MET	-	expression tag	UNP A0R1E8
E	2021	GLN	-	expression tag	UNP A0R1E8
F	882	SER	-	expression tag	UNP A0R1E8
F	883	MET	-	expression tag	UNP A0R1E8
F	2021	GLN	-	expression tag	UNP A0R1E8
G	882	SER	-	expression tag	UNP A0R1E8
G	883	MET	-	expression tag	UNP A0R1E8
G	2021	GLN	-	expression tag	UNP A0R1E8
H	882	SER	-	expression tag	UNP A0R1E8
H	883	MET	-	expression tag	UNP A0R1E8
H	2021	GLN	-	expression tag	UNP A0R1E8
I	882	SER	-	expression tag	UNP A0R1E8
I	883	MET	-	expression tag	UNP A0R1E8
I	2021	GLN	-	expression tag	UNP A0R1E8
J	882	SER	-	expression tag	UNP A0R1E8
J	883	MET	-	expression tag	UNP A0R1E8
J	2021	GLN	-	expression tag	UNP A0R1E8
K	882	SER	-	expression tag	UNP A0R1E8
K	883	MET	-	expression tag	UNP A0R1E8
K	2021	GLN	-	expression tag	UNP A0R1E8
L	882	SER	-	expression tag	UNP A0R1E8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	883	MET	-	expression tag	UNP A0R1E8
L	2021	GLN	-	expression tag	UNP A0R1E8
M	882	SER	-	expression tag	UNP A0R1E8
M	883	MET	-	expression tag	UNP A0R1E8
M	2021	GLN	-	expression tag	UNP A0R1E8
N	882	SER	-	expression tag	UNP A0R1E8
N	883	MET	-	expression tag	UNP A0R1E8
N	2021	GLN	-	expression tag	UNP A0R1E8
O	882	SER	-	expression tag	UNP A0R1E8
O	883	MET	-	expression tag	UNP A0R1E8
O	2021	GLN	-	expression tag	UNP A0R1E8
P	882	SER	-	expression tag	UNP A0R1E8
P	883	MET	-	expression tag	UNP A0R1E8
P	2021	GLN	-	expression tag	UNP A0R1E8
Q	882	SER	-	expression tag	UNP A0R1E8
Q	883	MET	-	expression tag	UNP A0R1E8
Q	2021	GLN	-	expression tag	UNP A0R1E8
R	882	SER	-	expression tag	UNP A0R1E8
R	883	MET	-	expression tag	UNP A0R1E8
R	2021	GLN	-	expression tag	UNP A0R1E8

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



Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	B	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	C	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	C	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	0
2	D	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	D	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	E	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	F	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	G	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	G	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	H	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	H	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	I	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	J	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	J	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	K	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	K	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	L	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	M	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

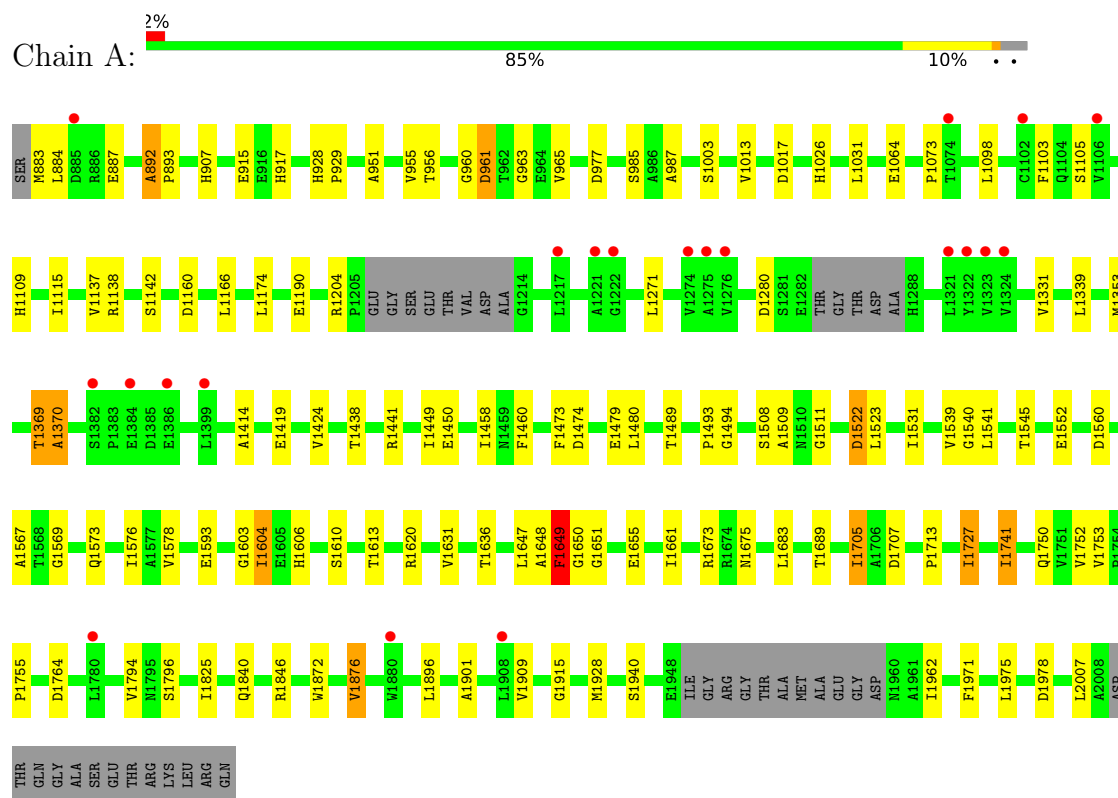
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	M	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	N	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	N	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	O	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	P	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	P	1	Total 38	C 10	H 11	N 5	O 10	P 2	0	0
2	Q	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
2	R	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

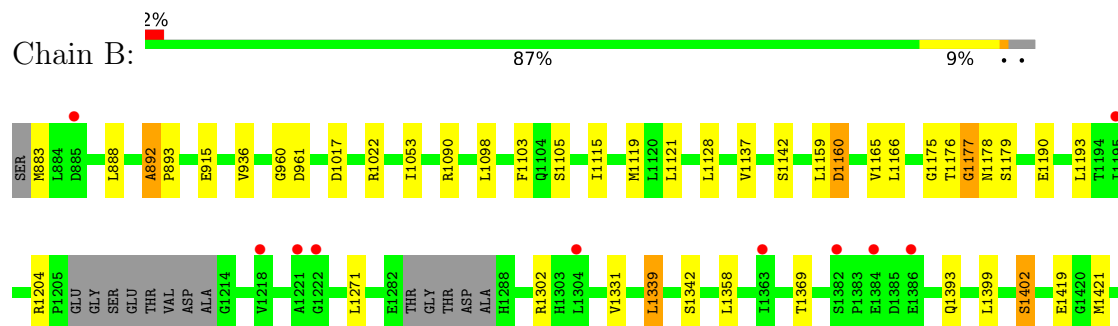
3 Residue-property plots [i](#)

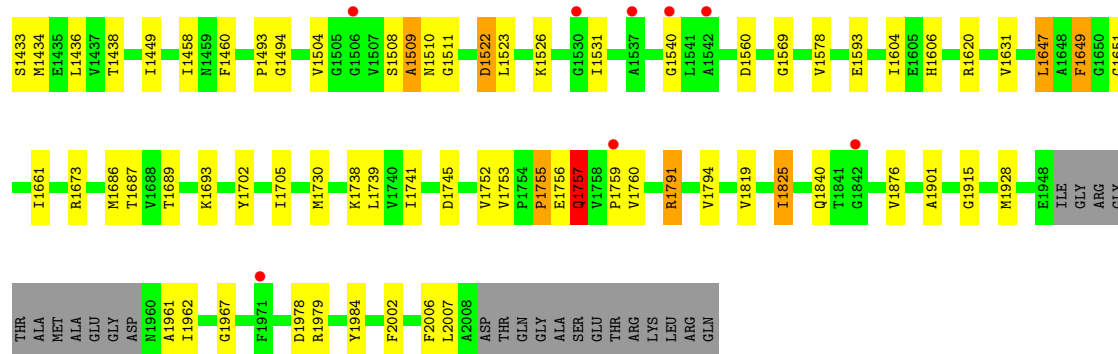
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Mycocerosic acid synthase

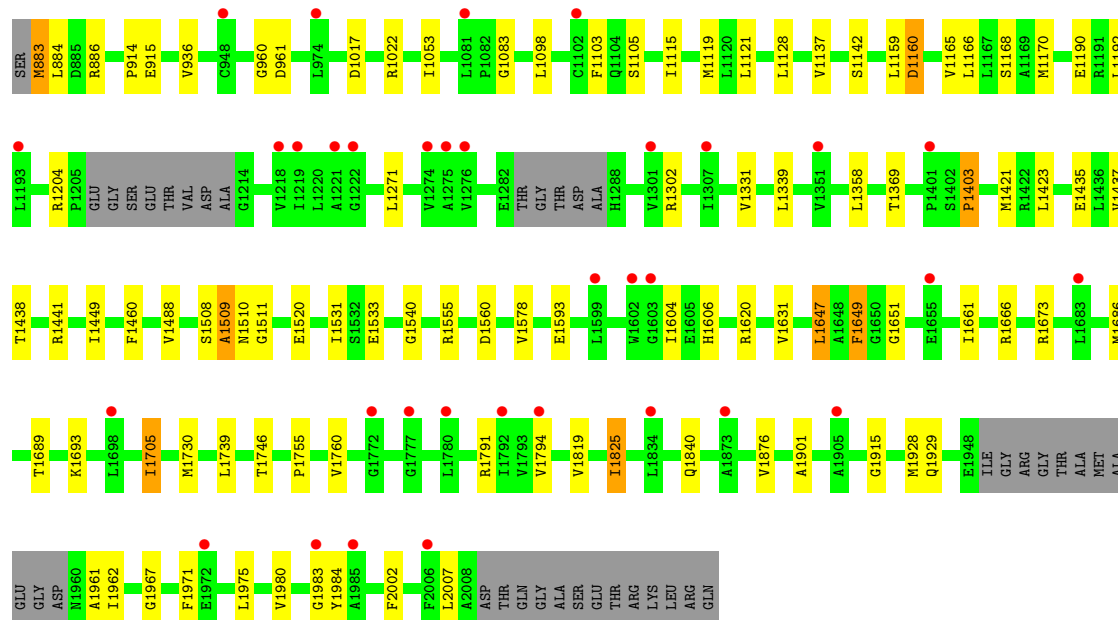
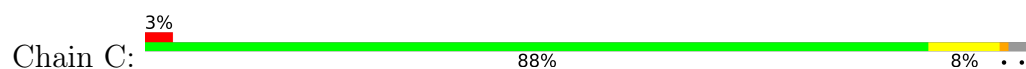


• Molecule 1: Mycocerosic acid synthase

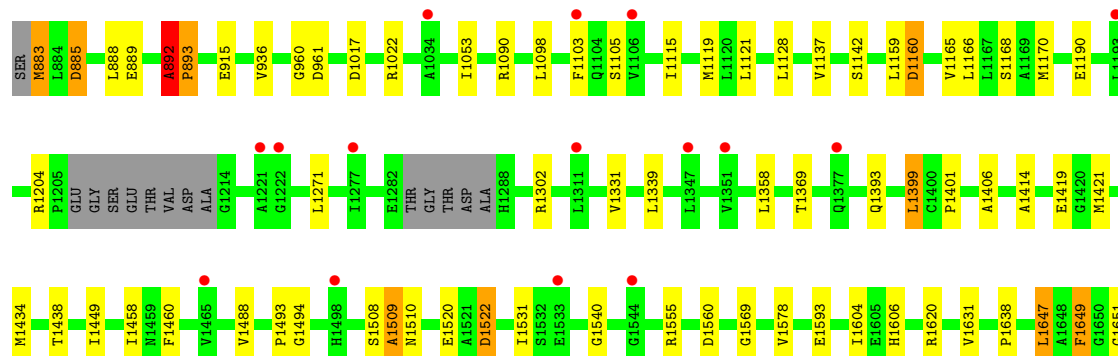
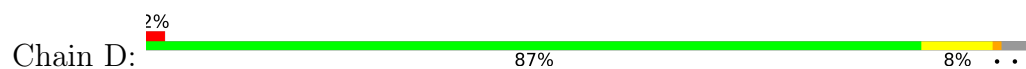


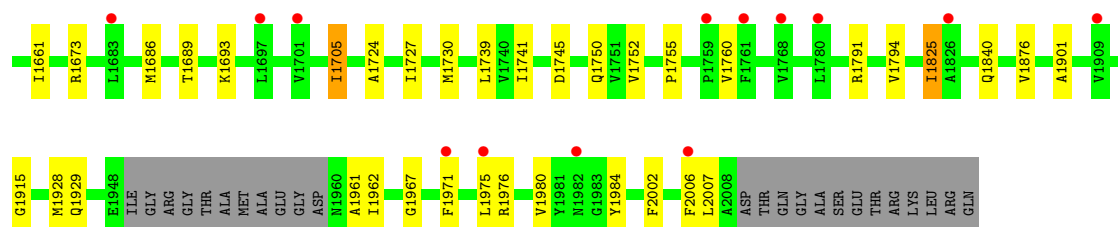


• Molecule 1: Mycocerosic acid synthase

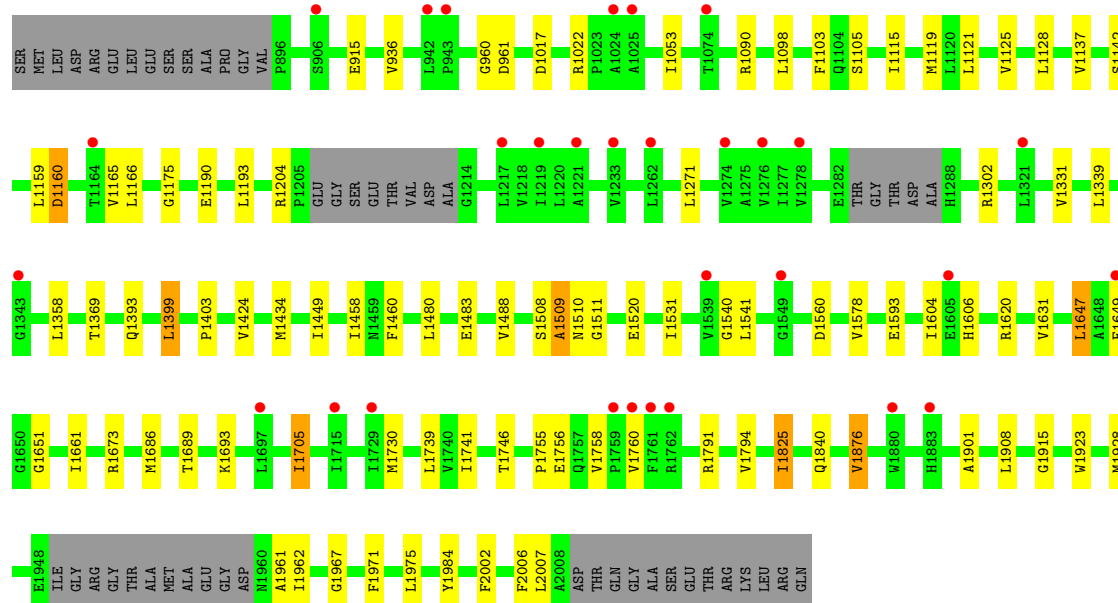
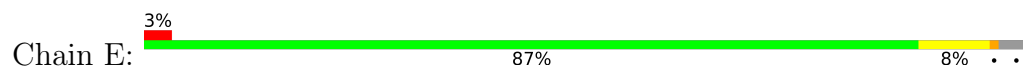


• Molecule 1: Mycocerosic acid synthase

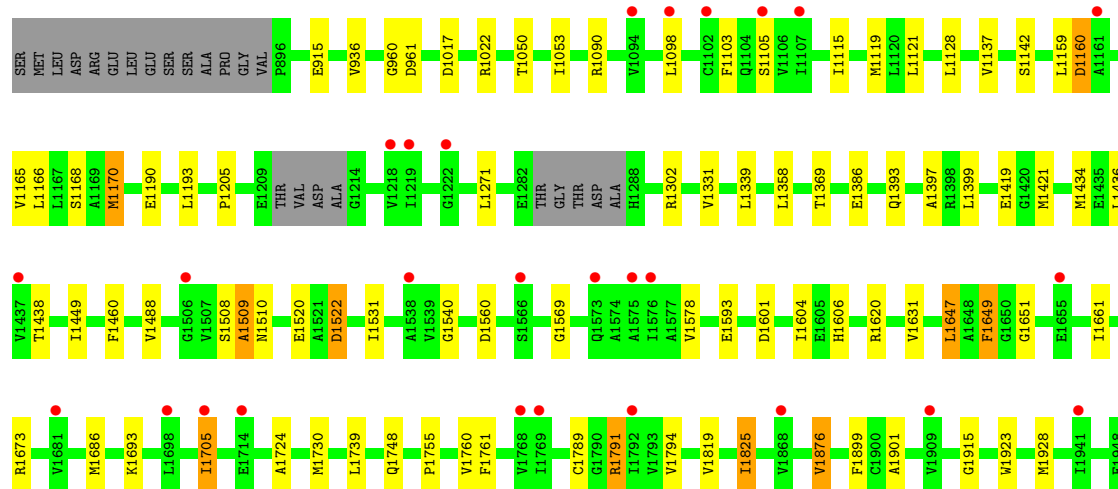
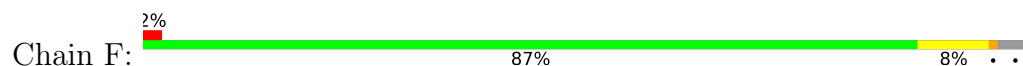




• Molecule 1: Mycocerosic acid synthase

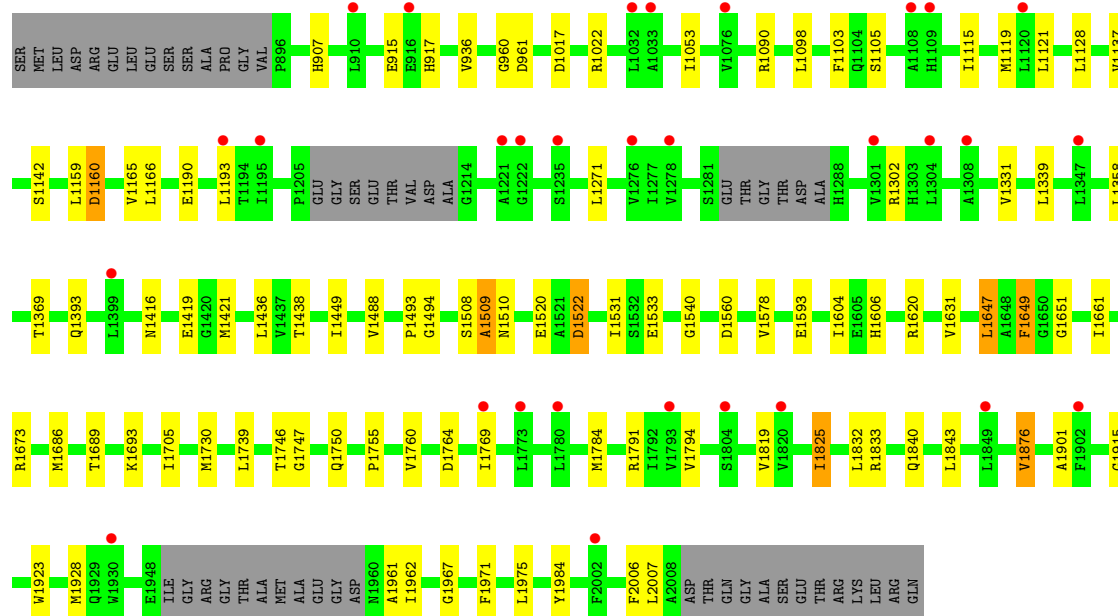
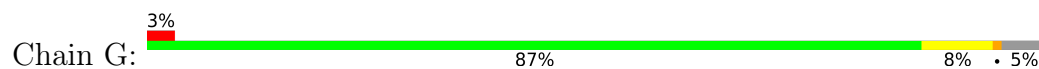


• Molecule 1: Mycocerosic acid synthase

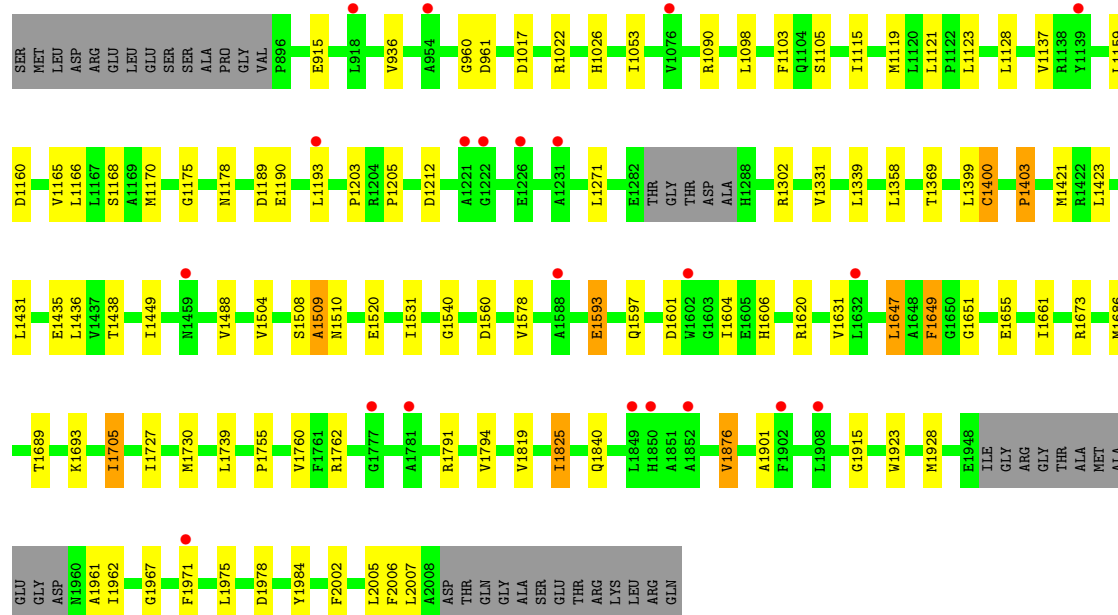
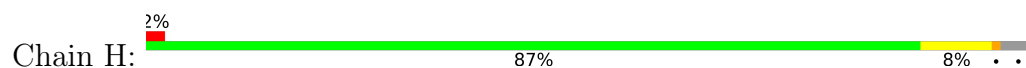




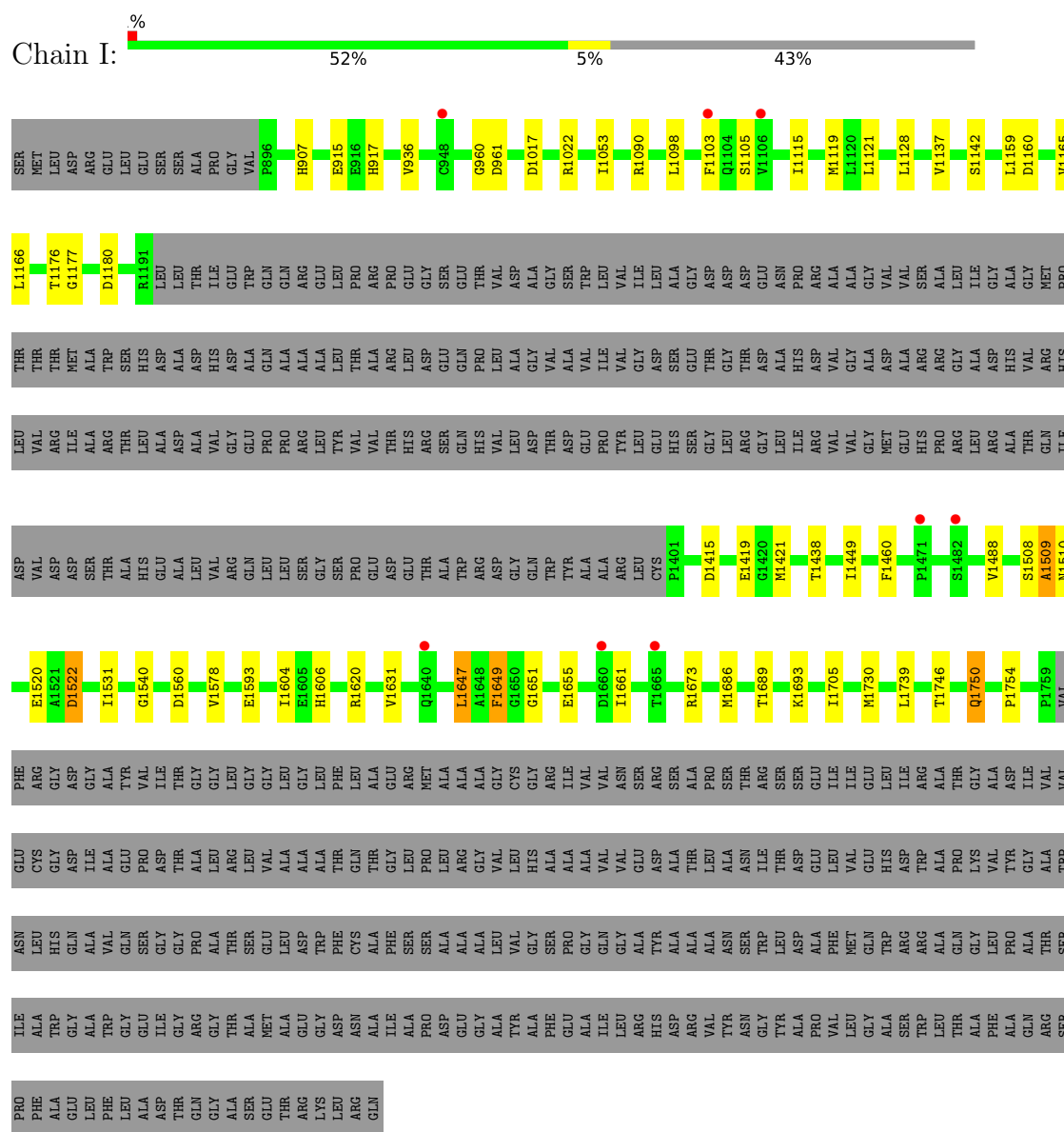
• Molecule 1: Mycocerosic acid synthase



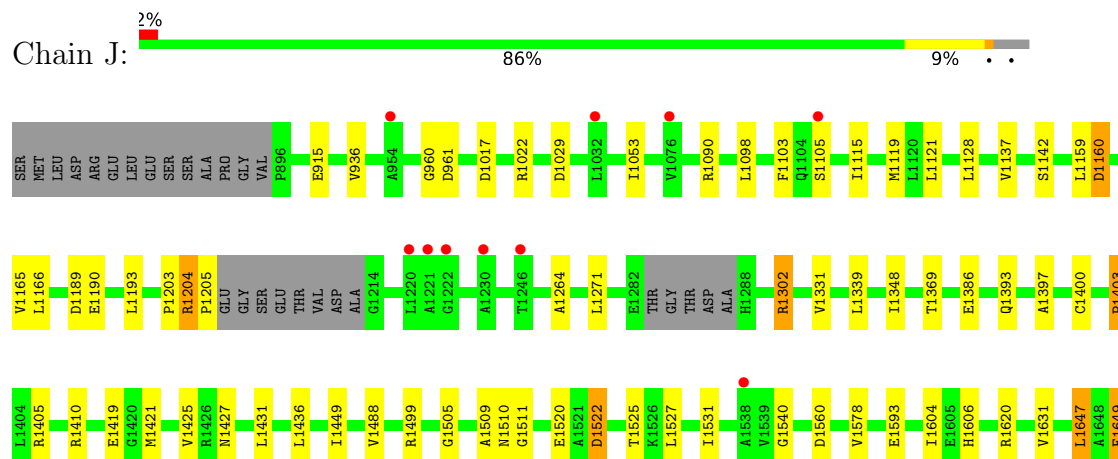
• Molecule 1: Mycocerosic acid synthase

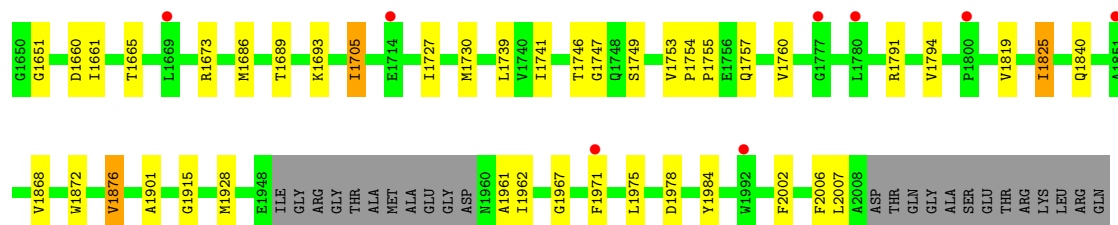


• Molecule 1: Mycocerosic acid synthase

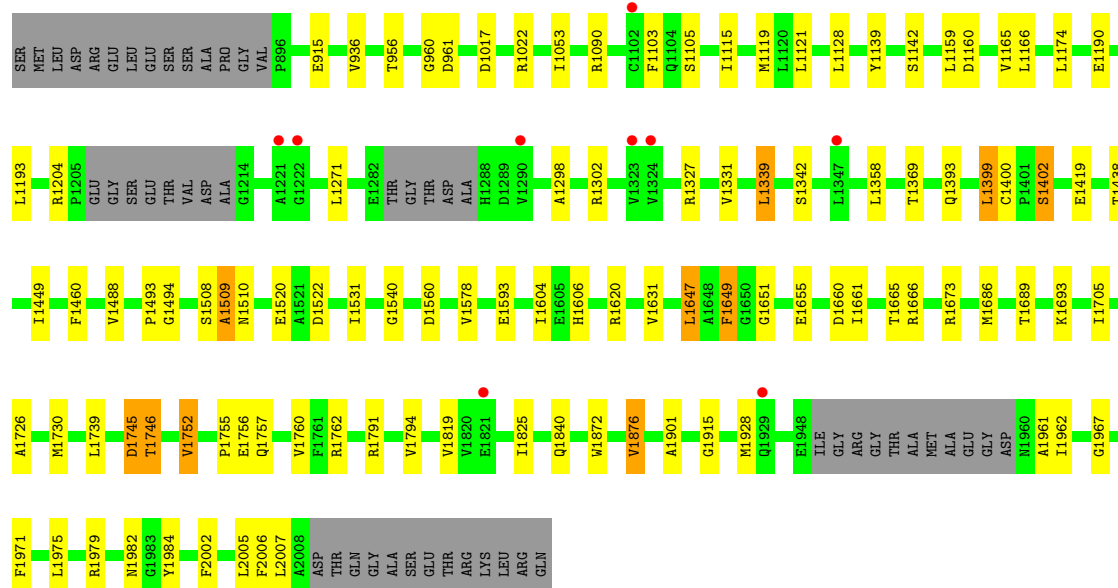
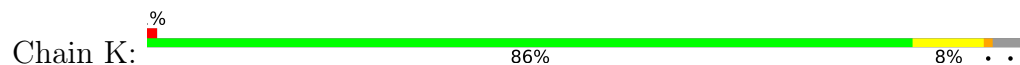


• Molecule 1: Mycocerosic acid synthase

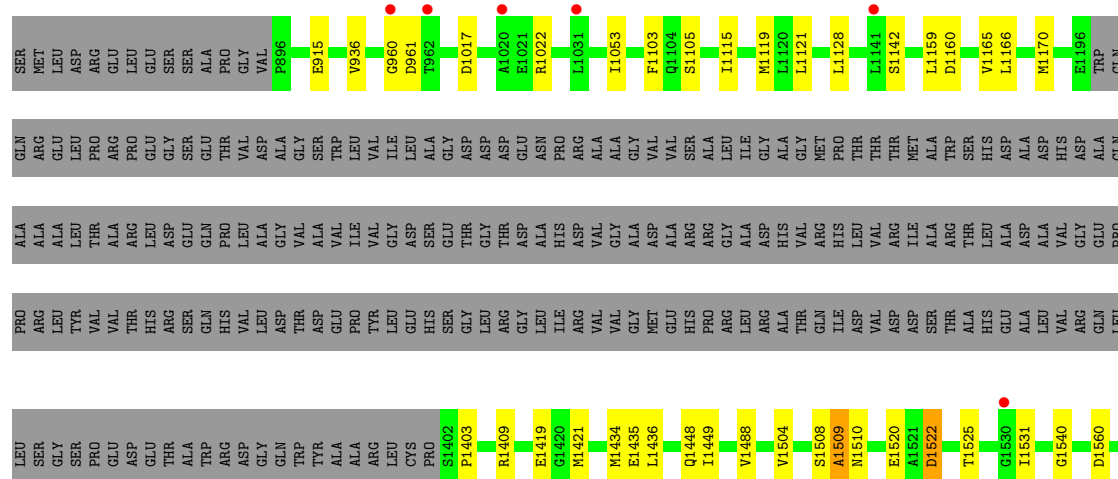


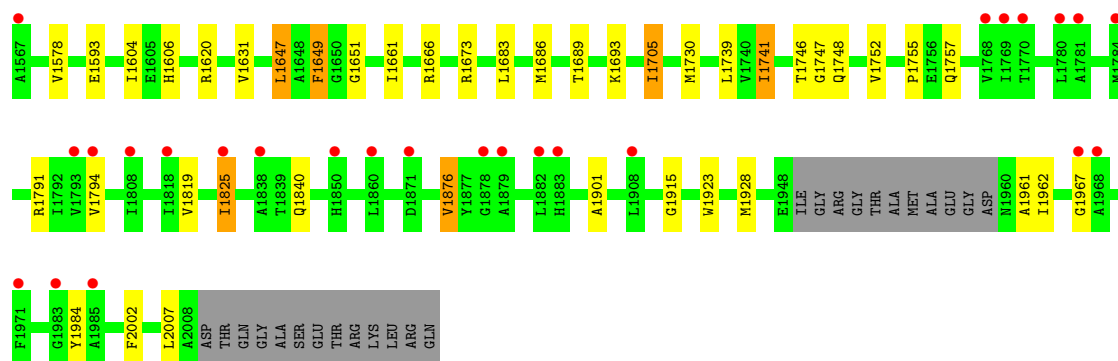


• Molecule 1: Mycocerosic acid synthase

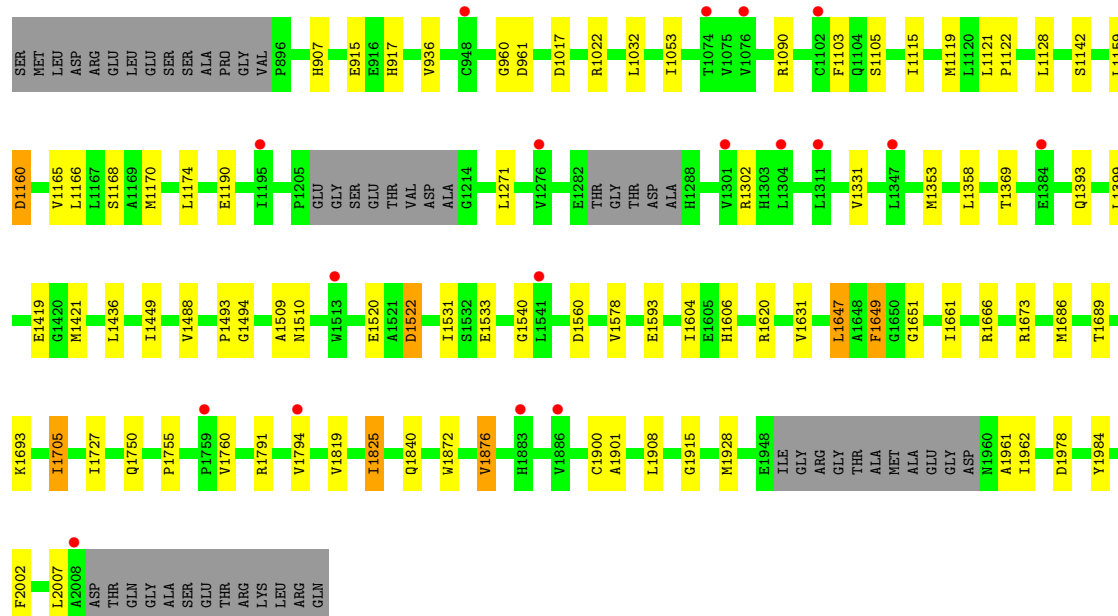
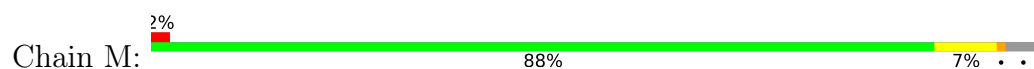


• Molecule 1: Mycocerosic acid synthase

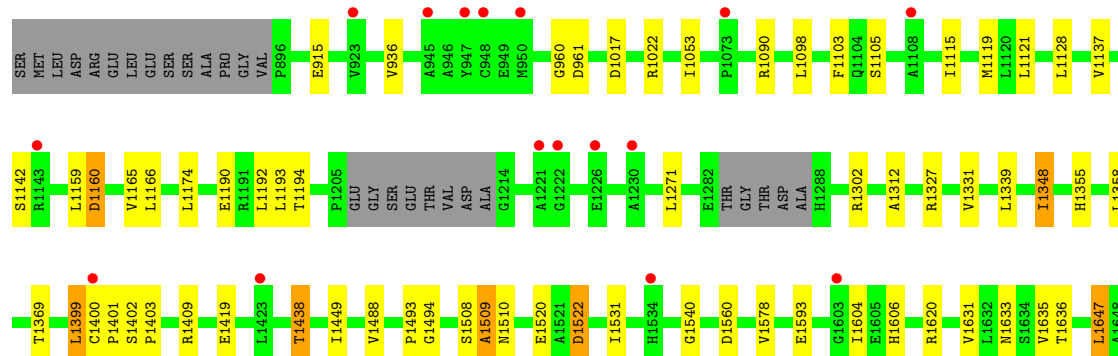
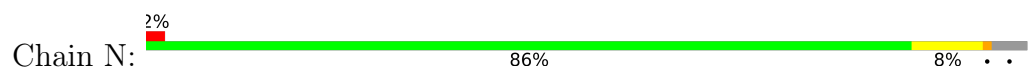


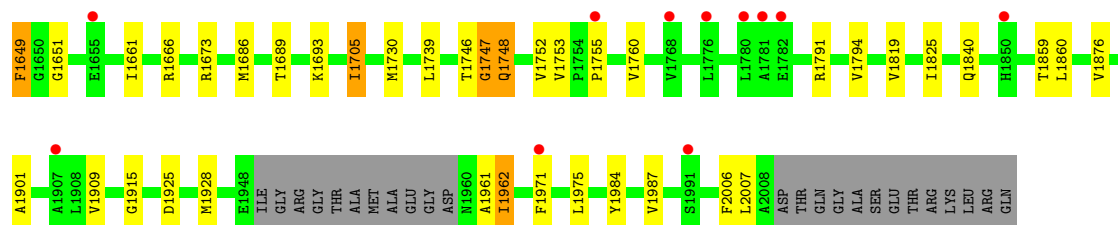


• Molecule 1: Mycocerosic acid synthase



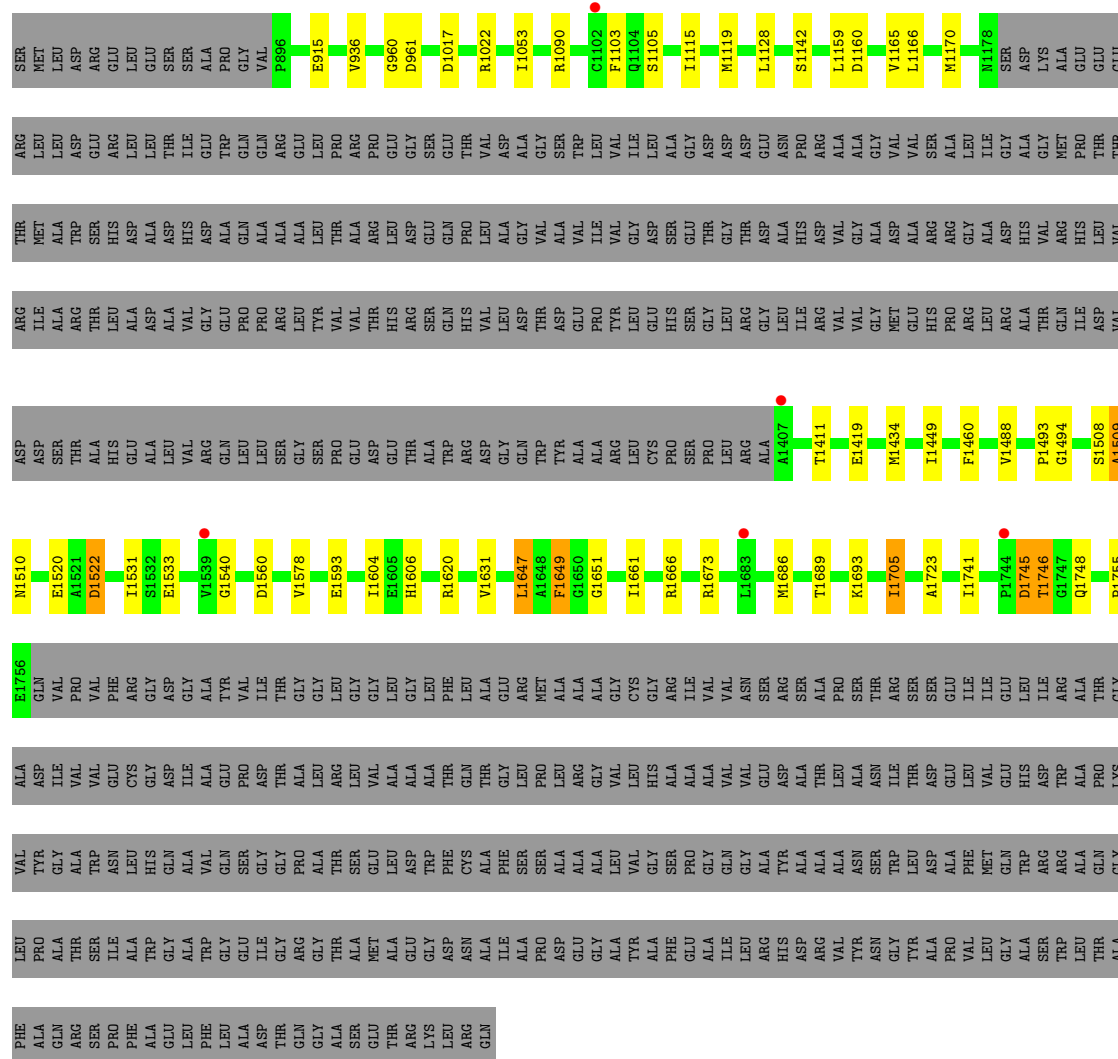
• Molecule 1: Mycocerosic acid synthase





● Molecule 1: Mycocerosic acid synthase

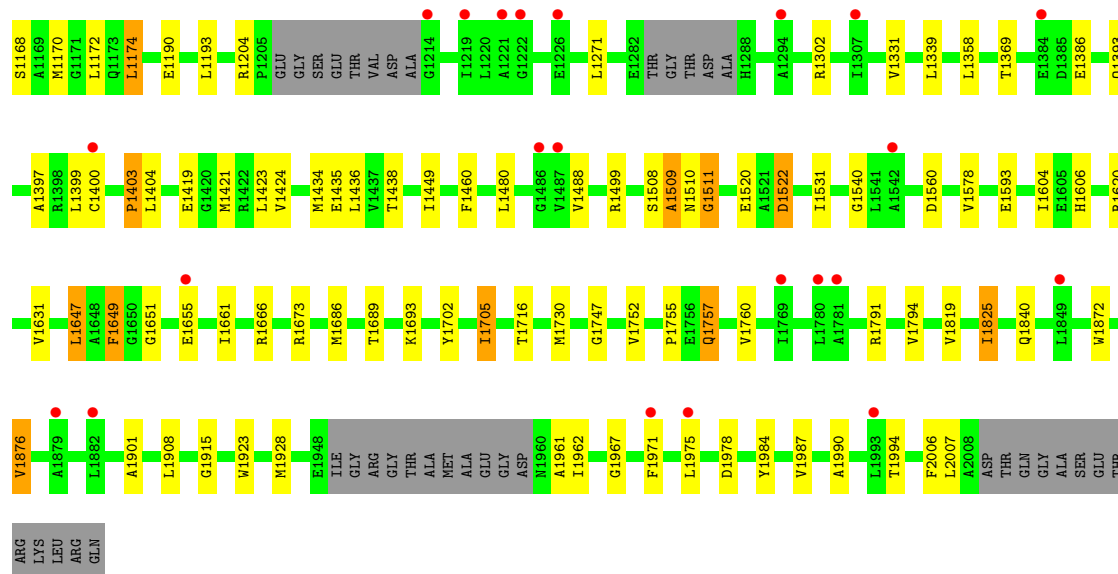
Chain O: 50% 44%



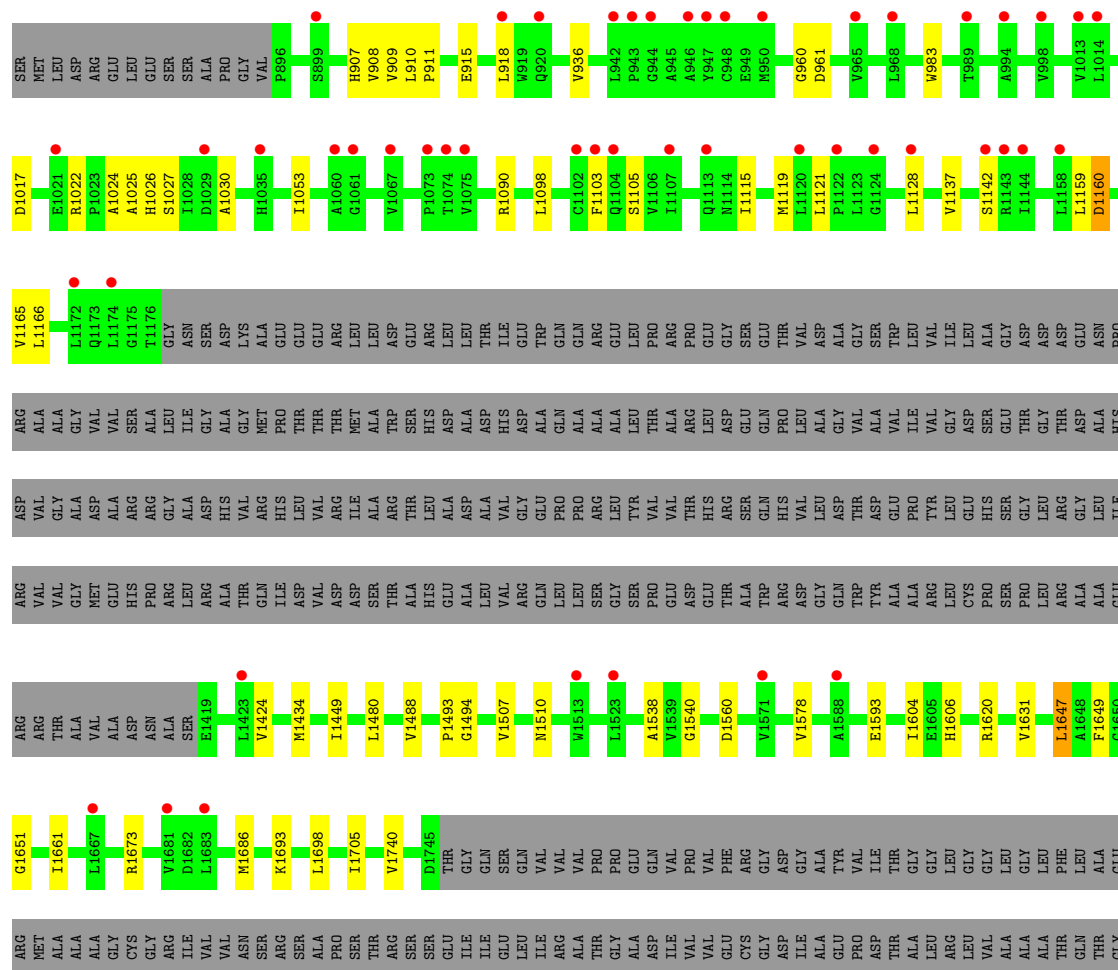
● Molecule 1: Mycocerosic acid synthase

Chain P: 2% 86% 9%





• Molecule 1: Mycocerosic acid synthase



LEU	PRO	ALA	ARG	GLY	VAL	LEU	HIS	ALA	ALA	VAL	VAL	GLU	ASP	ALA	THR	ALA	ASN	ILE	THR	ALA	PRO	LYS	VAL	VAL	GLY	ALA	GLY	THR	TRP	ASN	LEU	HIS	GLN	ALA	VAL	VAL	GLN	VAL	THR	ALA	THR	ALA	THR	ASP	ASN	CYS	ALA	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	ALA	ASP	GLY	ALA	LEU	VAL	GLY	SER	ALA	PRO	GLY	ALA	GLN	VAL	GLY	ALA	ASN	SER	TRP	ILE	GLN	THR	ALA	ASP	ALA	THR	ALA	GLY	TRP	ARG	GLY	GLN	TRP	GLY	ASP	THR	ALA	SER	GLY	THR	ALA	GLY	THR	ASP	ASN	GLY	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	PRO	GLU	ASP	GLY	ALA	TYR	ALA	PHE	GLU	SER	ALA	GLY	ILE	PRO	GLY	ARG	HIS	THR	ASN	TYR	VAL	THR	ALA	ARG	ALA	THR	GLY	ALA	GLY	SER	TRP	ARG	GLY	GLN	LEU	PHE	THR	LEU	GLY	THR	ALA	SER	GLY	THR	ALA	GLY	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Mycocerosic acid synthase



SER	MET	LEU	ASP	GLY	ARG	LEU	GLU	GLU	ALA	ALA	PRO	GLY	VAL	P896	H906	H907	V908	V909	E915	E916	H917	L918	V919	Q920	V936	L942	G960	D961	N983	D1017	R1022	R1090	V1094	L1098	L1099	D1100	F1103	Q1104	S1105	I1115	M1119	L1128	V1137
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

S1142	L1159	D1160	V1165	L1166	E1190	R1191	LEU	THR	ILE	TRP	GLN	GLN	ARG	GLU	PRO	GLY	SER	THR	VAL	ASP	ALA	ASP	ALA	ASP	GLU	ASP	GLU	ASN	PRO	ARG	ALA	ALA	GLY	VAL	VAL	SER	ALA	LEU	ILE	GLY	ALA
-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY	MET	PRO	THR	THR	THR	MET	ALA	TRP	SER	HIS	HIS	ASP	ALA	ASP	HIS	GLY	ALA	GLN	PRO	ALA	ALA	LEU	THR	VAL	THR	GLN	PRO	THR	VAL	THR	ILE	VAL	GLY	ASP	THR	ALA	GLY	ALA	ASP	VAL	ALA	ARG	GLY	ALA	ASP	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	ARG	HIS	LEU	VAL	ARG	ILE	ALA	ARG	THR	ALA	LEU	ASP	ALA	VAL	GLY	GLU	PRO	ALA	ARG	ALA	LEU	THR	VAL	THR	ALA	GLY	THR	VAL	THR	GLY	PRO	GLY	THR	ARG	GLY	VAL	GLY	THR	VAL	GLY	THR	VAL	GLY	ARG	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	GLN	ILE	ASP	VAL	ASP	SER	THR	THR	HIS	GLU	ALA	LEU	VAL	GLN	ARG	LEU	LEU	SER	GLY	THR	PRO	ASP	GLU	THR	ALA	TRP	ARG	THR	ASP	GLY	GLN	CYS	PRO	SER	PRO	LEU	ARG	ALA	VAL	VAL	VAL	ASN	ALA	SER	E1419	G1420
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------

M1421	M1434	E1435	L1436	I1449	V1488	P1493	G1494	S1508	A1509	M1510	E1520	I1531	S1532	E1533	G1540	D1560	V1578	E1593	I1604	E1605	H1606	R1620	V1631	Q1640	L1647	F1648	F1649	G1650	G1651	V1654	E1655	D1660	I1661	R1666	L1669	R1673	V1681
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

B1682	L1683	M1686	K1693	I1705	M1730	L1739	Q1748	S1749	Q1750	E1756	Q1757	V1758	P1759	PHE	ARG	GLY	ASP	THR	GLY	GLY	ALA	TYR	VAL	ILE	THR	GLY	LEU	PHE	LEU	ALA	GLY	ALA	GLY	CYS	THR	ALA	ARG	ILE	VAL	VAL	ASN	SER	ARG	SER
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	PRO	SER	THR	SER	GLY	ILE	ILE	GLU	GLU	ILE	ALA	ASP	ILE	VAL	VAL	GLU	CYS	GLY	ASP	THR	GLN	ILE	ALA	ALA	LEU	ALA	THR	ALA	THR	GLY	LEU	PRO	ALA	GLY	VAL	LEU	HIS	ALA	ARG	ALA	THR	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	LEU	ALA	ASN	THR	ILE	THR	ASP	GLY	LEU	VAL	VAL	GLY	VAL	ASN	LEU	HIS	GLN	GLY	GLY	PRO	GLY	THR	ALA	VAL	GLY	THR	ALA	THR	ALA	ALA	PHE	GLY	PRO	SER	ALA	ALA	LEU	VAL	GLY	THR	ALA	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	ALA	ASN	SER	TRP	GLY	LEU	ASP	ALA	PHE	VAL	GLY	TRP	ARG	GLN	GLY	LEU	PRO	ALA	GLN	THR	ILE	ALA	THR	GLY	ALA	GLY	ALA	THR	ALA	ALA	ILE	ALA	ASP	GLY	GLY	TYR	ALA	PHE	THR	ALA	GLY	THR	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ARG	VAL	TYR	ASN	GLY	TYR	ALA	PRO	VAL	GLY	ALA	PHE	THR	LEU	THR	THR	ALA	ALA	GLN	GLY	ARG	PRO	PHE	ALA	GLY	GLY	THR	GLN	ARG	LYS	LEU	ARG	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	151.38Å 190.37Å 270.84Å 95.58° 91.92° 103.65°	Depositor
Resolution (Å)	78.62 – 3.75 78.62 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (78.62-3.75) 98.9 (78.62-3.75)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.78Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.230 , 0.240 0.247 , 0.258	Depositor DCC
R_{free} test set	2985 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 153.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	262498	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% 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: NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.89	4/8420 (0.0%)	1.16	20/11488 (0.2%)
1	B	0.80	1/8420 (0.0%)	1.12	12/11488 (0.1%)
1	C	0.75	1/8420 (0.0%)	1.09	6/11488 (0.1%)
1	D	0.76	3/8420 (0.0%)	1.10	12/11488 (0.1%)
1	E	0.74	1/8323 (0.0%)	1.08	7/11356 (0.1%)
1	F	0.73	1/8351 (0.0%)	1.08	9/11393 (0.1%)
1	G	0.76	2/8314 (0.0%)	1.09	7/11344 (0.1%)
1	H	0.75	1/8379 (0.0%)	1.09	10/11434 (0.1%)
1	I	0.73	0/4977	1.08	7/6783 (0.1%)
1	J	0.76	2/8323 (0.0%)	1.10	10/11356 (0.1%)
1	K	0.78	1/8323 (0.0%)	1.10	10/11356 (0.1%)
1	L	0.79	2/6815 (0.0%)	1.10	10/9296 (0.1%)
1	M	0.74	1/8323 (0.0%)	1.08	8/11356 (0.1%)
1	N	0.75	1/8323 (0.0%)	1.10	10/11356 (0.1%)
1	O	0.77	1/4797 (0.0%)	1.08	5/6540 (0.1%)
1	P	0.77	2/8323 (0.0%)	1.11	12/11356 (0.1%)
1	Q	0.74	0/4617	1.07	5/6293 (0.1%)
1	R	0.74	0/4844	1.08	5/6602 (0.1%)
All	All	0.77	24/134712 (0.0%)	1.10	165/183773 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1348	ILE	CG1-CD1	7.42	1.80	1.51
1	K	1730	MET	SD-CE	6.98	1.97	1.79
1	L	1170	MET	SD-CE	6.96	1.97	1.79
1	A	1013	VAL	CA-C	-6.62	1.44	1.52
1	O	1170	MET	SD-CE	5.76	1.94	1.79
1	P	1730	MET	SD-CE	5.52	1.93	1.79
1	D	883	MET	SD-CE	-5.47	1.65	1.79
1	A	987	ALA	CA-C	-5.39	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	892	ALA	CA-C	5.38	1.59	1.52
1	A	1604	ILE	CA-CB	5.38	1.60	1.53
1	B	1825	ILE	CG1-CD1	-5.24	1.31	1.51
1	F	1825	ILE	CG1-CD1	-5.22	1.31	1.51
1	L	1825	ILE	CG1-CD1	-5.21	1.31	1.51
1	H	1825	ILE	CG1-CD1	-5.18	1.31	1.51
1	J	1825	ILE	CG1-CD1	-5.17	1.31	1.51
1	M	1825	ILE	CG1-CD1	-5.12	1.31	1.51
1	D	1825	ILE	CG1-CD1	-5.10	1.31	1.51
1	P	1825	ILE	CG1-CD1	-5.08	1.31	1.51
1	C	1825	ILE	CG1-CD1	-5.08	1.31	1.51
1	E	1825	ILE	CG1-CD1	-5.07	1.31	1.51
1	A	1539	VAL	CA-C	5.07	1.59	1.52
1	G	1825	ILE	CG1-CD1	-5.05	1.32	1.51
1	G	1832	LEU	C-N	5.00	1.40	1.33
1	J	1348	ILE	CG1-CD1	5.00	1.71	1.51

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1522	ASP	CA-CB-CG	8.74	121.34	112.60
1	B	1522	ASP	CA-CB-CG	8.53	121.12	112.60
1	D	893	PRO	CA-C-N	7.47	127.33	122.18
1	D	893	PRO	C-N-CA	7.47	127.33	122.18
1	J	1522	ASP	CA-CB-CG	7.20	119.80	112.60
1	L	1522	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	1560	ASP	CA-CB-CG	7.08	119.68	112.60
1	H	1504	VAL	CA-C-N	7.07	126.45	121.65
1	H	1504	VAL	C-N-CA	7.07	126.45	121.65
1	B	1178	ASN	CA-C-N	6.93	134.78	121.54
1	B	1178	ASN	C-N-CA	6.93	134.78	121.54
1	J	1978	ASP	CA-CB-CG	6.91	119.51	112.60
1	D	1522	ASP	CA-CB-CG	6.76	119.36	112.60
1	P	1522	ASP	CA-CB-CG	6.70	119.30	112.60
1	J	1425	VAL	N-CA-CB	6.68	117.81	110.53
1	F	1522	ASP	CA-CB-CG	6.65	119.25	112.60
1	N	1925	ASP	CA-CB-CG	6.62	119.22	112.60
1	J	2002	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	1017	ASP	CA-CB-CG	6.56	119.16	112.60
1	M	1522	ASP	CA-CB-CG	6.56	119.16	112.60
1	O	1522	ASP	CA-CB-CG	6.45	119.05	112.60
1	I	1522	ASP	CA-CB-CG	6.40	119.00	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1522	ASP	CA-CB-CG	6.40	119.00	112.60
1	O	1560	ASP	CA-CB-CG	6.34	118.94	112.60
1	Q	1560	ASP	CA-CB-CG	6.34	118.94	112.60
1	N	1522	ASP	CA-CB-CG	6.29	118.89	112.60
1	C	1560	ASP	CA-CB-CG	6.28	118.88	112.60
1	L	1560	ASP	CA-CB-CG	6.28	118.88	112.60
1	R	1560	ASP	CA-CB-CG	6.22	118.82	112.60
1	L	1504	VAL	CA-C-N	6.21	125.88	121.65
1	L	1504	VAL	C-N-CA	6.21	125.88	121.65
1	N	1560	ASP	CA-CB-CG	6.21	118.81	112.60
1	E	1560	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	1675	ASN	CA-CB-CG	6.16	118.76	112.60
1	H	1560	ASP	CA-CB-CG	6.16	118.76	112.60
1	D	1560	ASP	CA-CB-CG	6.13	118.73	112.60
1	F	1560	ASP	CA-CB-CG	6.12	118.72	112.60
1	M	1560	ASP	CA-CB-CG	6.11	118.71	112.60
1	H	2002	PHE	CA-CB-CG	6.11	119.91	113.80
1	L	1741	ILE	CB-CA-C	6.11	118.00	110.73
1	G	1560	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	1474	ASP	CA-CB-CG	6.10	118.70	112.60
1	K	1560	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	1560	ASP	CA-CB-CG	6.09	118.69	112.60
1	E	1175	GLY	N-CA-C	6.08	121.49	111.59
1	J	1560	ASP	CA-CB-CG	6.08	118.67	112.60
1	P	1560	ASP	CA-CB-CG	6.07	118.67	112.60
1	I	1560	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	1649	PHE	CA-CB-CG	-5.81	107.99	113.80
1	H	1978	ASP	CA-CB-CG	5.80	118.40	112.60
1	M	1978	ASP	CA-CB-CG	5.72	118.32	112.60
1	O	1649	PHE	CA-CB-CG	-5.71	108.09	113.80
1	M	1103	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	1017	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	1636	THR	N-CA-C	5.69	118.84	109.85
1	B	1175	GLY	N-CA-C	5.69	118.87	110.63
1	A	1539	VAL	N-CA-C	5.68	115.87	110.42
1	N	1649	PHE	CA-CB-CG	-5.67	108.13	113.80
1	M	1649	PHE	CA-CB-CG	-5.67	108.14	113.80
1	G	1649	PHE	CA-CB-CG	-5.66	108.14	113.80
1	I	1649	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	2002	PHE	CA-CB-CG	5.63	119.43	113.80
1	D	1103	PHE	CA-CB-CG	5.63	119.43	113.80
1	M	2002	PHE	CA-CB-CG	5.63	119.43	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1764	ASP	CA-CB-CG	5.62	118.22	112.60
1	R	1649	PHE	CA-CB-CG	-5.62	108.18	113.80
1	P	1403	PRO	CA-C-N	5.61	132.26	121.54
1	P	1403	PRO	C-N-CA	5.61	132.26	121.54
1	P	1978	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	1473	PHE	CA-C-N	5.61	127.79	120.28
1	A	1473	PHE	C-N-CA	5.61	127.79	120.28
1	Q	1649	PHE	CA-CB-CG	-5.60	108.20	113.80
1	L	2002	PHE	CA-CB-CG	5.58	119.38	113.80
1	D	1649	PHE	CA-CB-CG	-5.57	108.23	113.80
1	J	1649	PHE	CA-CB-CG	-5.57	108.23	113.80
1	P	1649	PHE	CA-CB-CG	-5.56	108.24	113.80
1	E	1649	PHE	CA-CB-CG	-5.55	108.25	113.80
1	N	1103	PHE	CA-CB-CG	5.55	119.35	113.80
1	K	1103	PHE	CA-CB-CG	5.54	119.34	113.80
1	P	1103	PHE	CA-CB-CG	5.53	119.33	113.80
1	I	1017	ASP	CA-CB-CG	5.50	118.10	112.60
1	P	1757	GLN	N-CA-C	-5.50	105.79	112.88
1	F	1017	ASP	CA-CB-CG	5.49	118.09	112.60
1	F	1649	PHE	CA-CB-CG	-5.48	108.32	113.80
1	K	1522	ASP	CA-CB-CG	5.48	118.08	112.60
1	O	1103	PHE	CA-CB-CG	5.48	119.28	113.80
1	H	1649	PHE	CA-CB-CG	-5.46	108.34	113.80
1	F	1205	PRO	CA-C-N	5.46	131.52	121.70
1	F	1205	PRO	C-N-CA	5.46	131.52	121.70
1	G	1103	PHE	CA-CB-CG	5.45	119.25	113.80
1	I	1103	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	884	LEU	N-CA-C	-5.43	105.01	111.69
1	O	1017	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	1745	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	1160	ASP	CA-CB-CG	5.42	118.03	112.60
1	N	1160	ASP	CA-CB-CG	5.42	118.02	112.60
1	F	2002	PHE	CA-CB-CG	5.41	119.21	113.80
1	L	1103	PHE	CA-CB-CG	5.41	119.21	113.80
1	C	2002	PHE	CA-CB-CG	5.41	119.21	113.80
1	R	1017	ASP	CA-CB-CG	5.40	118.00	112.60
1	E	2002	PHE	CA-CB-CG	5.40	119.20	113.80
1	C	1103	PHE	CA-CB-CG	5.39	119.19	113.80
1	L	1649	PHE	CA-CB-CG	-5.39	108.41	113.80
1	J	1103	PHE	CA-CB-CG	5.38	119.18	113.80
1	H	1017	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	1103	PHE	CA-CB-CG	5.37	119.17	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	893	PRO	N-CA-C	5.36	119.02	110.40
1	D	1160	ASP	CA-CB-CG	5.35	117.95	112.60
1	N	1017	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	1649	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	1707	ASP	CA-CB-CG	5.32	117.92	112.60
1	P	1460	PHE	CA-CB-CG	-5.32	108.48	113.80
1	B	1978	ASP	CA-CB-CG	5.31	117.91	112.60
1	F	1103	PHE	CA-CB-CG	5.29	119.09	113.80
1	K	2002	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	1103	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	2002	PHE	CA-CB-CG	5.29	119.09	113.80
1	H	1103	PHE	CA-CB-CG	5.28	119.08	113.80
1	R	1103	PHE	CA-CB-CG	5.26	119.06	113.80
1	G	1017	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	1280	ASP	CA-CB-CG	5.25	117.84	112.60
1	K	1017	ASP	CA-CB-CG	5.25	117.84	112.60
1	Q	1017	ASP	CA-CB-CG	5.25	117.84	112.60
1	K	1756	GLU	N-CA-C	-5.23	106.96	113.55
1	A	1962	ILE	N-CA-CB	5.23	116.42	110.72
1	J	1017	ASP	CA-CB-CG	5.22	117.82	112.60
1	N	1633	ASN	N-CA-C	5.22	116.76	108.67
1	B	1757	GLN	N-CA-C	-5.22	106.69	113.16
1	J	1757	GLN	N-CA-C	-5.21	106.76	113.02
1	M	1017	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	1648	ALA	N-CA-C	5.21	117.56	108.76
1	I	1415	ASP	CA-CB-CG	5.20	117.80	112.60
1	G	1416	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	1649	PHE	CA-CB-CG	-5.20	108.60	113.80
1	C	1160	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	1017	ASP	CA-CB-CG	5.18	117.78	112.60
1	L	1017	ASP	CA-CB-CG	5.17	117.77	112.60
1	Q	1160	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	1017	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	885	ASP	N-CA-C	-5.14	105.76	111.36
1	H	1655	GLU	CB-CG-CD	5.14	121.33	112.60
1	D	1017	ASP	CA-CB-CG	5.13	117.73	112.60
1	K	1649	PHE	CA-CB-CG	-5.13	108.67	113.80
1	G	1160	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	1523	LEU	N-CA-C	5.12	118.66	112.93
1	F	1160	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	1103	PHE	CA-CB-CG	5.11	118.91	113.80
1	H	1178	ASN	CA-CB-CG	5.10	117.70	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1160	ASP	CA-CB-CG	5.10	117.70	112.60
1	Q	1103	PHE	CA-CB-CG	5.10	118.90	113.80
1	K	1327	ARG	CA-C-N	5.09	127.41	120.54
1	K	1327	ARG	C-N-CA	5.09	127.41	120.54
1	K	1655	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	961	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	1160	ASP	CA-CB-CG	5.08	117.67	112.60
1	R	1160	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	1978	ASP	CA-CB-CG	5.05	117.65	112.60
1	J	1160	ASP	CA-CB-CG	5.04	117.64	112.60
1	I	1655	GLU	CB-CG-CD	5.03	121.16	112.60
1	P	1160	ASP	CA-CB-CG	5.03	117.63	112.60
1	P	1655	GLU	CB-CG-CD	5.03	121.15	112.60
1	P	1017	ASP	CA-CB-CG	5.02	117.62	112.60
1	L	1757	GLN	N-CA-C	-5.01	107.01	112.72
1	N	1327	ARG	CA-C-N	5.01	127.30	120.54
1	N	1327	ARG	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8245	8038	8072	39	0
1	B	8245	8038	8072	44	0
1	C	8245	8038	8072	31	1
1	D	8245	8038	8072	38	0
1	E	8149	7945	7979	31	0
1	F	8177	7965	7999	36	0
1	G	8140	7939	7973	32	0
1	H	8204	7991	8025	44	0
1	I	4879	4801	4822	19	0
1	J	8149	7945	7979	37	1
1	K	8149	7945	7979	36	0
1	L	6674	6535	6560	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	8149	7945	7979	28	0
1	N	8149	7945	7979	32	0
1	O	4702	4625	4646	17	0
1	P	8149	7945	7979	36	0
1	Q	4524	4455	4476	36	0
1	R	4748	4669	4690	28	0
2	A	75	36	36	2	0
2	B	75	36	36	2	0
2	C	79	36	36	1	0
2	D	75	36	36	2	0
2	E	48	25	25	1	0
2	F	75	36	36	2	0
2	G	75	36	36	0	0
2	H	75	36	36	0	0
2	I	48	25	25	1	0
2	J	75	36	36	0	0
2	K	75	36	36	2	0
2	L	48	25	25	1	0
2	M	75	36	36	0	0
2	N	75	36	36	0	0
2	O	48	25	25	1	0
2	P	75	36	36	0	0
2	Q	48	25	25	0	0
2	R	48	25	25	0	0
All	All	133114	129384	129935	540	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 2.

All (540) 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:N:1348:ILE:CD1	1:N:1348:ILE:CG1	1.80	1.59
1:F:1730:MET:HE3	1:F:1739:LEU:HD22	1.58	0.85
1:L:1730:MET:HE3	1:L:1739:LEU:HD22	1.63	0.80
1:J:1730:MET:HE3	1:J:1739:LEU:HD22	1.64	0.79
1:N:1901:ALA:HB2	1:N:1928:MET:HE3	1.63	0.78
1:C:1730:MET:HE3	1:C:1739:LEU:HD22	1.65	0.77
1:Q:908:VAL:HG13	1:R:920:GLN:HB2	1.68	0.75
1:N:1193:LEU:HD22	1:N:1399:LEU:HD22	1.70	0.73
1:C:914:PRO:HD3	1:D:1638:PRO:HG3	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:909:VAL:O	1:R:983:TRP:NE1	2.21	0.71
1:A:1098:LEU:HD21	1:A:1137:VAL:HG11	1.73	0.71
1:A:1631:VAL:HG23	1:A:1647:LEU:HD23	1.73	0.70
1:B:1901:ALA:HB2	1:B:1928:MET:HE3	1.74	0.70
1:M:1901:ALA:HB2	1:M:1928:MET:HE3	1.74	0.69
1:F:1050:THR:O	1:F:1988:LEU:HD22	1.92	0.69
1:C:1901:ALA:HB2	1:C:1928:MET:HE3	1.75	0.69
1:J:1901:ALA:HB2	1:J:1928:MET:HE3	1.75	0.69
1:G:1962:ILE:HD12	1:G:1984:TYR:CE1	2.28	0.69
1:L:1901:ALA:HB2	1:L:1928:MET:HE3	1.75	0.69
1:P:1901:ALA:HB2	1:P:1928:MET:HE3	1.74	0.69
1:F:1901:ALA:HB2	1:F:1928:MET:HE3	1.75	0.69
1:K:1901:ALA:HB2	1:K:1928:MET:HE3	1.75	0.68
1:D:1901:ALA:HB2	1:D:1928:MET:HE3	1.75	0.68
1:H:1901:ALA:HB2	1:H:1928:MET:HE3	1.75	0.68
1:G:1901:ALA:HB2	1:G:1928:MET:HE3	1.76	0.66
1:E:1901:ALA:HB2	1:E:1928:MET:HE3	1.76	0.66
1:P:1421:MET:HE3	1:P:1436:LEU:HD21	1.76	0.66
1:L:1421:MET:HB2	1:L:1436:LEU:HD21	1.78	0.65
1:K:1438:THR:HB	1:K:1752:VAL:HG11	1.81	0.63
1:O:1649:PHE:CD1	1:P:1689:THR:HG21	2.33	0.63
1:E:1689:THR:HG21	1:F:1649:PHE:CD1	2.34	0.63
1:Q:909:VAL:HB	1:R:920:GLN:NE2	2.14	0.63
1:N:1730:MET:HE3	1:N:1739:LEU:HD22	1.80	0.62
1:Q:1507:VAL:HG23	1:Q:1698:LEU:HD11	1.80	0.62
1:A:1567:ALA:HB1	1:A:1576:ILE:HD11	1.80	0.62
1:A:1971:PHE:CZ	1:A:1975:LEU:HD11	2.35	0.61
1:B:1421:MET:CE	1:B:1436:LEU:HD21	2.30	0.61
1:H:1593:GLU:OE1	1:Q:1024:ALA:HB3	2.00	0.61
1:Q:911:PRO:HD3	1:R:983:TRP:CD1	2.35	0.61
1:Q:918:LEU:HD21	1:R:908:VAL:HG11	1.84	0.60
1:B:1193:LEU:HD22	1:B:1399:LEU:HD11	1.85	0.59
1:H:1730:MET:HE3	1:H:1739:LEU:HD22	1.84	0.59
1:K:1666:ARG:HB3	1:L:1666:ARG:HB3	1.85	0.59
1:E:1193:LEU:HD22	1:E:1399:LEU:HD22	1.84	0.58
1:G:1421:MET:CE	1:G:1436:LEU:HD21	2.33	0.58
1:H:1597:GLN:HG2	1:Q:1026:HIS:HA	1.84	0.58
1:C:883:MET:HE2	1:D:885:ASP:OD2	2.02	0.58
1:I:1730:MET:HE3	1:I:1739:LEU:HD22	1.85	0.58
1:H:1193:LEU:HD22	1:H:1399:LEU:HD11	1.87	0.57
1:M:1689:THR:HG21	1:N:1649:PHE:CD1	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:MET:HE1	1:B:883:MET:HE3	1.86	0.57
1:J:1421:MET:CE	1:J:1436:LEU:HD21	2.35	0.57
1:F:1791:ARG:CZ	1:F:1819:VAL:HG21	2.35	0.56
1:Q:918:LEU:CD2	1:R:908:VAL:HG11	2.36	0.56
1:A:892:ALA:HB3	1:A:893:PRO:HD3	1.87	0.56
1:H:1601:ASP:HB3	1:Q:1030:ALA:HB3	1.88	0.56
1:M:1962:ILE:HD12	1:M:1984:TYR:CE1	2.41	0.56
1:P:1119:MET:HE2	1:P:1121:LEU:HD11	1.88	0.56
1:Q:909:VAL:HB	1:R:920:GLN:HE22	1.71	0.55
1:E:1730:MET:HE3	1:E:1739:LEU:HD22	1.89	0.55
1:N:1119:MET:HE2	1:N:1121:LEU:HD11	1.89	0.55
1:K:936:VAL:HG13	1:K:1119:MET:HE1	1.89	0.55
1:K:1119:MET:HE2	1:K:1121:LEU:HD11	1.89	0.55
1:Q:1119:MET:HE2	1:Q:1121:LEU:HD11	1.88	0.55
1:E:1119:MET:HE2	1:E:1121:LEU:HD11	1.89	0.55
1:A:1689:THR:HG21	1:B:1649:PHE:CD1	2.41	0.55
1:H:1119:MET:HE2	1:H:1121:LEU:HD11	1.89	0.55
1:O:936:VAL:HG13	1:O:1119:MET:HE1	1.88	0.55
1:J:1119:MET:HE2	1:J:1121:LEU:HD11	1.89	0.54
1:A:1901:ALA:HB2	1:A:1928:MET:HE3	1.88	0.54
1:C:1119:MET:HE2	1:C:1121:LEU:HD11	1.89	0.54
1:M:936:VAL:HG13	1:M:1119:MET:HE1	1.90	0.54
1:K:1649:PHE:CD1	1:L:1689:THR:HG21	2.43	0.54
1:B:1962:ILE:HD12	1:B:1984:TYR:CE1	2.43	0.54
1:C:936:VAL:HG13	1:C:1119:MET:HE1	1.90	0.54
1:I:1119:MET:HE2	1:I:1121:LEU:HD11	1.89	0.54
1:O:1689:THR:HG21	1:P:1649:PHE:CD1	2.43	0.54
1:F:1119:MET:HE2	1:F:1121:LEU:HD11	1.88	0.54
1:G:1119:MET:HE2	1:G:1121:LEU:HD11	1.89	0.54
1:B:1119:MET:HE2	1:B:1121:LEU:HD11	1.89	0.53
1:C:1649:PHE:CD1	1:D:1689:THR:HG21	2.42	0.53
1:L:1119:MET:HE2	1:L:1121:LEU:HD11	1.90	0.53
1:D:1119:MET:HE2	1:D:1121:LEU:HD11	1.89	0.53
1:M:1119:MET:HE2	1:M:1121:LEU:HD11	1.89	0.53
1:E:936:VAL:HG13	1:E:1119:MET:HE1	1.90	0.53
1:H:1601:ASP:HB3	1:Q:1030:ALA:CB	2.38	0.53
1:D:1531:ILE:HG21	1:D:1705:ILE:HG23	1.90	0.53
1:C:1168:SER:HB2	1:C:1170:MET:HE3	1.90	0.53
1:D:1962:ILE:HD12	1:D:1984:TYR:CE1	2.44	0.53
1:J:936:VAL:HG13	1:J:1119:MET:HE1	1.90	0.53
1:N:1747:GLY:O	1:N:1748:GLN:C	2.50	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ALA:HB3	1:B:893:PRO:CD	2.38	0.53
1:H:936:VAL:HG13	1:H:1119:MET:HE1	1.91	0.53
1:I:936:VAL:HG13	1:I:1119:MET:HE1	1.91	0.53
1:Q:936:VAL:HG13	1:Q:1119:MET:HE1	1.91	0.53
1:A:1569:GLY:O	1:A:1573:GLN:HG3	2.09	0.53
1:D:1730:MET:HE3	1:D:1739:LEU:HD22	1.91	0.53
1:H:1531:ILE:HG21	1:H:1705:ILE:HG23	1.88	0.53
1:K:1686:MET:HE1	1:K:1693:LYS:HG2	1.91	0.53
1:F:1168:SER:HB2	1:F:1170:MET:HE3	1.91	0.53
1:L:936:VAL:HG13	1:L:1119:MET:HE1	1.91	0.53
1:H:1593:GLU:HB3	1:Q:1024:ALA:HB2	1.91	0.52
1:L:1962:ILE:HD12	1:L:1984:TYR:CE1	2.44	0.52
1:N:936:VAL:HG13	1:N:1119:MET:HE1	1.90	0.52
1:P:1399:LEU:HD21	1:P:1908:LEU:HD21	1.91	0.52
1:B:1686:MET:HE1	1:B:1693:LYS:HG2	1.92	0.52
1:D:1929:GLN:HG2	1:D:1980:VAL:HG11	1.91	0.52
1:G:1686:MET:HE1	1:G:1693:LYS:HG2	1.92	0.52
1:Q:1686:MET:HE1	1:Q:1693:LYS:HG2	1.91	0.52
1:A:1438:THR:HB	1:A:1752:VAL:HG11	1.90	0.52
1:D:1686:MET:HE1	1:D:1693:LYS:HG2	1.91	0.52
1:I:1686:MET:HE1	1:I:1693:LYS:HG2	1.92	0.52
1:J:1421:MET:HE3	1:J:1436:LEU:HD21	1.92	0.52
1:F:1421:MET:HE3	1:F:1436:LEU:HD21	1.91	0.52
1:M:1649:PHE:CD1	1:N:1689:THR:HG21	2.43	0.52
1:P:1168:SER:HB2	1:P:1170:MET:HE3	1.92	0.52
1:P:936:VAL:HG13	1:P:1119:MET:HE1	1.90	0.52
1:D:1971:PHE:CZ	1:D:1975:LEU:HD11	2.45	0.52
1:E:1962:ILE:HD12	1:E:1984:TYR:CE1	2.44	0.52
1:J:1686:MET:HE1	1:J:1693:LYS:HG2	1.91	0.52
1:J:1962:ILE:HD12	1:J:1984:TYR:CE1	2.45	0.52
1:N:1686:MET:HE1	1:N:1693:LYS:HG2	1.91	0.52
1:B:1193:LEU:HD21	1:B:2006:PHE:CZ	2.45	0.52
1:F:1962:ILE:HD12	1:F:1984:TYR:CE1	2.45	0.52
1:H:1962:ILE:HD12	1:H:1984:TYR:CE1	2.44	0.52
1:Q:909:VAL:H	1:R:920:GLN:CD	2.18	0.52
1:K:1631:VAL:HG23	1:K:1647:LEU:HD23	1.92	0.51
1:K:1962:ILE:HD12	1:K:1984:TYR:CE1	2.45	0.51
1:P:1053:ILE:HG13	1:P:1119:MET:HE3	1.92	0.51
1:C:1962:ILE:HD12	1:C:1984:TYR:CE1	2.45	0.51
1:G:936:VAL:HG13	1:G:1119:MET:HE1	1.91	0.51
1:M:1686:MET:HE1	1:M:1693:LYS:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:936:VAL:HG13	1:F:1119:MET:HE1	1.91	0.51
1:P:1686:MET:HE1	1:P:1693:LYS:HG2	1.92	0.51
1:F:1569:GLY:HA3	2:F:3001:NAP:O1A	2.11	0.51
1:F:1686:MET:HE1	1:F:1693:LYS:HG2	1.92	0.51
1:G:1971:PHE:CZ	1:G:1975:LEU:HD11	2.45	0.51
1:E:1531:ILE:HG21	1:E:1705:ILE:HG23	1.93	0.51
1:F:1421:MET:CE	1:F:1436:LEU:HD21	2.40	0.51
1:M:907:HIS:HE2	1:M:917:HIS:HD1	1.58	0.51
1:E:1971:PHE:CZ	1:E:1975:LEU:HD11	2.45	0.51
1:R:907:HIS:HE2	1:R:917:HIS:HD1	1.59	0.51
1:A:1073:PRO:HA	1:A:1109:HIS:HE2	1.76	0.51
1:F:1971:PHE:CZ	1:F:1975:LEU:HD11	2.46	0.51
1:G:1649:PHE:CD1	1:H:1689:THR:HG21	2.46	0.51
1:I:907:HIS:HE2	1:I:917:HIS:HD1	1.59	0.51
1:O:1631:VAL:HG23	1:O:1647:LEU:HD23	1.93	0.51
1:L:1686:MET:HE1	1:L:1693:LYS:HG2	1.92	0.51
1:G:1631:VAL:HG23	1:G:1647:LEU:HD23	1.93	0.51
1:Q:1631:VAL:HG23	1:Q:1647:LEU:HD23	1.93	0.51
1:G:1730:MET:HE3	1:G:1739:LEU:HD22	1.93	0.50
1:I:1631:VAL:HG23	1:I:1647:LEU:HD23	1.93	0.50
1:K:1053:ILE:HG13	1:K:1119:MET:HE3	1.93	0.50
1:O:1686:MET:HE1	1:O:1693:LYS:HG2	1.92	0.50
1:B:1569:GLY:HA3	2:B:3001:NAP:O1A	2.11	0.50
1:D:936:VAL:HG13	1:D:1119:MET:HE1	1.91	0.50
1:E:1631:VAL:HG23	1:E:1647:LEU:HD23	1.93	0.50
1:G:907:HIS:HE2	1:G:917:HIS:HD1	1.59	0.50
1:N:1901:ALA:CB	1:N:1928:MET:HE3	2.35	0.50
1:R:1631:VAL:HG23	1:R:1647:LEU:HD23	1.94	0.50
1:B:936:VAL:HG13	1:B:1119:MET:HE1	1.93	0.50
1:C:1053:ILE:HG13	1:C:1119:MET:HE3	1.94	0.50
1:C:1686:MET:HE1	1:C:1693:LYS:HG2	1.93	0.50
1:R:1686:MET:HE1	1:R:1693:LYS:HG2	1.93	0.50
1:A:1531:ILE:HG21	1:A:1705:ILE:HG23	1.93	0.50
1:A:1603:GLY:HA2	1:J:1029:ASP:HB2	1.92	0.50
1:G:1053:ILE:HG13	1:G:1119:MET:HE3	1.94	0.50
1:H:1053:ILE:HG13	1:H:1119:MET:HE3	1.94	0.50
1:H:1168:SER:HB2	1:H:1170:MET:HE3	1.94	0.50
1:A:1441:ARG:NH2	1:A:1489:THR:HG21	2.26	0.50
1:A:1458:ILE:HD11	1:A:1741:ILE:HD13	1.94	0.50
1:D:1631:VAL:HG23	1:D:1647:LEU:HD23	1.94	0.50
1:E:1053:ILE:HG13	1:E:1119:MET:HE3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1631:VAL:HG23	1:H:1647:LEU:HD23	1.93	0.50
1:J:1193:LEU:HD21	1:J:2006:PHE:CZ	2.47	0.50
1:N:1631:VAL:HG23	1:N:1647:LEU:HD23	1.93	0.50
1:Q:1053:ILE:HG13	1:Q:1119:MET:HE3	1.94	0.50
1:B:1339:LEU:HA	1:B:1342:SER:OG	2.12	0.50
1:G:1193:LEU:HD21	1:G:2006:PHE:CZ	2.47	0.50
1:P:1480:LEU:O	1:P:1511:GLY:HA2	2.12	0.50
1:P:1631:VAL:HG23	1:P:1647:LEU:HD23	1.93	0.50
1:N:1971:PHE:CZ	1:N:1975:LEU:HD11	2.47	0.50
1:C:1971:PHE:CZ	1:C:1975:LEU:HD11	2.47	0.50
1:K:1971:PHE:CZ	1:K:1975:LEU:HD11	2.46	0.50
1:N:1438:THR:HB	1:N:1752:VAL:HG11	1.94	0.50
1:O:1053:ILE:HG13	1:O:1119:MET:HE3	1.94	0.50
1:B:1631:VAL:HG23	1:B:1647:LEU:HD23	1.93	0.49
1:D:1399:LEU:HD13	1:D:2006:PHE:CZ	2.45	0.49
1:F:1631:VAL:HG23	1:F:1647:LEU:HD23	1.93	0.49
1:G:1531:ILE:HG21	1:G:1705:ILE:HG23	1.94	0.49
1:B:1053:ILE:HG13	1:B:1119:MET:HE3	1.93	0.49
1:H:1193:LEU:HD21	1:H:2006:PHE:CZ	2.47	0.49
1:K:1689:THR:HG21	1:L:1649:PHE:CD1	2.47	0.49
1:L:1631:VAL:HG23	1:L:1647:LEU:HD23	1.93	0.49
1:Q:1449:ILE:HG23	1:Q:1488:VAL:HG13	1.93	0.49
1:R:1421:MET:HE2	1:R:1436:LEU:HD21	1.93	0.49
1:B:1458:ILE:HD11	1:B:1741:ILE:HD13	1.94	0.49
1:K:1193:LEU:HD21	1:K:2006:PHE:CZ	2.48	0.49
1:N:1531:ILE:HG21	1:N:1705:ILE:HG23	1.94	0.49
1:R:1756:GLU:HA	1:R:1757:GLN:C	2.37	0.49
1:D:1053:ILE:HG13	1:D:1119:MET:HE3	1.94	0.49
1:F:1193:LEU:HD21	1:F:2006:PHE:CZ	2.47	0.49
1:H:1686:MET:HE1	1:H:1693:LYS:HG2	1.92	0.49
1:J:1531:ILE:HG21	1:J:1705:ILE:HG23	1.93	0.49
1:C:1631:VAL:HG23	1:C:1647:LEU:HD23	1.93	0.49
1:J:1753:VAL:HG23	1:J:1753:VAL:O	2.12	0.49
1:J:1971:PHE:CZ	1:J:1975:LEU:HD11	2.47	0.49
1:M:1631:VAL:HG23	1:M:1647:LEU:HD23	1.93	0.49
1:B:892:ALA:HB3	1:B:893:PRO:HD3	1.93	0.49
1:D:1460:PHE:CD1	2:D:3001:NAP:H52A	2.46	0.49
1:E:1686:MET:HE1	1:E:1693:LYS:HG2	1.92	0.49
1:F:1434:MET:HE3	1:F:1724:ALA:HA	1.95	0.49
1:I:1649:PHE:CD1	1:J:1689:THR:HG21	2.48	0.49
1:J:1053:ILE:HG13	1:J:1119:MET:HE3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1448:GLN:C	1:L:1449:ILE:HD12	2.37	0.49
1:N:1053:ILE:HG13	1:N:1119:MET:HE3	1.93	0.49
1:J:1631:VAL:HG23	1:J:1647:LEU:HD23	1.93	0.49
1:K:1901:ALA:CB	1:K:1928:MET:HE3	2.42	0.49
1:B:1438:THR:HB	1:B:1752:VAL:HG11	1.95	0.49
1:H:1601:ASP:OD2	1:Q:1027:SER:HB3	2.13	0.49
1:M:1053:ILE:HG13	1:M:1119:MET:HE3	1.94	0.49
1:P:1971:PHE:CZ	1:P:1975:LEU:HD11	2.47	0.49
1:O:1531:ILE:HG21	1:O:1705:ILE:HG23	1.94	0.49
1:A:883:MET:CE	1:B:883:MET:HE3	2.42	0.48
1:M:1531:ILE:HG21	1:M:1705:ILE:HG23	1.94	0.48
1:B:1531:ILE:HG21	1:B:1705:ILE:HG23	1.95	0.48
1:I:1053:ILE:HG13	1:I:1119:MET:HE3	1.94	0.48
1:J:1189:ASP:HA	1:J:1403:PRO:HB3	1.95	0.48
1:K:1531:ILE:HG21	1:K:1705:ILE:HG23	1.95	0.48
1:D:1449:ILE:HG23	1:D:1488:VAL:HG13	1.96	0.48
1:I:1449:ILE:HG23	1:I:1488:VAL:HG13	1.96	0.48
1:I:1531:ILE:HG21	1:I:1705:ILE:HG23	1.94	0.48
1:L:1053:ILE:HG13	1:L:1119:MET:HE3	1.94	0.48
1:L:1531:ILE:HG21	1:L:1705:ILE:HG23	1.94	0.48
1:M:1449:ILE:HG23	1:M:1488:VAL:HG13	1.96	0.48
1:E:1193:LEU:HD21	1:E:2006:PHE:CZ	2.49	0.48
1:F:1053:ILE:HG13	1:F:1119:MET:HE3	1.94	0.48
1:A:1424:VAL:HA	1:A:1480:LEU:HD12	1.96	0.48
1:C:1449:ILE:HG23	1:C:1488:VAL:HG13	1.96	0.48
1:C:1460:PHE:CD1	2:C:3001:NAP:H52A	2.48	0.48
1:C:1531:ILE:HG21	1:C:1705:ILE:HG23	1.95	0.48
1:H:1431:LEU:HD21	1:H:1727:ILE:HG21	1.95	0.48
1:Q:1538:ALA:HB2	1:Q:1740:VAL:CG2	2.43	0.48
1:A:883:MET:SD	1:B:883:MET:HE3	2.54	0.48
1:E:1449:ILE:HG23	1:E:1488:VAL:HG13	1.96	0.48
1:H:1189:ASP:HA	1:H:1403:PRO:HB3	1.94	0.48
1:A:955:VAL:HG11	1:A:963:GLY:HA3	1.96	0.48
1:E:1901:ALA:CB	1:E:1928:MET:HE3	2.43	0.48
1:I:1460:PHE:CD1	2:I:3001:NAP:H52A	2.48	0.48
1:N:1962:ILE:HD12	1:N:1984:TYR:CE1	2.49	0.48
1:F:1449:ILE:HG23	1:F:1488:VAL:HG13	1.96	0.48
1:R:1531:ILE:HG21	1:R:1705:ILE:HG23	1.94	0.48
1:B:1901:ALA:CB	1:B:1928:MET:HE3	2.41	0.48
1:J:1431:LEU:HD21	1:J:1727:ILE:HG21	1.96	0.48
1:K:1449:ILE:HG23	1:K:1488:VAL:HG13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1449:ILE:HG23	1:P:1488:VAL:HG13	1.96	0.48
1:G:1449:ILE:HG23	1:G:1488:VAL:HG13	1.96	0.47
1:K:1402:SER:O	1:K:1979:ARG:NH2	2.46	0.47
1:J:1410:ARG:O	1:J:1754:PRO:HD2	2.14	0.47
1:P:1053:ILE:CG1	1:P:1119:MET:HE3	2.45	0.47
1:L:1901:ALA:CB	1:L:1928:MET:HE3	2.42	0.47
1:N:1449:ILE:HG23	1:N:1488:VAL:HG13	1.96	0.47
1:G:1689:THR:HG21	1:H:1649:PHE:CD1	2.50	0.47
1:B:1504:VAL:HG12	1:B:1526:LYS:HA	1.97	0.47
1:J:1053:ILE:CG1	1:J:1119:MET:HE3	2.45	0.47
1:O:1449:ILE:HG23	1:O:1488:VAL:HG13	1.96	0.47
1:R:1449:ILE:HG23	1:R:1488:VAL:HG13	1.96	0.47
1:A:1441:ARG:HH22	1:A:1489:THR:HG21	1.80	0.47
1:C:886:ARG:NE	1:D:885:ASP:OD2	2.48	0.47
1:D:1160:ASP:HB3	1:D:1166:LEU:HD11	1.97	0.47
1:G:1901:ALA:CB	1:G:1928:MET:HE3	2.43	0.47
1:J:1204:ARG:HB3	1:J:1205:PRO:HA	1.97	0.47
1:B:1193:LEU:HD21	1:B:2006:PHE:HZ	1.80	0.47
1:B:1730:MET:HE3	1:B:1739:LEU:HD22	1.95	0.47
1:J:1901:ALA:CB	1:J:1928:MET:HE3	2.42	0.47
1:E:1053:ILE:CG1	1:E:1119:MET:HE3	2.45	0.47
1:F:1901:ALA:CB	1:F:1928:MET:HE3	2.42	0.46
1:M:1901:ALA:CB	1:M:1928:MET:HE3	2.42	0.46
1:N:1053:ILE:CG1	1:N:1119:MET:HE3	2.45	0.46
1:P:1901:ALA:CB	1:P:1928:MET:HE3	2.42	0.46
1:R:916:GLU:OE2	1:R:1666:ARG:NH2	2.48	0.46
1:B:1962:ILE:HD12	1:B:1984:TYR:CD1	2.50	0.46
1:G:1962:ILE:HD12	1:G:1984:TYR:CD1	2.49	0.46
1:Q:1053:ILE:CG1	1:Q:1119:MET:HE3	2.45	0.46
1:H:1901:ALA:CB	1:H:1928:MET:HE3	2.43	0.46
1:O:1666:ARG:HB3	1:P:1666:ARG:HB3	1.97	0.46
1:C:1791:ARG:CZ	1:C:1819:VAL:HG21	2.46	0.46
1:D:1421:MET:HE1	1:D:1750:GLN:HB3	1.98	0.46
1:F:1053:ILE:CG1	1:F:1119:MET:HE3	2.45	0.46
1:L:1962:ILE:HD12	1:L:1984:TYR:CD1	2.50	0.46
1:C:1901:ALA:CB	1:C:1928:MET:HE3	2.42	0.46
1:D:1053:ILE:CG1	1:D:1119:MET:HE3	2.45	0.46
1:G:1053:ILE:CG1	1:G:1119:MET:HE3	2.45	0.46
1:G:1421:MET:HE3	1:G:1436:LEU:HD21	1.97	0.46
1:H:1449:ILE:HG23	1:H:1488:VAL:HG13	1.96	0.46
1:K:1053:ILE:CG1	1:K:1119:MET:HE3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:ILE:CG1	1:C:1119:MET:HE3	2.45	0.46
1:C:1689:THR:HG21	1:D:1649:PHE:CD1	2.51	0.46
1:J:1449:ILE:HG23	1:J:1488:VAL:HG13	1.97	0.46
1:Q:911:PRO:HB3	1:R:983:TRP:CD2	2.51	0.46
1:D:1901:ALA:CB	1:D:1928:MET:HE3	2.43	0.46
1:G:1421:MET:HE1	1:G:1750:GLN:HB3	1.97	0.46
1:H:1193:LEU:HD22	1:H:1399:LEU:CD1	2.46	0.46
1:E:1483:GLU:HB3	1:E:1541:LEU:HD13	1.98	0.46
1:D:1962:ILE:HD12	1:D:1984:TYR:CD1	2.51	0.46
1:L:1053:ILE:CG1	1:L:1119:MET:HE3	2.46	0.46
1:O:1723:ALA:HB2	1:O:1741:ILE:HD11	1.98	0.46
1:A:1569:GLY:HA3	2:A:3001:NAP:O1A	2.16	0.46
1:F:1761:PHE:HB3	1:F:1789:CYS:SG	2.56	0.45
1:B:1402:SER:O	1:B:1979:ARG:NH1	2.48	0.45
1:B:1755:PRO:HD2	1:B:1757:GLN:HG3	1.97	0.45
1:F:1962:ILE:HD12	1:F:1984:TYR:CD1	2.51	0.45
1:G:1769:ILE:HD11	1:G:1784:MET:SD	2.56	0.45
1:H:1160:ASP:HB3	1:H:1166:LEU:HD11	1.98	0.45
1:M:1053:ILE:CG1	1:M:1119:MET:HE3	2.46	0.45
1:N:1312:ALA:HB1	1:N:1355:HIS:CE1	2.51	0.45
1:E:1399:LEU:HD21	1:E:1908:LEU:HD21	1.98	0.45
1:H:1053:ILE:CG1	1:H:1119:MET:HE3	2.46	0.45
1:I:1421:MET:HE1	1:I:1750:GLN:HB2	1.98	0.45
1:M:1399:LEU:HD21	1:M:1908:LEU:HD11	1.98	0.45
1:M:1421:MET:CE	1:M:1436:LEU:HD21	2.46	0.45
1:O:1745:ASP:O	1:O:1746:THR:C	2.60	0.45
1:A:1353:MET:HE2	1:A:1909:VAL:HG12	1.98	0.45
1:B:1160:ASP:HB3	1:B:1166:LEU:HD11	1.98	0.45
1:B:1508:SER:O	1:B:1509:ALA:HB3	2.16	0.45
1:G:1764:ASP:C	1:G:1843:LEU:HD22	2.40	0.45
1:J:1160:ASP:HB3	1:J:1166:LEU:HD11	1.98	0.45
1:L:1160:ASP:HB3	1:L:1166:LEU:HD11	1.97	0.45
1:M:1791:ARG:CZ	1:M:1819:VAL:HG21	2.46	0.45
1:B:1176:THR:O	1:B:1177:GLY:C	2.59	0.45
1:O:1053:ILE:CG1	1:O:1119:MET:HE3	2.45	0.45
1:Q:1160:ASP:HB3	1:Q:1166:LEU:HD11	1.99	0.45
1:E:1962:ILE:HD12	1:E:1984:TYR:CD1	2.51	0.45
1:J:1499:ARG:HD3	1:K:1139:TYR:OH	2.16	0.45
1:K:1160:ASP:HB3	1:K:1166:LEU:HD11	1.98	0.45
1:M:1493:PRO:HA	1:M:1494:GLY:HA2	1.86	0.45
1:E:1458:ILE:HD11	1:E:1741:ILE:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1160:ASP:HB3	1:F:1166:LEU:HD11	1.99	0.45
1:K:1193:LEU:HD22	1:K:1399:LEU:HD22	1.99	0.45
1:O:1460:PHE:CD1	2:O:3001:NAP:H52A	2.52	0.45
1:R:1730:MET:HE3	1:R:1739:LEU:HD22	1.99	0.45
1:O:1160:ASP:HB3	1:O:1166:LEU:HD11	1.99	0.45
1:P:1160:ASP:HB3	1:P:1166:LEU:HD11	1.99	0.45
1:P:1962:ILE:HD12	1:P:1984:TYR:CE2	2.52	0.45
1:B:1053:ILE:CG1	1:B:1119:MET:HE3	2.46	0.45
1:C:1192:LEU:HD12	1:C:1403:PRO:HB3	1.99	0.45
1:I:1053:ILE:CG1	1:I:1119:MET:HE3	2.46	0.45
1:M:1421:MET:HE3	1:M:1436:LEU:HD21	1.98	0.45
1:R:936:VAL:HG13	1:R:1119:MET:HE1	1.98	0.45
1:E:1125:VAL:HG11	1:E:1128:LEU:HG	1.99	0.44
1:F:1531:ILE:HG21	1:F:1705:ILE:HG23	1.98	0.44
1:G:1193:LEU:HD21	1:G:2006:PHE:HZ	1.81	0.44
1:H:1791:ARG:CZ	1:H:1819:VAL:HG21	2.47	0.44
1:H:1962:ILE:HD12	1:H:1984:TYR:CD1	2.51	0.44
1:K:1339:LEU:HA	1:K:1342:SER:OG	2.17	0.44
1:P:1791:ARG:CZ	1:P:1819:VAL:HG21	2.46	0.44
1:C:1962:ILE:HD12	1:C:1984:TYR:CD1	2.52	0.44
1:N:1160:ASP:HB3	1:N:1166:LEU:HD11	1.98	0.44
1:N:1752:VAL:HG12	1:N:1753:VAL:H	1.82	0.44
1:N:1962:ILE:HD12	1:N:1984:TYR:CD1	2.52	0.44
1:C:1160:ASP:HB3	1:C:1166:LEU:HD11	1.98	0.44
1:D:1493:PRO:HA	1:D:1494:GLY:HA2	1.86	0.44
1:J:1505:GLY:HA3	1:J:1527:LEU:HD21	1.99	0.44
1:J:1791:ARG:CZ	1:J:1819:VAL:HG21	2.47	0.44
1:E:1160:ASP:HB3	1:E:1166:LEU:HD11	1.98	0.44
1:K:1962:ILE:HD12	1:K:1984:TYR:CD1	2.52	0.44
1:L:1791:ARG:CZ	1:L:1819:VAL:HG21	2.47	0.44
1:N:1859:THR:O	1:N:1860:LEU:C	2.60	0.44
1:Q:910:LEU:HD22	1:R:918:LEU:HD21	2.00	0.44
1:J:1962:ILE:HD12	1:J:1984:TYR:CD1	2.52	0.44
1:K:1962:ILE:HD11	1:K:1967:GLY:CA	2.48	0.44
1:P:1193:LEU:HD22	1:P:1399:LEU:HD22	1.99	0.44
1:P:1962:ILE:HD12	1:P:1984:TYR:CD2	2.52	0.44
1:G:1791:ARG:CZ	1:G:1819:VAL:HG21	2.48	0.44
1:H:1193:LEU:HD21	1:H:2006:PHE:HZ	1.82	0.44
1:H:1421:MET:HE3	1:H:1436:LEU:HD21	1.99	0.44
1:K:1791:ARG:CZ	1:K:1819:VAL:HG21	2.48	0.44
1:N:1791:ARG:CZ	1:N:1819:VAL:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1424:VAL:HA	1:P:1480:LEU:HD12	2.00	0.44
1:A:1649:PHE:CD1	1:B:1689:THR:HG21	2.53	0.44
1:F:1962:ILE:HD11	1:F:1967:GLY:CA	2.48	0.44
1:H:1962:ILE:HD11	1:H:1967:GLY:CA	2.48	0.44
1:P:1962:ILE:HD11	1:P:1967:GLY:CA	2.48	0.44
1:A:1026:HIS:HB3	1:A:1031:LEU:HD11	1.99	0.44
1:R:1160:ASP:HB3	1:R:1166:LEU:HD11	1.98	0.44
1:G:1160:ASP:HB3	1:G:1166:LEU:HD11	1.99	0.44
1:L:1159:LEU:CD2	1:L:1165:VAL:HG22	2.48	0.43
1:M:1160:ASP:HB3	1:M:1166:LEU:HD11	1.99	0.43
1:M:1399:LEU:HD11	1:M:1908:LEU:HD21	2.00	0.43
1:H:1593:GLU:HB3	1:Q:1024:ALA:CB	2.48	0.43
1:I:1160:ASP:HB3	1:I:1166:LEU:HD11	1.99	0.43
1:J:1386:GLU:HB3	1:J:1397:ALA:HB3	2.00	0.43
1:K:1193:LEU:HD21	1:K:2006:PHE:HZ	1.82	0.43
1:A:1369:THR:O	1:A:1370:ALA:HB3	2.18	0.43
1:D:1962:ILE:HD11	1:D:1967:GLY:CA	2.48	0.43
1:G:1962:ILE:HD11	1:G:1967:GLY:CA	2.48	0.43
1:H:1971:PHE:CZ	1:H:1975:LEU:HD11	2.53	0.43
1:A:1460:PHE:CD1	2:A:3001:NAP:H52A	2.53	0.43
1:B:1962:ILE:HD11	1:B:1967:GLY:CA	2.48	0.43
1:E:1460:PHE:CD1	2:E:3001:NAP:H51A	2.53	0.43
1:J:1962:ILE:HD11	1:J:1967:GLY:CA	2.49	0.43
1:M:1122:PRO:HA	1:M:1174:LEU:HD23	2.01	0.43
1:F:1601:ASP:OD2	1:H:1026:HIS:HA	2.19	0.43
1:M:1168:SER:HB2	1:M:1170:MET:HE3	2.00	0.43
1:C:1962:ILE:HD11	1:C:1967:GLY:CA	2.48	0.43
1:E:1962:ILE:HD11	1:E:1967:GLY:CA	2.48	0.43
1:C:1929:GLN:HG3	1:C:1980:VAL:HG11	2.01	0.43
1:E:1159:LEU:CD2	1:E:1165:VAL:HG22	2.49	0.43
1:L:1962:ILE:HD11	1:L:1967:GLY:CA	2.48	0.43
1:Q:1159:LEU:CD2	1:Q:1165:VAL:HG22	2.49	0.43
1:A:1545:THR:OG1	1:A:1683:LEU:HD22	2.19	0.43
1:A:1752:VAL:HG12	1:A:1753:VAL:H	1.84	0.43
1:C:1159:LEU:CD2	1:C:1165:VAL:HG22	2.49	0.43
1:P:1531:ILE:HG21	1:P:1705:ILE:HG23	2.01	0.43
1:C:1555:ARG:NH2	1:D:1555:ARG:NH2	2.66	0.43
1:B:1193:LEU:HD22	1:B:1399:LEU:CD1	2.48	0.42
1:F:1193:LEU:HD21	1:F:2006:PHE:HZ	1.82	0.42
1:K:1745:ASP:O	1:K:1746:THR:O	2.38	0.42
1:L:1449:ILE:HG23	1:L:1488:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1493:PRO:HA	1:R:1494:GLY:HA2	1.85	0.42
1:A:1026:HIS:CB	1:A:1031:LEU:HD11	2.48	0.42
1:D:1569:GLY:HA3	2:D:3001:NAP:O1A	2.18	0.42
1:O:1159:LEU:CD2	1:O:1165:VAL:HG22	2.49	0.42
1:F:1193:LEU:HD22	1:F:1399:LEU:HD11	2.01	0.42
1:K:1460:PHE:CD1	2:K:3001:NAP:H52A	2.54	0.42
1:P:1159:LEU:CD2	1:P:1165:VAL:HG22	2.49	0.42
1:B:1159:LEU:CD2	1:B:1165:VAL:HG22	2.49	0.42
1:H:1597:GLN:HG2	1:Q:1025:ALA:O	2.20	0.42
1:I:1159:LEU:CD2	1:I:1165:VAL:HG22	2.49	0.42
1:J:1660:ASP:OD1	1:J:1665:THR:HG21	2.19	0.42
1:K:1298:ALA:HB2	1:K:1872:TRP:NE1	2.34	0.42
1:M:1159:LEU:CD2	1:M:1165:VAL:HG22	2.49	0.42
1:D:1414:ALA:HB3	1:D:1752:VAL:HG21	2.01	0.42
1:E:1098:LEU:HD21	1:E:1137:VAL:HG11	2.02	0.42
1:G:1159:LEU:CD2	1:G:1165:VAL:HG22	2.49	0.42
1:B:1421:MET:HE3	1:B:1436:LEU:HD21	2.01	0.42
1:C:1423:LEU:HD12	1:C:1435:GLU:O	2.19	0.42
1:K:1400:CYS:HB3	1:K:2005:LEU:HD12	2.02	0.42
1:L:1436:LEU:HD23	1:L:1752:VAL:HG13	2.01	0.42
1:F:1159:LEU:CD2	1:F:1165:VAL:HG22	2.49	0.42
1:J:1159:LEU:CD2	1:J:1165:VAL:HG22	2.50	0.42
1:K:1508:SER:O	1:K:1509:ALA:HB3	2.19	0.42
1:F:1386:GLU:HB3	1:F:1397:ALA:HB3	2.01	0.42
1:I:1689:THR:HG21	1:J:1649:PHE:CD1	2.55	0.42
1:A:928:HIS:O	1:A:929:PRO:C	2.62	0.42
1:B:1523:LEU:HD22	1:B:1687:THR:HG23	2.02	0.42
1:D:1159:LEU:CD2	1:D:1165:VAL:HG22	2.49	0.42
1:D:1168:SER:HB2	1:D:1170:MET:HE3	2.02	0.42
1:F:1508:SER:O	1:F:1509:ALA:HB3	2.20	0.42
1:K:1159:LEU:CD2	1:K:1165:VAL:HG22	2.50	0.42
1:M:1900:CYS:SG	1:M:1901:ALA:N	2.93	0.42
1:O:1508:SER:O	1:O:1509:ALA:HB3	2.20	0.42
1:C:1098:LEU:HD21	1:C:1137:VAL:HG11	2.02	0.41
1:D:1458:ILE:O	1:D:1730:MET:HE1	2.20	0.41
1:D:1458:ILE:HD11	1:D:1741:ILE:HD13	2.02	0.41
1:H:1123:LEU:HD11	1:H:1175:GLY:O	2.19	0.41
1:H:1159:LEU:CD2	1:H:1165:VAL:HG22	2.49	0.41
1:L:1508:SER:O	1:L:1509:ALA:HB3	2.19	0.41
1:L:1876:VAL:HB	1:L:1923:TRP:CE3	2.55	0.41
1:Q:1098:LEU:HD21	1:Q:1137:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:ALA:HB3	1:A:1752:VAL:HG21	2.02	0.41
1:D:892:ALA:CB	1:D:893:PRO:CD	2.99	0.41
1:G:1493:PRO:HA	1:G:1494:GLY:HA2	1.86	0.41
1:I:1176:THR:HG21	1:I:1180:ASP:OD1	2.20	0.41
1:A:1493:PRO:HA	1:A:1494:GLY:HA2	1.84	0.41
1:J:1098:LEU:HD21	1:J:1137:VAL:HG11	2.03	0.41
1:J:1302:ARG:HG3	1:J:1868:VAL:HG11	2.01	0.41
1:A:1727:ILE:HD13	1:A:1727:ILE:N	2.36	0.41
1:A:1846:ARG:HA	1:A:1896:LEU:HA	2.02	0.41
1:F:1876:VAL:HB	1:F:1923:TRP:CE3	2.56	0.41
1:N:1159:LEU:CD2	1:N:1165:VAL:HG22	2.50	0.41
1:N:1635:VAL:HG22	1:N:1636:THR:H	1.85	0.41
1:R:1159:LEU:CD2	1:R:1165:VAL:HG22	2.49	0.41
1:B:1098:LEU:HD21	1:B:1137:VAL:HG11	2.03	0.41
1:B:1493:PRO:HA	1:B:1494:GLY:HA2	1.85	0.41
1:E:1756:GLU:C	1:E:1758:VAL:H	2.28	0.41
1:I:1098:LEU:HD21	1:I:1137:VAL:HG11	2.03	0.41
1:M:1032:LEU:HD13	1:P:1499:ARG:HD2	2.02	0.41
1:A:1872:TRP:NE1	1:A:1876:VAL:HG21	2.35	0.41
1:B:1755:PRO:O	1:B:1756:GLU:OE1	2.39	0.41
1:D:1098:LEU:HD21	1:D:1137:VAL:HG11	2.02	0.41
1:E:1424:VAL:HA	1:E:1480:LEU:HD12	2.02	0.41
1:F:1460:PHE:CD1	2:F:3001:NAP:H52A	2.56	0.41
1:H:1098:LEU:HD21	1:H:1137:VAL:HG11	2.02	0.41
1:H:1876:VAL:HB	1:H:1923:TRP:CE3	2.56	0.41
1:P:1386:GLU:HB3	1:P:1397:ALA:HB3	2.03	0.41
1:Q:907:HIS:O	1:R:906:SER:OG	2.30	0.41
1:A:951:ALA:HB1	1:A:965:VAL:HG11	2.02	0.41
1:C:1508:SER:O	1:C:1509:ALA:HB3	2.21	0.41
1:D:1434:MET:HE3	1:D:1724:ALA:HA	2.02	0.41
1:Q:1424:VAL:HA	1:Q:1480:LEU:HD12	2.03	0.41
1:R:1508:SER:O	1:R:1509:ALA:HB3	2.21	0.41
1:A:1649:PHE:O	1:A:1650:GLY:C	2.64	0.41
1:B:1791:ARG:CZ	1:B:1819:VAL:HG21	2.51	0.41
1:G:1876:VAL:HB	1:G:1923:TRP:CE3	2.56	0.41
1:J:1193:LEU:HD21	1:J:2006:PHE:HZ	1.84	0.41
1:K:1872:TRP:NE1	1:K:1876:VAL:HG21	2.35	0.41
1:L:1683:LEU:H	2:L:3001:NAP:H72N	1.67	0.41
1:M:1872:TRP:NE1	1:M:1876:VAL:HG21	2.36	0.41
1:N:1098:LEU:HD21	1:N:1137:VAL:HG11	2.02	0.41
1:N:1193:LEU:HD21	1:N:2006:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1493:PRO:HA	1:O:1494:GLY:HA2	1.86	0.41
1:P:1872:TRP:NE1	1:P:1876:VAL:HG21	2.36	0.41
1:Q:983:TRP:NE1	1:R:909:VAL:O	2.54	0.41
1:B:1460:PHE:CD1	2:B:3001:NAP:H52A	2.55	0.41
1:D:1434:MET:CE	1:D:1724:ALA:HA	2.51	0.41
1:P:1876:VAL:HB	1:P:1923:TRP:CE3	2.56	0.41
1:D:1508:SER:O	1:D:1509:ALA:HB3	2.21	0.40
1:H:1508:SER:O	1:H:1509:ALA:HB3	2.21	0.40
2:K:3001:NAP:O1A	2:K:3001:NAP:H4B	2.19	0.40
1:N:1493:PRO:HA	1:N:1494:GLY:HA2	1.86	0.40
1:P:1122:PRO:HA	1:P:1174:LEU:HB3	2.02	0.40
1:P:1508:SER:O	1:P:1509:ALA:HB3	2.21	0.40
1:A:1160:ASP:HB3	1:A:1166:LEU:HD11	2.03	0.40
1:G:1098:LEU:HD21	1:G:1137:VAL:HG11	2.03	0.40
1:H:1400:CYS:HB3	1:H:2005:LEU:HD22	2.03	0.40
1:H:1597:GLN:CG	1:Q:1026:HIS:HA	2.50	0.40
1:J:1872:TRP:NE1	1:J:1876:VAL:HG21	2.37	0.40
1:K:1493:PRO:HA	1:K:1494:GLY:HA2	1.86	0.40
1:K:1660:ASP:OD1	1:K:1665:THR:HG21	2.22	0.40
1:N:1508:SER:O	1:N:1509:ALA:HB3	2.21	0.40
1:Q:908:VAL:HG13	1:R:920:GLN:CB	2.46	0.40
1:Q:1493:PRO:HA	1:Q:1494:GLY:HA2	1.85	0.40
1:R:1098:LEU:HD21	1:R:1137:VAL:HG11	2.02	0.40
1:E:1508:SER:O	1:E:1509:ALA:HB3	2.22	0.40
1:G:1508:SER:O	1:G:1509:ALA:HB3	2.21	0.40
1:H:1423:LEU:HD12	1:H:1435:GLU:O	2.22	0.40
1:M:1666:ARG:HB3	1:N:1666:ARG:HB3	2.03	0.40
1:P:1098:LEU:HD21	1:P:1137:VAL:HG11	2.03	0.40
1:B:1531:ILE:HD11	1:B:1702:TYR:HB3	2.03	0.40
1:E:1876:VAL:HB	1:E:1923:TRP:CE3	2.56	0.40
1:F:1098:LEU:HD21	1:F:1137:VAL:HG11	2.02	0.40
1:P:1103:PHE:CD1	1:P:1172:LEU:HD22	2.57	0.40
1:P:1423:LEU:HD12	1:P:1435:GLU:O	2.21	0.40
1:P:1531:ILE:HD11	1:P:1702:TYR:HB3	2.03	0.40
1:A:907:HIS:NE2	1:A:917:HIS:ND1	2.69	0.40
1:E:1193:LEU:HD21	1:E:2006:PHE:HZ	1.85	0.40
1:F:1899:PHE:CE1	1:F:1928:MET:HE1	2.57	0.40
1:I:1508:SER:O	1:I:1509:ALA:HB3	2.21	0.40
1:K:1726:ALA:HB1	1:K:1739:LEU:HD23	2.04	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:1083:GLY:HA2	1:J:1264:ALA:HB1[1_565]	1.34	0.26

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	1094/1140 (96%)	995 (91%)	79 (7%)	20 (2%)	6	32
1	B	1094/1140 (96%)	1002 (92%)	69 (6%)	23 (2%)	5	30
1	C	1094/1140 (96%)	1002 (92%)	73 (7%)	19 (2%)	7	33
1	D	1094/1140 (96%)	1001 (92%)	72 (7%)	21 (2%)	6	32
1	E	1081/1140 (95%)	993 (92%)	68 (6%)	20 (2%)	6	32
1	F	1085/1140 (95%)	995 (92%)	74 (7%)	16 (2%)	8	35
1	G	1080/1140 (95%)	990 (92%)	72 (7%)	18 (2%)	7	33
1	H	1091/1140 (96%)	996 (91%)	76 (7%)	19 (2%)	7	33
1	I	651/1140 (57%)	601 (92%)	39 (6%)	11 (2%)	7	33
1	J	1081/1140 (95%)	991 (92%)	68 (6%)	22 (2%)	6	31
1	K	1081/1140 (95%)	990 (92%)	71 (7%)	20 (2%)	6	32
1	L	891/1140 (78%)	815 (92%)	61 (7%)	15 (2%)	7	33
1	M	1081/1140 (95%)	995 (92%)	71 (7%)	15 (1%)	9	36
1	N	1081/1140 (95%)	982 (91%)	76 (7%)	23 (2%)	5	30
1	O	629/1140 (55%)	580 (92%)	37 (6%)	12 (2%)	6	32
1	P	1081/1140 (95%)	986 (91%)	72 (7%)	23 (2%)	5	30
1	Q	604/1140 (53%)	562 (93%)	35 (6%)	7 (1%)	10	39
1	R	633/1140 (56%)	582 (92%)	39 (6%)	12 (2%)	6	32
All	All	17526/20520 (85%)	16058 (92%)	1152 (7%)	316 (2%)	6	32

All (316) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1755	PRO
1	B	892	ALA
1	B	1179	SER
1	C	1755	PRO
1	D	892	ALA
1	D	1755	PRO
1	E	1755	PRO
1	F	1755	PRO
1	G	1755	PRO
1	H	1403	PRO
1	H	1755	PRO
1	J	1403	PRO
1	K	1746	THR
1	K	1755	PRO
1	M	1755	PRO
1	N	1747	GLY
1	N	1748	GLN
1	N	1755	PRO
1	O	1746	THR
1	P	1404	LEU
1	P	1540	GLY
1	P	1755	PRO
1	A	892	ALA
1	A	915	GLU
1	A	960	GLY
1	A	1115	ILE
1	A	1339	LEU
1	A	1509	ALA
1	A	1651	GLY
1	A	1915	GLY
1	B	1177	GLY
1	B	1419	GLU
1	B	1540	GLY
1	B	1606	HIS
1	B	1651	GLY
1	B	1760	VAL
1	B	1840	GLN
1	B	1915	GLY
1	B	1961	ALA
1	C	1540	GLY
1	C	1606	HIS
1	C	1651	GLY
1	C	1840	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1915	GLY
1	C	1961	ALA
1	D	1419	GLU
1	D	1540	GLY
1	D	1606	HIS
1	D	1651	GLY
1	D	1915	GLY
1	D	1961	ALA
1	E	1540	GLY
1	E	1606	HIS
1	E	1651	GLY
1	E	1915	GLY
1	E	1961	ALA
1	F	1540	GLY
1	F	1606	HIS
1	F	1651	GLY
1	F	1915	GLY
1	F	1961	ALA
1	G	1419	GLU
1	G	1540	GLY
1	G	1606	HIS
1	G	1651	GLY
1	G	1747	GLY
1	G	1915	GLY
1	G	1961	ALA
1	H	1540	GLY
1	H	1606	HIS
1	H	1651	GLY
1	H	1840	GLN
1	H	1915	GLY
1	H	1961	ALA
1	I	1540	GLY
1	I	1606	HIS
1	I	1651	GLY
1	J	1540	GLY
1	J	1606	HIS
1	J	1651	GLY
1	J	1746	THR
1	J	1755	PRO
1	J	1840	GLN
1	J	1915	GLY
1	J	1961	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	1419	GLU
1	K	1540	GLY
1	K	1606	HIS
1	K	1651	GLY
1	K	1757	GLN
1	K	1840	GLN
1	K	1915	GLY
1	K	1961	ALA
1	L	1419	GLU
1	L	1540	GLY
1	L	1606	HIS
1	L	1651	GLY
1	L	1755	PRO
1	L	1840	GLN
1	L	1915	GLY
1	L	1961	ALA
1	M	1540	GLY
1	M	1606	HIS
1	M	1651	GLY
1	M	1840	GLN
1	M	1915	GLY
1	M	1961	ALA
1	N	1419	GLU
1	N	1540	GLY
1	N	1606	HIS
1	N	1651	GLY
1	N	1840	GLN
1	N	1915	GLY
1	N	1987	VAL
1	O	1540	GLY
1	O	1606	HIS
1	O	1651	GLY
1	O	1745	ASP
1	P	1419	GLU
1	P	1606	HIS
1	P	1651	GLY
1	P	1747	GLY
1	P	1840	GLN
1	P	1915	GLY
1	P	1961	ALA
1	P	1987	VAL
1	Q	1540	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	1606	HIS
1	Q	1651	GLY
1	R	1540	GLY
1	R	1606	HIS
1	R	1651	GLY
1	A	1419	GLU
1	A	1540	GLY
1	A	1606	HIS
1	A	1840	GLN
1	B	1509	ALA
1	B	1755	PRO
1	C	1746	THR
1	D	1401	PRO
1	D	1840	GLN
1	E	1840	GLN
1	F	1419	GLU
1	G	1339	LEU
1	G	1746	THR
1	G	1840	GLN
1	H	1205	PRO
1	I	1419	GLU
1	J	1419	GLU
1	J	1747	GLY
1	K	1339	LEU
1	M	1419	GLU
1	N	1401	PRO
1	O	1419	GLU
1	P	1403	PRO
1	P	1990	ALA
1	R	1750	GLN
1	A	1369	THR
1	A	1649	PHE
1	B	915	GLU
1	B	960	GLY
1	B	1090	ARG
1	B	1339	LEU
1	C	915	GLU
1	C	960	GLY
1	C	1509	ALA
1	D	915	GLU
1	D	960	GLY
1	D	1090	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1509	ALA
1	D	1760	VAL
1	E	960	GLY
1	E	1090	ARG
1	E	1509	ALA
1	E	1746	THR
1	F	915	GLU
1	F	960	GLY
1	F	1090	ARG
1	F	1509	ALA
1	G	915	GLU
1	G	960	GLY
1	G	1090	ARG
1	G	1509	ALA
1	H	1090	ARG
1	H	1509	ALA
1	I	915	GLU
1	I	960	GLY
1	I	1090	ARG
1	I	1509	ALA
1	I	1754	PRO
1	J	915	GLU
1	J	960	GLY
1	J	1090	ARG
1	J	1509	ALA
1	K	915	GLU
1	K	960	GLY
1	K	1090	ARG
1	K	1509	ALA
1	K	1760	VAL
1	L	1509	ALA
1	M	915	GLU
1	M	1090	ARG
1	M	1509	ALA
1	N	915	GLU
1	N	1090	ARG
1	N	1509	ALA
1	N	1746	THR
1	N	1961	ALA
1	O	915	GLU
1	O	960	GLY
1	O	1090	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	1509	ALA
1	P	1090	ARG
1	P	1509	ALA
1	Q	915	GLU
1	Q	960	GLY
1	Q	1090	ARG
1	R	915	GLU
1	R	1090	ARG
1	R	1509	ALA
1	R	1748	GLN
1	A	1370	ALA
1	B	1115	ILE
1	B	1369	THR
1	B	1791	ARG
1	C	1115	ILE
1	C	1339	LEU
1	C	1369	THR
1	C	1403	PRO
1	D	1115	ILE
1	D	1339	LEU
1	D	1369	THR
1	D	1406	ALA
1	D	1791	ARG
1	E	915	GLU
1	E	1115	ILE
1	E	1339	LEU
1	E	1369	THR
1	E	1791	ARG
1	F	1115	ILE
1	F	1339	LEU
1	F	1369	THR
1	F	1791	ARG
1	G	1115	ILE
1	H	915	GLU
1	H	960	GLY
1	H	1115	ILE
1	H	1212	ASP
1	H	1339	LEU
1	H	1369	THR
1	I	1115	ILE
1	J	1115	ILE
1	J	1204	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	1339	LEU
1	J	1369	THR
1	K	1115	ILE
1	K	1369	THR
1	K	1745	ASP
1	L	915	GLU
1	L	1115	ILE
1	L	1746	THR
1	M	960	GLY
1	M	1115	ILE
1	M	1369	THR
1	N	960	GLY
1	N	1115	ILE
1	N	1339	LEU
1	N	1369	THR
1	N	1402	SER
1	O	1115	ILE
1	O	1755	PRO
1	P	915	GLU
1	P	960	GLY
1	P	1115	ILE
1	P	1339	LEU
1	P	1369	THR
1	Q	1115	ILE
1	R	960	GLY
1	R	1756	GLU
1	R	1758	VAL
1	A	1508	SER
1	B	1204	ARG
1	C	1511	GLY
1	E	1760	VAL
1	G	1369	THR
1	I	1177	GLY
1	J	1203	PRO
1	J	1760	VAL
1	L	960	GLY
1	L	1403	PRO
1	P	1760	VAL
1	R	1115	ILE
1	C	1760	VAL
1	E	1403	PRO
1	E	1511	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1760	VAL
1	G	1760	VAL
1	M	1760	VAL
1	A	1511	GLY
1	C	1204	ARG
1	D	1204	ARG
1	E	1204	ARG
1	H	1203	PRO
1	K	1204	ARG
1	P	1204	ARG
1	B	1759	PRO
1	C	1983	GLY
1	L	1747	GLY
1	N	1403	PRO
1	N	1760	VAL
1	A	1204	ARG
1	A	1713	PRO
1	B	1511	GLY
1	H	1760	VAL
1	J	1511	GLY
1	P	1511	GLY

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	836/863 (97%)	797 (95%)	39 (5%)	23	47
1	B	836/863 (97%)	803 (96%)	33 (4%)	28	51
1	C	836/863 (97%)	804 (96%)	32 (4%)	29	52
1	D	836/863 (97%)	803 (96%)	33 (4%)	28	51
1	E	825/863 (96%)	799 (97%)	26 (3%)	34	55
1	F	828/863 (96%)	799 (96%)	29 (4%)	32	53
1	G	824/863 (96%)	796 (97%)	28 (3%)	32	54
1	H	831/863 (96%)	805 (97%)	26 (3%)	35	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	503/863 (58%)	485 (96%)	18 (4%)	31	53
1	J	825/863 (96%)	794 (96%)	31 (4%)	29	52
1	K	825/863 (96%)	794 (96%)	31 (4%)	29	52
1	L	674/863 (78%)	648 (96%)	26 (4%)	28	51
1	M	825/863 (96%)	795 (96%)	30 (4%)	31	53
1	N	825/863 (96%)	791 (96%)	34 (4%)	27	51
1	O	483/863 (56%)	463 (96%)	20 (4%)	27	51
1	P	825/863 (96%)	790 (96%)	35 (4%)	26	50
1	Q	464/863 (54%)	449 (97%)	15 (3%)	34	55
1	R	490/863 (57%)	472 (96%)	18 (4%)	30	52
All	All	13391/15534 (86%)	12887 (96%)	504 (4%)	29	52

All (504) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	887	GLU
1	A	956	THR
1	A	961	ASP
1	A	977	ASP
1	A	985	SER
1	A	1003	SER
1	A	1064	GLU
1	A	1105	SER
1	A	1138	ARG
1	A	1142	SER
1	A	1174	LEU
1	A	1190	GLU
1	A	1271	LEU
1	A	1331	VAL
1	A	1449	ILE
1	A	1450	GLU
1	A	1479	GLU
1	A	1522	ASP
1	A	1541	LEU
1	A	1552	GLU
1	A	1578	VAL
1	A	1593	GLU
1	A	1604	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1610	SER
1	A	1613	THR
1	A	1620	ARG
1	A	1655	GLU
1	A	1661	ILE
1	A	1673	ARG
1	A	1705	ILE
1	A	1727	ILE
1	A	1741	ILE
1	A	1750	GLN
1	A	1794	VAL
1	A	1796	SER
1	A	1825	ILE
1	A	1876	VAL
1	A	1940	SER
1	A	2007	LEU
1	B	888	LEU
1	B	961	ASP
1	B	1022	ARG
1	B	1105	SER
1	B	1128	LEU
1	B	1142	SER
1	B	1190	GLU
1	B	1271	LEU
1	B	1302	ARG
1	B	1331	VAL
1	B	1358	LEU
1	B	1393	GLN
1	B	1402	SER
1	B	1433	SER
1	B	1434	MET
1	B	1449	ILE
1	B	1510	ASN
1	B	1522	ASP
1	B	1578	VAL
1	B	1593	GLU
1	B	1604	ILE
1	B	1620	ARG
1	B	1647	LEU
1	B	1661	ILE
1	B	1673	ARG
1	B	1738	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1745	ASP
1	B	1753	VAL
1	B	1757	GLN
1	B	1794	VAL
1	B	1825	ILE
1	B	1876	VAL
1	B	2007	LEU
1	C	883	MET
1	C	884	LEU
1	C	961	ASP
1	C	1022	ARG
1	C	1105	SER
1	C	1128	LEU
1	C	1142	SER
1	C	1190	GLU
1	C	1271	LEU
1	C	1302	ARG
1	C	1331	VAL
1	C	1358	LEU
1	C	1421	MET
1	C	1437	VAL
1	C	1438	THR
1	C	1441	ARG
1	C	1510	ASN
1	C	1520	GLU
1	C	1533	GLU
1	C	1578	VAL
1	C	1593	GLU
1	C	1604	ILE
1	C	1620	ARG
1	C	1647	LEU
1	C	1661	ILE
1	C	1666	ARG
1	C	1673	ARG
1	C	1705	ILE
1	C	1794	VAL
1	C	1825	ILE
1	C	1876	VAL
1	C	2007	LEU
1	D	883	MET
1	D	888	LEU
1	D	889	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	961	ASP
1	D	1022	ARG
1	D	1105	SER
1	D	1128	LEU
1	D	1142	SER
1	D	1190	GLU
1	D	1271	LEU
1	D	1302	ARG
1	D	1331	VAL
1	D	1358	LEU
1	D	1393	GLN
1	D	1399	LEU
1	D	1438	THR
1	D	1510	ASN
1	D	1520	GLU
1	D	1522	ASP
1	D	1578	VAL
1	D	1593	GLU
1	D	1604	ILE
1	D	1620	ARG
1	D	1647	LEU
1	D	1661	ILE
1	D	1673	ARG
1	D	1705	ILE
1	D	1727	ILE
1	D	1794	VAL
1	D	1825	ILE
1	D	1876	VAL
1	D	1976	ARG
1	D	2007	LEU
1	E	961	ASP
1	E	1022	ARG
1	E	1105	SER
1	E	1142	SER
1	E	1190	GLU
1	E	1271	LEU
1	E	1302	ARG
1	E	1331	VAL
1	E	1358	LEU
1	E	1393	GLN
1	E	1399	LEU
1	E	1434	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1510	ASN
1	E	1520	GLU
1	E	1578	VAL
1	E	1593	GLU
1	E	1604	ILE
1	E	1620	ARG
1	E	1647	LEU
1	E	1661	ILE
1	E	1673	ARG
1	E	1705	ILE
1	E	1794	VAL
1	E	1825	ILE
1	E	1876	VAL
1	E	2007	LEU
1	F	961	ASP
1	F	1022	ARG
1	F	1105	SER
1	F	1128	LEU
1	F	1142	SER
1	F	1170	MET
1	F	1190	GLU
1	F	1271	LEU
1	F	1302	ARG
1	F	1331	VAL
1	F	1358	LEU
1	F	1393	GLN
1	F	1438	THR
1	F	1510	ASN
1	F	1520	GLU
1	F	1522	ASP
1	F	1578	VAL
1	F	1593	GLU
1	F	1604	ILE
1	F	1620	ARG
1	F	1647	LEU
1	F	1661	ILE
1	F	1673	ARG
1	F	1705	ILE
1	F	1748	GLN
1	F	1794	VAL
1	F	1825	ILE
1	F	1876	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	2007	LEU
1	G	961	ASP
1	G	1022	ARG
1	G	1105	SER
1	G	1128	LEU
1	G	1142	SER
1	G	1190	GLU
1	G	1271	LEU
1	G	1302	ARG
1	G	1331	VAL
1	G	1358	LEU
1	G	1393	GLN
1	G	1438	THR
1	G	1510	ASN
1	G	1520	GLU
1	G	1522	ASP
1	G	1533	GLU
1	G	1578	VAL
1	G	1593	GLU
1	G	1604	ILE
1	G	1620	ARG
1	G	1647	LEU
1	G	1661	ILE
1	G	1673	ARG
1	G	1794	VAL
1	G	1825	ILE
1	G	1833	ARG
1	G	1876	VAL
1	G	2007	LEU
1	H	961	ASP
1	H	1022	ARG
1	H	1105	SER
1	H	1128	LEU
1	H	1190	GLU
1	H	1271	LEU
1	H	1302	ARG
1	H	1331	VAL
1	H	1358	LEU
1	H	1400	CYS
1	H	1438	THR
1	H	1510	ASN
1	H	1520	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1578	VAL
1	H	1593	GLU
1	H	1604	ILE
1	H	1620	ARG
1	H	1647	LEU
1	H	1661	ILE
1	H	1673	ARG
1	H	1705	ILE
1	H	1762	ARG
1	H	1794	VAL
1	H	1825	ILE
1	H	1876	VAL
1	H	2007	LEU
1	I	961	ASP
1	I	1022	ARG
1	I	1105	SER
1	I	1128	LEU
1	I	1142	SER
1	I	1438	THR
1	I	1510	ASN
1	I	1520	GLU
1	I	1522	ASP
1	I	1578	VAL
1	I	1593	GLU
1	I	1604	ILE
1	I	1620	ARG
1	I	1647	LEU
1	I	1661	ILE
1	I	1673	ARG
1	I	1746	THR
1	I	1750	GLN
1	J	961	ASP
1	J	1022	ARG
1	J	1105	SER
1	J	1128	LEU
1	J	1142	SER
1	J	1190	GLU
1	J	1271	LEU
1	J	1302	ARG
1	J	1331	VAL
1	J	1393	GLN
1	J	1400	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	1405	ARG
1	J	1427	ASN
1	J	1510	ASN
1	J	1520	GLU
1	J	1522	ASP
1	J	1525	THR
1	J	1578	VAL
1	J	1593	GLU
1	J	1604	ILE
1	J	1620	ARG
1	J	1647	LEU
1	J	1661	ILE
1	J	1673	ARG
1	J	1705	ILE
1	J	1741	ILE
1	J	1749	SER
1	J	1794	VAL
1	J	1825	ILE
1	J	1876	VAL
1	J	2007	LEU
1	K	956	THR
1	K	961	ASP
1	K	1022	ARG
1	K	1105	SER
1	K	1128	LEU
1	K	1142	SER
1	K	1174	LEU
1	K	1190	GLU
1	K	1271	LEU
1	K	1302	ARG
1	K	1331	VAL
1	K	1358	LEU
1	K	1393	GLN
1	K	1399	LEU
1	K	1402	SER
1	K	1510	ASN
1	K	1520	GLU
1	K	1578	VAL
1	K	1593	GLU
1	K	1604	ILE
1	K	1620	ARG
1	K	1647	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	1661	ILE
1	K	1673	ARG
1	K	1752	VAL
1	K	1762	ARG
1	K	1794	VAL
1	K	1825	ILE
1	K	1876	VAL
1	K	1982	ASN
1	K	2007	LEU
1	L	961	ASP
1	L	1022	ARG
1	L	1105	SER
1	L	1128	LEU
1	L	1142	SER
1	L	1409	ARG
1	L	1434	MET
1	L	1435	GLU
1	L	1510	ASN
1	L	1520	GLU
1	L	1522	ASP
1	L	1525	THR
1	L	1578	VAL
1	L	1593	GLU
1	L	1604	ILE
1	L	1620	ARG
1	L	1647	LEU
1	L	1661	ILE
1	L	1673	ARG
1	L	1705	ILE
1	L	1741	ILE
1	L	1748	GLN
1	L	1794	VAL
1	L	1825	ILE
1	L	1876	VAL
1	L	2007	LEU
1	M	961	ASP
1	M	1022	ARG
1	M	1105	SER
1	M	1128	LEU
1	M	1142	SER
1	M	1190	GLU
1	M	1271	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	1302	ARG
1	M	1331	VAL
1	M	1353	MET
1	M	1358	LEU
1	M	1393	GLN
1	M	1510	ASN
1	M	1520	GLU
1	M	1522	ASP
1	M	1533	GLU
1	M	1578	VAL
1	M	1593	GLU
1	M	1604	ILE
1	M	1620	ARG
1	M	1647	LEU
1	M	1661	ILE
1	M	1673	ARG
1	M	1705	ILE
1	M	1727	ILE
1	M	1750	GLN
1	M	1794	VAL
1	M	1825	ILE
1	M	1876	VAL
1	M	2007	LEU
1	N	961	ASP
1	N	1022	ARG
1	N	1105	SER
1	N	1128	LEU
1	N	1142	SER
1	N	1174	LEU
1	N	1190	GLU
1	N	1192	LEU
1	N	1194	THR
1	N	1271	LEU
1	N	1302	ARG
1	N	1331	VAL
1	N	1358	LEU
1	N	1399	LEU
1	N	1400	CYS
1	N	1409	ARG
1	N	1438	THR
1	N	1510	ASN
1	N	1520	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	1522	ASP
1	N	1578	VAL
1	N	1593	GLU
1	N	1604	ILE
1	N	1620	ARG
1	N	1647	LEU
1	N	1661	ILE
1	N	1673	ARG
1	N	1705	ILE
1	N	1794	VAL
1	N	1825	ILE
1	N	1876	VAL
1	N	1909	VAL
1	N	1962	ILE
1	N	2007	LEU
1	O	961	ASP
1	O	1022	ARG
1	O	1105	SER
1	O	1128	LEU
1	O	1142	SER
1	O	1411	THR
1	O	1434	MET
1	O	1510	ASN
1	O	1520	GLU
1	O	1522	ASP
1	O	1533	GLU
1	O	1578	VAL
1	O	1593	GLU
1	O	1604	ILE
1	O	1620	ARG
1	O	1647	LEU
1	O	1661	ILE
1	O	1673	ARG
1	O	1705	ILE
1	O	1748	GLN
1	P	961	ASP
1	P	1022	ARG
1	P	1105	SER
1	P	1128	LEU
1	P	1142	SER
1	P	1174	LEU
1	P	1190	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	1271	LEU
1	P	1302	ARG
1	P	1331	VAL
1	P	1358	LEU
1	P	1393	GLN
1	P	1400	CYS
1	P	1434	MET
1	P	1438	THR
1	P	1510	ASN
1	P	1520	GLU
1	P	1522	ASP
1	P	1578	VAL
1	P	1593	GLU
1	P	1604	ILE
1	P	1620	ARG
1	P	1647	LEU
1	P	1661	ILE
1	P	1673	ARG
1	P	1705	ILE
1	P	1716	THR
1	P	1752	VAL
1	P	1757	GLN
1	P	1794	VAL
1	P	1825	ILE
1	P	1876	VAL
1	P	1994	THR
1	P	2006	PHE
1	P	2007	LEU
1	Q	961	ASP
1	Q	1022	ARG
1	Q	1105	SER
1	Q	1128	LEU
1	Q	1142	SER
1	Q	1434	MET
1	Q	1510	ASN
1	Q	1578	VAL
1	Q	1593	GLU
1	Q	1604	ILE
1	Q	1620	ARG
1	Q	1647	LEU
1	Q	1661	ILE
1	Q	1673	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	1705	ILE
1	R	961	ASP
1	R	1022	ARG
1	R	1105	SER
1	R	1128	LEU
1	R	1142	SER
1	R	1190	GLU
1	R	1434	MET
1	R	1510	ASN
1	R	1520	GLU
1	R	1533	GLU
1	R	1578	VAL
1	R	1593	GLU
1	R	1604	ILE
1	R	1620	ARG
1	R	1647	LEU
1	R	1661	ILE
1	R	1673	ARG
1	R	1705	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	971	HIS
1	A	1002	GLN
1	A	1198	GLN
1	A	1227	ASN
1	A	1633	ASN
1	A	1640	GLN
1	A	1914	GLN
1	B	1008	GLN
1	B	1198	GLN
1	B	1227	ASN
1	B	1330	HIS
1	B	1498	HIS
1	B	1597	GLN
1	B	1633	ASN
1	B	1735	HIS
1	C	1008	GLN
1	C	1089	GLN
1	C	1227	ASN
1	C	1330	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1459	ASN
1	C	1597	GLN
1	C	1633	ASN
1	D	1008	GLN
1	D	1227	ASN
1	D	1330	HIS
1	D	1597	GLN
1	D	1633	ASN
1	D	1735	HIS
1	E	1008	GLN
1	E	1227	ASN
1	E	1330	HIS
1	E	1459	ASN
1	E	1597	GLN
1	E	1633	ASN
1	F	1008	GLN
1	F	1198	GLN
1	F	1227	ASN
1	F	1330	HIS
1	F	1448	GLN
1	F	1597	GLN
1	F	1633	ASN
1	F	1735	HIS
1	G	912	GLN
1	G	1008	GLN
1	G	1227	ASN
1	G	1330	HIS
1	G	1448	GLN
1	G	1597	GLN
1	G	1633	ASN
1	H	1008	GLN
1	H	1227	ASN
1	H	1459	ASN
1	H	1597	GLN
1	H	1606	HIS
1	H	1633	ASN
1	I	1008	GLN
1	I	1448	GLN
1	I	1459	ASN
1	I	1597	GLN
1	I	1633	ASN
1	J	1008	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	1227	ASN
1	J	1330	HIS
1	J	1459	ASN
1	J	1597	GLN
1	J	1633	ASN
1	K	1008	GLN
1	K	1227	ASN
1	K	1330	HIS
1	K	1633	ASN
1	L	1008	GLN
1	L	1089	GLN
1	L	1178	ASN
1	L	1416	ASN
1	L	1448	GLN
1	L	1459	ASN
1	L	1498	HIS
1	L	1597	GLN
1	L	1633	ASN
1	L	1735	HIS
1	L	1757	GLN
1	M	912	GLN
1	M	1008	GLN
1	M	1227	ASN
1	M	1330	HIS
1	M	1448	GLN
1	M	1459	ASN
1	M	1597	GLN
1	M	1633	ASN
1	N	1008	GLN
1	N	1037	ASN
1	N	1227	ASN
1	N	1330	HIS
1	N	1416	ASN
1	N	1448	GLN
1	N	1597	GLN
1	N	1633	ASN
1	O	1008	GLN
1	O	1448	GLN
1	O	1459	ASN
1	O	1597	GLN
1	O	1633	ASN
1	P	1008	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	1089	GLN
1	P	1227	ASN
1	P	1330	HIS
1	P	1448	GLN
1	P	1597	GLN
1	P	1633	ASN
1	Q	1008	GLN
1	Q	1448	GLN
1	Q	1597	GLN
1	Q	1633	ASN
1	R	1008	GLN
1	R	1448	GLN
1	R	1459	ASN
1	R	1597	GLN
1	R	1633	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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	3001	-	50,52,52	0.96	1 (2%)	71,80,80	0.85	2 (2%)
2	NAP	M	3001	-	50,52,52	0.90	3 (6%)	71,80,80	1.03	4 (5%)
2	NAP	B	3001	-	50,52,52	0.83	2 (4%)	71,80,80	1.06	5 (7%)
2	NAP	E	3001	-	50,52,52	0.85	2 (4%)	71,80,80	0.89	4 (5%)
2	NAP	I	3001	-	50,52,52	0.78	1 (2%)	71,80,80	0.81	2 (2%)
2	NAP	L	3001	-	50,52,52	0.85	2 (4%)	71,80,80	1.01	5 (7%)
2	NAP	F	3002	-	29,29,52	0.55	0	44,45,80	0.99	5 (11%)
2	NAP	O	3001	-	50,52,52	0.93	3 (6%)	71,80,80	0.99	3 (4%)
2	NAP	R	3001	-	50,52,52	0.67	1 (2%)	71,80,80	0.71	2 (2%)
2	NAP	F	3001	-	50,52,52	1.05	2 (4%)	71,80,80	0.99	4 (5%)
2	NAP	K	3001	-	50,52,52	1.43	2 (4%)	71,80,80	0.89	3 (4%)
2	NAP	Q	3001	-	50,52,52	0.90	1 (2%)	71,80,80	0.90	3 (4%)
2	NAP	C	3001	-	50,52,52	0.65	1 (2%)	71,80,80	0.78	1 (1%)
2	NAP	B	3002	-	29,29,52	0.65	0	44,45,80	1.11	3 (6%)
2	NAP	H	3002	-	29,29,52	0.54	0	44,45,80	0.95	4 (9%)
2	NAP	N	3002	-	29,29,52	0.70	1 (3%)	44,45,80	1.15	2 (4%)
2	NAP	G	3001	-	50,52,52	0.86	1 (2%)	71,80,80	0.93	3 (4%)
2	NAP	P	3002	-	29,29,52	0.56	0	44,45,80	1.07	4 (9%)
2	NAP	C	3002	-	32,33,52	0.64	0	50,52,80	0.93	4 (8%)
2	NAP	D	3002	-	29,29,52	0.58	0	44,45,80	1.00	4 (9%)
2	NAP	J	3001	-	50,52,52	0.72	1 (2%)	71,80,80	1.40	4 (5%)
2	NAP	K	3002	-	29,29,52	0.42	0	44,45,80	1.03	5 (11%)
2	NAP	G	3002	-	29,29,52	0.48	0	44,45,80	1.00	3 (6%)
2	NAP	N	3001	-	50,52,52	0.90	2 (4%)	71,80,80	0.95	3 (4%)
2	NAP	M	3002	-	29,29,52	0.75	1 (3%)	44,45,80	0.94	2 (4%)
2	NAP	P	3001	-	50,52,52	0.83	2 (4%)	71,80,80	1.13	3 (4%)
2	NAP	D	3001	-	50,52,52	0.83	1 (2%)	71,80,80	0.95	1 (1%)
2	NAP	J	3002	-	29,29,52	0.60	0	44,45,80	1.07	3 (6%)
2	NAP	H	3001	-	50,52,52	0.74	1 (2%)	71,80,80	0.94	3 (4%)
2	NAP	A	3002	-	29,29,52	0.49	0	44,45,80	0.96	2 (4%)

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	3001	-	-	13/35/67/67	0/5/5/5
2	NAP	M	3001	-	-	9/35/67/67	0/5/5/5
2	NAP	B	3001	-	-	11/35/67/67	0/5/5/5
2	NAP	E	3001	-	-	8/35/67/67	0/5/5/5
2	NAP	I	3001	-	-	10/35/67/67	0/5/5/5
2	NAP	L	3001	-	-	8/35/67/67	0/5/5/5
2	NAP	F	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	O	3001	-	-	10/35/67/67	0/5/5/5
2	NAP	R	3001	-	-	10/35/67/67	0/5/5/5
2	NAP	F	3001	-	-	12/35/67/67	0/5/5/5
2	NAP	K	3001	-	-	11/35/67/67	0/5/5/5
2	NAP	Q	3001	-	-	6/35/67/67	0/5/5/5
2	NAP	C	3001	-	-	8/35/67/67	0/5/5/5
2	NAP	B	3002	-	-	4/15/31/67	0/3/3/5
2	NAP	H	3002	-	-	3/15/31/67	0/3/3/5
2	NAP	N	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	G	3001	-	-	8/35/67/67	0/5/5/5
2	NAP	P	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	C	3002	-	-	4/21/37/67	0/3/3/5
2	NAP	D	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	J	3001	-	-	3/35/67/67	0/5/5/5
2	NAP	K	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	G	3002	-	-	3/15/31/67	0/3/3/5
2	NAP	N	3001	-	-	9/35/67/67	0/5/5/5
2	NAP	M	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	P	3001	-	-	4/35/67/67	0/5/5/5
2	NAP	D	3001	-	-	10/35/67/67	0/5/5/5
2	NAP	J	3002	-	-	5/15/31/67	0/3/3/5
2	NAP	H	3001	-	-	9/35/67/67	0/5/5/5
2	NAP	A	3002	-	-	6/15/31/67	0/3/3/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3001	NAP	C2N-N1N	8.93	1.44	1.35
2	F	3001	NAP	C2N-N1N	5.83	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3001	NAP	C2N-N1N	5.40	1.40	1.35
2	A	3001	NAP	C2N-N1N	5.18	1.40	1.35
2	G	3001	NAP	C2N-N1N	5.06	1.40	1.35
2	D	3001	NAP	C2N-N1N	4.79	1.40	1.35
2	N	3001	NAP	C2N-N1N	4.72	1.40	1.35
2	E	3001	NAP	C2N-N1N	4.55	1.40	1.35
2	I	3001	NAP	C2N-N1N	4.37	1.39	1.35
2	P	3001	NAP	C2N-N1N	4.33	1.39	1.35
2	J	3001	NAP	C2N-N1N	4.05	1.39	1.35
2	L	3001	NAP	P2B-O1X	3.94	1.62	1.50
2	O	3001	NAP	P2B-O1X	3.87	1.62	1.50
2	R	3001	NAP	C2N-N1N	3.76	1.39	1.35
2	B	3001	NAP	C2N-N1N	3.45	1.38	1.35
2	M	3001	NAP	C2N-N1N	3.43	1.38	1.35
2	O	3001	NAP	C2N-N1N	3.37	1.38	1.35
2	H	3001	NAP	C2N-N1N	3.35	1.38	1.35
2	K	3001	NAP	O7N-C7N	-3.22	1.18	1.24
2	N	3002	NAP	PA-O1A	3.21	1.60	1.50
2	M	3002	NAP	PA-O1A	3.20	1.60	1.50
2	B	3001	NAP	O4D-C1D	-3.05	1.36	1.40
2	M	3001	NAP	C7N-N7N	-3.04	1.27	1.33
2	C	3001	NAP	C2N-N1N	2.97	1.38	1.35
2	N	3001	NAP	O4D-C1D	-2.96	1.37	1.40
2	L	3001	NAP	C2N-N1N	2.83	1.38	1.35
2	F	3001	NAP	C3N-C7N	2.79	1.54	1.50
2	M	3001	NAP	O4D-C1D	-2.76	1.37	1.40
2	E	3001	NAP	P2B-O1X	-2.38	1.43	1.50
2	P	3001	NAP	P2B-O1X	2.36	1.57	1.50
2	O	3001	NAP	C7N-N7N	-2.10	1.29	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3001	NAP	O2A-PA-O3	-9.53	81.52	107.27
2	P	3001	NAP	O2A-PA-O3	-7.13	88.01	107.27
2	N	3001	NAP	O2A-PA-O3	-5.24	93.11	107.27
2	M	3001	NAP	O2A-PA-O3	-5.15	93.36	107.27
2	Q	3001	NAP	C4D-O4D-C1D	4.81	114.33	109.92
2	F	3001	NAP	C4D-O4D-C1D	-4.78	105.55	109.92
2	N	3002	NAP	O2B-P2B-O1X	-4.68	92.64	109.33
2	O	3001	NAP	P2B-O2B-C2B	4.10	134.37	123.43
2	D	3001	NAP	O2A-PA-O3	-4.07	96.26	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3001	NAP	O2A-PA-O3	-4.01	96.42	107.27
2	G	3001	NAP	C2B-C1B-N9A	3.94	120.24	113.75
2	A	3001	NAP	O2A-PA-O3	-3.94	96.64	107.27
2	B	3002	NAP	O5B-PA-O1A	-3.93	95.83	106.44
2	B	3001	NAP	O2A-PA-O3	-3.91	96.71	107.27
2	L	3001	NAP	C2B-C1B-N9A	3.90	120.16	113.75
2	P	3002	NAP	O2B-P2B-O1X	-3.82	95.72	109.33
2	K	3001	NAP	O2A-PA-O5B	-3.81	90.31	107.57
2	B	3001	NAP	C4D-O4D-C1D	3.78	113.39	109.92
2	H	3001	NAP	O3-PA-O1A	3.70	121.83	110.70
2	J	3002	NAP	C2B-C1B-N9A	3.60	119.68	113.75
2	I	3001	NAP	O2A-PA-O3	-3.54	97.71	107.27
2	G	3001	NAP	O3-PA-O1A	3.45	121.08	110.70
2	O	3001	NAP	C2B-C1B-N9A	3.39	119.33	113.75
2	L	3001	NAP	P2B-O2B-C2B	3.33	132.32	123.43
2	E	3001	NAP	C2B-C1B-N9A	3.29	119.17	113.75
2	J	3001	NAP	O3-PA-O1A	3.29	120.59	110.70
2	F	3001	NAP	O3-PA-O1A	3.19	120.29	110.70
2	F	3001	NAP	O2A-PA-O3	-3.15	98.75	107.27
2	M	3001	NAP	P2B-O2B-C2B	3.08	131.66	123.43
2	K	3002	NAP	O2A-PA-O5B	-3.04	98.75	106.67
2	N	3001	NAP	O3-PA-O1A	3.01	119.75	110.70
2	J	3002	NAP	O3-PA-O5B	-2.94	99.01	106.67
2	L	3001	NAP	O3-PA-O1A	2.93	119.51	110.70
2	D	3002	NAP	O2X-P2B-O2B	-2.93	94.45	105.85
2	E	3001	NAP	O3-PA-O1A	2.90	119.41	110.70
2	C	3001	NAP	O2A-PA-O3	-2.87	99.51	107.27
2	H	3002	NAP	O5B-PA-O1A	-2.86	98.70	106.44
2	A	3002	NAP	C2B-C1B-N9A	2.82	118.39	113.75
2	F	3002	NAP	O3-PA-O5B	-2.75	99.51	106.67
2	H	3001	NAP	C2B-C1B-N9A	2.74	118.26	113.75
2	M	3002	NAP	C2B-C1B-N9A	2.74	118.26	113.75
2	G	3002	NAP	O2X-P2B-O2B	-2.70	95.31	105.85
2	K	3002	NAP	O2X-P2B-O2B	-2.70	95.31	105.85
2	B	3002	NAP	O3-PA-O5B	-2.64	99.77	106.67
2	I	3001	NAP	O3-PA-O1A	2.64	118.64	110.70
2	L	3001	NAP	O2A-PA-O5B	-2.63	95.66	107.57
2	N	3001	NAP	O3X-P2B-O2B	-2.60	95.72	105.85
2	F	3002	NAP	O2X-P2B-O2B	-2.58	95.78	105.85
2	E	3001	NAP	C4D-O4D-C1D	2.58	112.29	109.92
2	J	3001	NAP	P2B-O2B-C2B	2.58	130.32	123.43
2	D	3002	NAP	O3-PA-O2A	2.57	117.45	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3002	NAP	O3-PA-O5B	-2.56	100.00	106.67
2	P	3002	NAP	C2B-C1B-N9A	2.53	117.91	113.75
2	M	3002	NAP	O2B-P2B-O1X	-2.53	100.33	109.33
2	C	3002	NAP	O2X-P2B-O2B	-2.52	96.01	105.85
2	G	3001	NAP	P2B-O2B-C2B	2.50	130.12	123.43
2	P	3001	NAP	O3-PA-O1A	2.48	118.16	110.70
2	C	3002	NAP	C2B-C1B-N9A	2.45	117.78	113.75
2	G	3002	NAP	C2B-C1B-N9A	2.45	117.78	113.75
2	B	3001	NAP	P2B-O2B-C2B	2.44	129.96	123.43
2	D	3002	NAP	O3-PA-O5B	-2.40	100.41	106.67
2	B	3001	NAP	O3-PA-O1A	2.39	117.89	110.70
2	K	3002	NAP	O3-PA-O5B	-2.37	100.49	106.67
2	Q	3001	NAP	P2B-O2B-C2B	2.35	129.70	123.43
2	K	3001	NAP	O3X-P2B-O2B	-2.32	96.81	105.85
2	K	3001	NAP	O3-PA-O1A	2.32	117.67	110.70
2	H	3002	NAP	O2X-P2B-O2B	-2.31	96.85	105.85
2	J	3002	NAP	O2X-P2B-O2B	-2.30	96.89	105.85
2	R	3001	NAP	O3-PA-O1A	2.30	117.61	110.70
2	D	3002	NAP	C2B-C1B-N9A	2.29	117.52	113.75
2	H	3002	NAP	O2A-PA-O5B	2.28	112.60	106.67
2	H	3002	NAP	O3-PA-O2A	2.26	116.28	107.80
2	P	3002	NAP	O3-PA-O5B	-2.24	100.83	106.67
2	O	3001	NAP	O3X-P2B-O2B	-2.22	97.20	105.85
2	B	3002	NAP	O3-PA-O2A	2.21	116.09	107.80
2	F	3001	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
2	F	3002	NAP	O2A-PA-O5B	-2.18	100.99	106.67
2	A	3001	NAP	P2B-O2B-C2B	2.17	129.22	123.43
2	P	3001	NAP	P2B-O2B-C2B	2.15	129.17	123.43
2	P	3002	NAP	O3-PA-O2A	2.14	115.82	107.80
2	J	3001	NAP	O2D-C2D-C3D	2.13	118.64	111.82
2	M	3001	NAP	O3-PA-O1A	2.12	117.08	110.70
2	E	3001	NAP	P2B-O2B-C2B	2.11	129.06	123.43
2	N	3002	NAP	O3-PA-O2A	2.09	115.64	107.80
2	L	3001	NAP	O3X-P2B-O2B	-2.08	97.75	105.85
2	G	3002	NAP	O3X-P2B-O2B	2.07	113.92	105.85
2	K	3002	NAP	O3X-P2B-O2X	2.06	115.53	107.80
2	K	3002	NAP	O5B-PA-O1A	2.06	112.01	106.44
2	F	3002	NAP	O3X-P2B-O2B	2.06	113.88	105.85
2	C	3002	NAP	O2N-PN-O1N	2.06	118.86	110.83
2	C	3002	NAP	O3-PA-O1A	2.05	116.88	110.70
2	Q	3001	NAP	C6N-N1N-C2N	-2.04	120.14	121.88
2	B	3001	NAP	O3D-C3D-C2D	2.03	118.33	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3002	NAP	O5B-PA-O1A	2.02	111.91	106.44
2	R	3001	NAP	P2B-O2B-C2B	2.02	128.82	123.43
2	M	3001	NAP	C6N-N1N-C1D	2.02	123.69	119.73

There are no chirality outliers.

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	C5B-O5B-PA-O2A
2	A	3001	NAP	C5B-O5B-PA-O3
2	A	3001	NAP	C5D-O5D-PN-O1N
2	A	3001	NAP	C5D-O5D-PN-O2N
2	A	3001	NAP	O4D-C1D-N1N-C6N
2	A	3002	NAP	C5B-O5B-PA-O1A
2	A	3002	NAP	C5B-O5B-PA-O2A
2	A	3002	NAP	C5B-O5B-PA-O3
2	B	3001	NAP	C5B-O5B-PA-O2A
2	B	3001	NAP	C4B-C5B-O5B-PA
2	B	3001	NAP	C5D-O5D-PN-O3
2	B	3001	NAP	C5D-O5D-PN-O1N
2	B	3001	NAP	C5D-O5D-PN-O2N
2	B	3002	NAP	C5B-O5B-PA-O1A
2	B	3002	NAP	C5B-O5B-PA-O2A
2	B	3002	NAP	C5B-O5B-PA-O3
2	C	3001	NAP	C5B-O5B-PA-O2A
2	C	3001	NAP	C5D-O5D-PN-O1N
2	C	3001	NAP	C5D-O5D-PN-O2N
2	C	3002	NAP	C5B-O5B-PA-O1A
2	C	3002	NAP	C5B-O5B-PA-O2A
2	C	3002	NAP	C5B-O5B-PA-O3
2	D	3001	NAP	C5B-O5B-PA-O2A
2	D	3001	NAP	C4B-C5B-O5B-PA
2	D	3001	NAP	C5D-O5D-PN-O3
2	D	3001	NAP	C5D-O5D-PN-O1N
2	D	3001	NAP	C5D-O5D-PN-O2N
2	D	3002	NAP	C5B-O5B-PA-O1A
2	D	3002	NAP	C5B-O5B-PA-O2A
2	D	3002	NAP	C5B-O5B-PA-O3
2	E	3001	NAP	C5B-O5B-PA-O3
2	E	3001	NAP	PA-O3-PN-O5D
2	F	3001	NAP	C5D-O5D-PN-O1N
2	F	3001	NAP	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	3002	NAP	C5B-O5B-PA-O1A
2	F	3002	NAP	C5B-O5B-PA-O2A
2	F	3002	NAP	C5B-O5B-PA-O3
2	G	3001	NAP	C3B-C4B-C5B-O5B
2	G	3001	NAP	C5D-O5D-PN-O1N
2	G	3001	NAP	C5D-O5D-PN-O2N
2	G	3002	NAP	C5B-O5B-PA-O2A
2	G	3002	NAP	C5B-O5B-PA-O3
2	H	3001	NAP	C3B-C4B-C5B-O5B
2	H	3001	NAP	C5D-O5D-PN-O3
2	H	3001	NAP	C5D-O5D-PN-O2N
2	H	3002	NAP	C5B-O5B-PA-O1A
2	H	3002	NAP	C5B-O5B-PA-O2A
2	H	3002	NAP	C5B-O5B-PA-O3
2	I	3001	NAP	C5B-O5B-PA-O2A
2	I	3001	NAP	C5D-O5D-PN-O1N
2	I	3001	NAP	C5D-O5D-PN-O2N
2	J	3002	NAP	C5B-O5B-PA-O2A
2	J	3002	NAP	C5B-O5B-PA-O3
2	K	3001	NAP	C4B-C5B-O5B-PA
2	K	3001	NAP	C5D-O5D-PN-O3
2	K	3001	NAP	C5D-O5D-PN-O2N
2	K	3001	NAP	C4D-C5D-O5D-PN
2	K	3001	NAP	C2D-C1D-N1N-C2N
2	K	3001	NAP	C2D-C1D-N1N-C6N
2	K	3002	NAP	C5B-O5B-PA-O1A
2	K	3002	NAP	C5B-O5B-PA-O2A
2	K	3002	NAP	C5B-O5B-PA-O3
2	L	3001	NAP	O4D-C1D-N1N-C6N
2	M	3001	NAP	C5B-O5B-PA-O2A
2	M	3001	NAP	C5D-O5D-PN-O3
2	M	3001	NAP	C5D-O5D-PN-O1N
2	M	3001	NAP	C5D-O5D-PN-O2N
2	M	3002	NAP	C5B-O5B-PA-O2A
2	N	3001	NAP	C5B-O5B-PA-O2A
2	N	3001	NAP	C5D-O5D-PN-O1N
2	N	3001	NAP	C5D-O5D-PN-O2N
2	N	3002	NAP	C5B-O5B-PA-O1A
2	N	3002	NAP	C5B-O5B-PA-O2A
2	N	3002	NAP	C5B-O5B-PA-O3
2	O	3001	NAP	C3B-C4B-C5B-O5B
2	O	3001	NAP	O4D-C1D-N1N-C2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	O	3001	NAP	O4D-C1D-N1N-C6N
2	O	3001	NAP	C2D-C1D-N1N-C2N
2	P	3002	NAP	C5B-O5B-PA-O1A
2	P	3002	NAP	C5B-O5B-PA-O2A
2	P	3002	NAP	C5B-O5B-PA-O3
2	Q	3001	NAP	O4D-C1D-N1N-C6N
2	R	3001	NAP	C5B-O5B-PA-O2A
2	R	3001	NAP	C5D-O5D-PN-O3
2	R	3001	NAP	C5D-O5D-PN-O1N
2	R	3001	NAP	C5D-O5D-PN-O2N
2	A	3001	NAP	C3B-C4B-C5B-O5B
2	B	3001	NAP	C3B-C4B-C5B-O5B
2	C	3001	NAP	C3B-C4B-C5B-O5B
2	D	3001	NAP	C3B-C4B-C5B-O5B
2	F	3001	NAP	C3B-C4B-C5B-O5B
2	F	3001	NAP	O4D-C4D-C5D-O5D
2	H	3001	NAP	O4B-C4B-C5B-O5B
2	I	3001	NAP	C3B-C4B-C5B-O5B
2	K	3001	NAP	C3B-C4B-C5B-O5B
2	L	3001	NAP	C3B-C4B-C5B-O5B
2	L	3001	NAP	C3D-C4D-C5D-O5D
2	M	3001	NAP	C3B-C4B-C5B-O5B
2	N	3001	NAP	C3B-C4B-C5B-O5B
2	R	3001	NAP	C3B-C4B-C5B-O5B
2	I	3001	NAP	C4B-C5B-O5B-PA
2	M	3001	NAP	C4B-C5B-O5B-PA
2	P	3001	NAP	C4B-C5B-O5B-PA
2	A	3001	NAP	O4B-C4B-C5B-O5B
2	B	3001	NAP	O4B-C4B-C5B-O5B
2	C	3001	NAP	O4B-C4B-C5B-O5B
2	F	3001	NAP	O4B-C4B-C5B-O5B
2	G	3001	NAP	O4B-C4B-C5B-O5B
2	I	3001	NAP	O4B-C4B-C5B-O5B
2	K	3001	NAP	O4B-C4B-C5B-O5B
2	L	3001	NAP	O4B-C4B-C5B-O5B
2	L	3001	NAP	O4D-C4D-C5D-O5D
2	M	3001	NAP	O4B-C4B-C5B-O5B
2	N	3001	NAP	O4B-C4B-C5B-O5B
2	O	3001	NAP	O4B-C4B-C5B-O5B
2	O	3001	NAP	O4D-C4D-C5D-O5D
2	O	3001	NAP	C3D-C4D-C5D-O5D
2	R	3001	NAP	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	3001	NAP	O4B-C4B-C5B-O5B
2	A	3001	NAP	C4B-C5B-O5B-PA
2	C	3001	NAP	C4B-C5B-O5B-PA
2	G	3001	NAP	C4B-C5B-O5B-PA
2	H	3001	NAP	C4B-C5B-O5B-PA
2	R	3001	NAP	C4B-C5B-O5B-PA
2	F	3001	NAP	C3D-C4D-C5D-O5D
2	N	3001	NAP	C4B-C5B-O5B-PA
2	Q	3001	NAP	C3D-C4D-C5D-O5D
2	C	3001	NAP	C2B-O2B-P2B-O1X
2	F	3001	NAP	C2B-O2B-P2B-O1X
2	K	3001	NAP	C2B-O2B-P2B-O1X
2	J	3002	NAP	C5B-O5B-PA-O1A
2	Q	3001	NAP	O4D-C4D-C5D-O5D
2	F	3001	NAP	C4B-C5B-O5B-PA
2	L	3001	NAP	C4B-C5B-O5B-PA
2	O	3001	NAP	C4B-C5B-O5B-PA
2	B	3001	NAP	PN-O3-PA-O5B
2	E	3001	NAP	PN-O3-PA-O5B
2	L	3001	NAP	PN-O3-PA-O5B
2	M	3001	NAP	PN-O3-PA-O5B
2	M	3002	NAP	C5B-O5B-PA-O3
2	M	3002	NAP	C2B-C1B-N9A-C8A
2	O	3001	NAP	PA-O3-PN-O1N
2	P	3001	NAP	PA-O3-PN-O2N
2	R	3001	NAP	PA-O3-PN-O1N
2	F	3002	NAP	O4B-C4B-C5B-O5B
2	D	3001	NAP	C2B-O2B-P2B-O1X
2	J	3002	NAP	C2B-O2B-P2B-O1X
2	N	3001	NAP	C2B-O2B-P2B-O1X
2	O	3001	NAP	C2B-O2B-P2B-O1X
2	Q	3001	NAP	C2B-O2B-P2B-O1X
2	R	3001	NAP	C2B-O2B-P2B-O1X
2	A	3001	NAP	C5D-O5D-PN-O3
2	C	3001	NAP	C5D-O5D-PN-O3
2	E	3001	NAP	C5B-O5B-PA-O1A
2	F	3001	NAP	C5B-O5B-PA-O2A
2	F	3001	NAP	C5D-O5D-PN-O3
2	G	3001	NAP	C5D-O5D-PN-O3
2	H	3001	NAP	C5D-O5D-PN-O1N
2	I	3001	NAP	C5D-O5D-PN-O3
2	K	3001	NAP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	N	3001	NAP	C5D-O5D-PN-O3
2	P	3001	NAP	C5B-O5B-PA-O1A
2	Q	3001	NAP	C5D-O5D-PN-O1N
2	E	3001	NAP	C4B-C5B-O5B-PA
2	J	3001	NAP	C4B-C5B-O5B-PA
2	M	3002	NAP	C5B-O5B-PA-O1A
2	E	3001	NAP	O4B-C4B-C5B-O5B
2	F	3001	NAP	PA-O3-PN-O1N
2	A	3001	NAP	C2B-O2B-P2B-O3X
2	G	3002	NAP	C2B-O2B-P2B-O3X
2	H	3001	NAP	C2B-O2B-P2B-O3X
2	I	3001	NAP	C2B-O2B-P2B-O3X
2	J	3001	NAP	C2B-O2B-P2B-O3X
2	E	3001	NAP	C3B-C4B-C5B-O5B
2	F	3002	NAP	C3B-C4B-C5B-O5B
2	Q	3001	NAP	O4D-C1D-N1N-C2N
2	A	3001	NAP	C2B-O2B-P2B-O1X
2	B	3001	NAP	C2B-O2B-P2B-O1X
2	B	3002	NAP	C2B-O2B-P2B-O1X
2	D	3002	NAP	C2B-O2B-P2B-O1X
2	G	3001	NAP	C2B-O2B-P2B-O1X
2	H	3001	NAP	C2B-O2B-P2B-O1X
2	N	3002	NAP	C2B-O2B-P2B-O1X
2	P	3002	NAP	C2B-O2B-P2B-O1X
2	D	3001	NAP	PA-O3-PN-O1N
2	P	3001	NAP	PA-O3-PN-O1N
2	E	3001	NAP	O4D-C4D-C5D-O5D
2	K	3002	NAP	O4B-C4B-C5B-O5B
2	G	3001	NAP	O4B-C1B-N9A-C8A
2	I	3001	NAP	PA-O3-PN-O2N
2	K	3001	NAP	PN-O3-PA-O2A
2	H	3001	NAP	O4B-C1B-N9A-C8A
2	L	3001	NAP	O4B-C1B-N9A-C8A
2	M	3002	NAP	O4B-C1B-N9A-C8A
2	A	3002	NAP	O4B-C4B-C5B-O5B
2	C	3002	NAP	O4B-C4B-C5B-O5B
2	D	3002	NAP	O4B-C4B-C5B-O5B
2	J	3002	NAP	O4B-C4B-C5B-O5B
2	B	3001	NAP	C2B-O2B-P2B-O2X
2	K	3002	NAP	C2B-O2B-P2B-O2X
2	N	3002	NAP	C2B-O2B-P2B-O3X
2	A	3002	NAP	C2B-O2B-P2B-O1X

Continued on next page...

Continued from previous page...

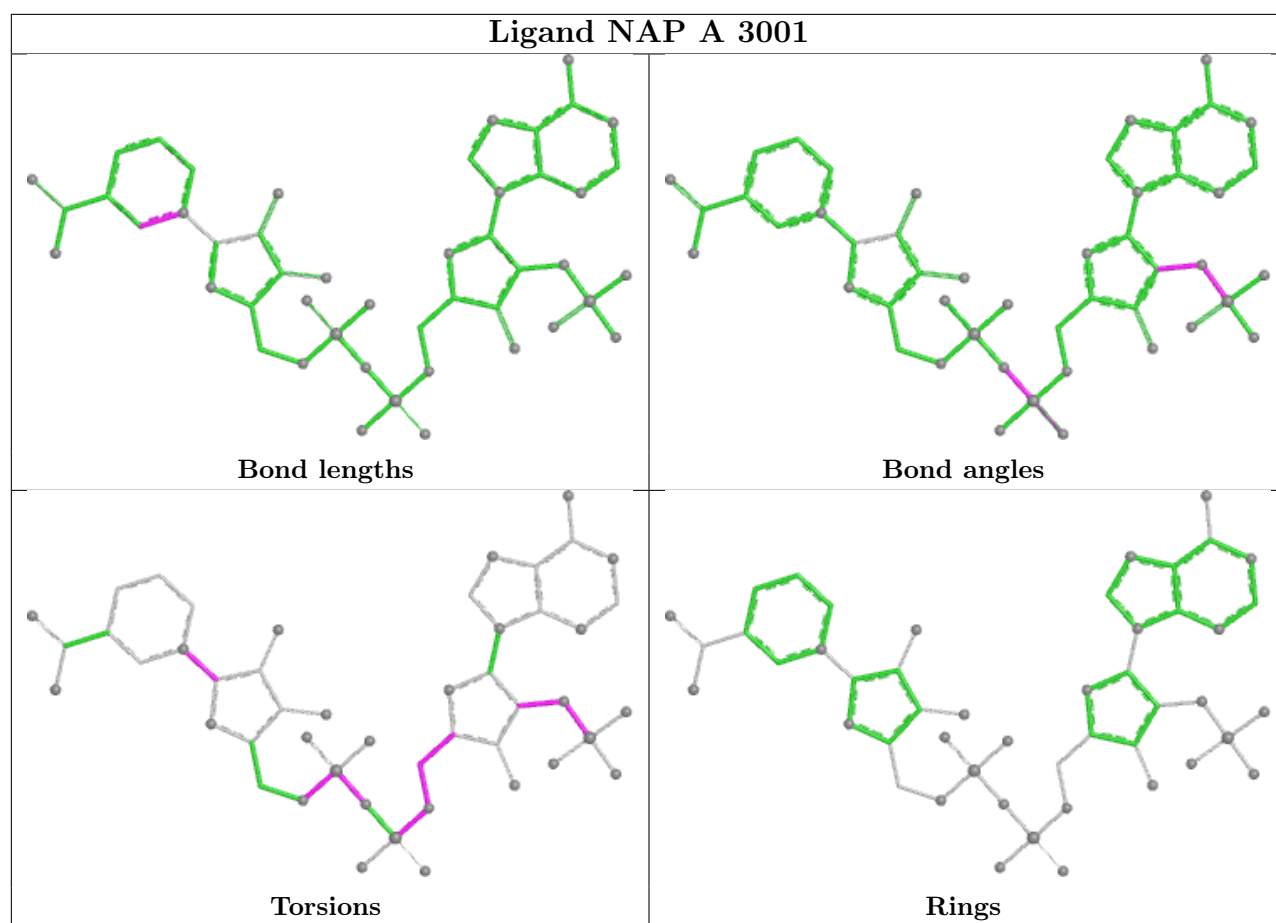
Mol	Chain	Res	Type	Atoms
2	I	3001	NAP	C2B-O2B-P2B-O1X
2	J	3001	NAP	C2B-O2B-P2B-O1X
2	A	3001	NAP	C3B-C2B-O2B-P2B
2	A	3002	NAP	C2B-C1B-N9A-C8A
2	P	3002	NAP	O4B-C4B-C5B-O5B
2	N	3001	NAP	O4B-C1B-N9A-C8A
2	A	3001	NAP	PA-O3-PN-O2N
2	B	3001	NAP	PA-O3-PN-O2N
2	D	3001	NAP	PA-O3-PN-O2N
2	F	3001	NAP	PA-O3-PN-O2N
2	M	3001	NAP	PA-O3-PN-O2N
2	R	3001	NAP	PA-O3-PN-O2N

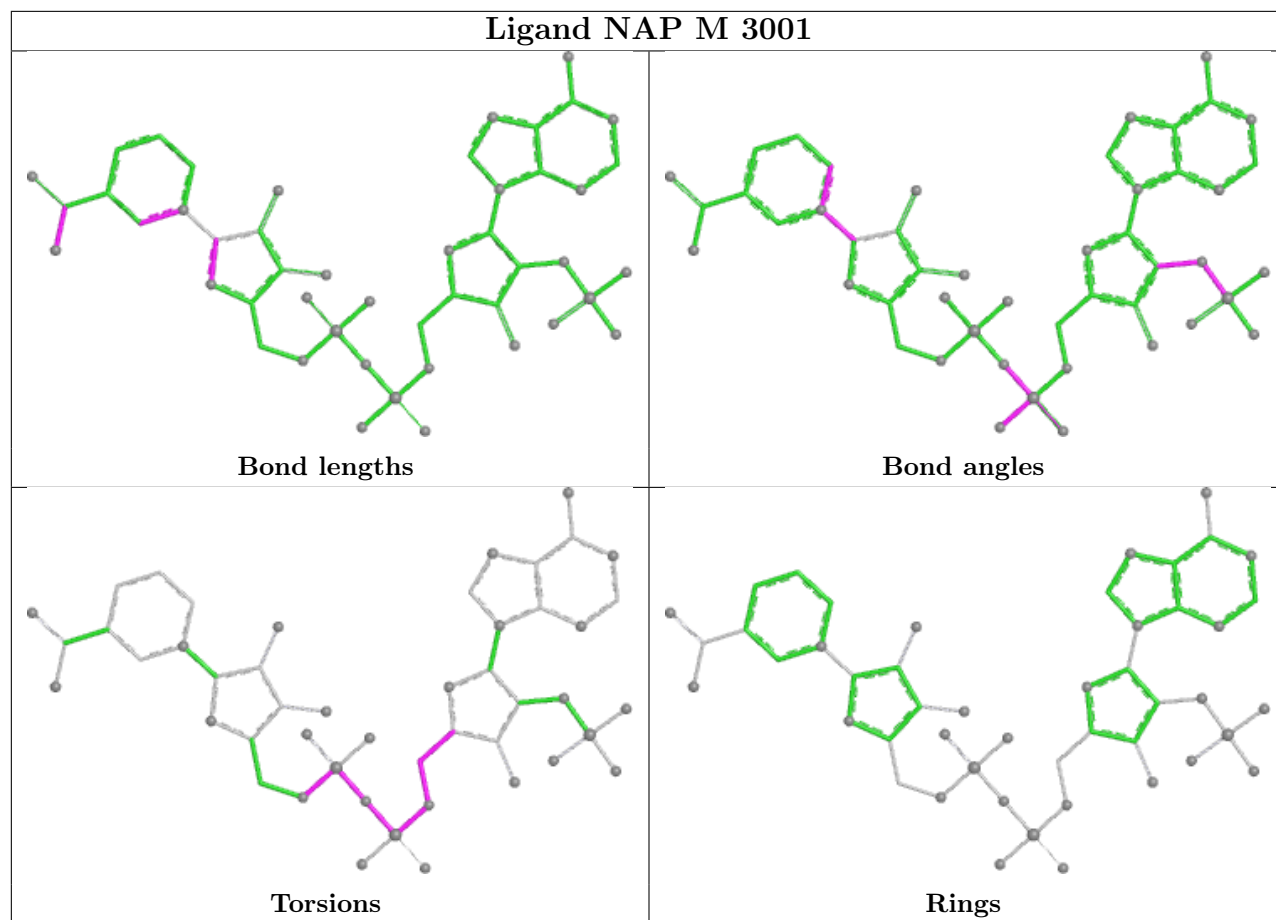
There are no ring outliers.

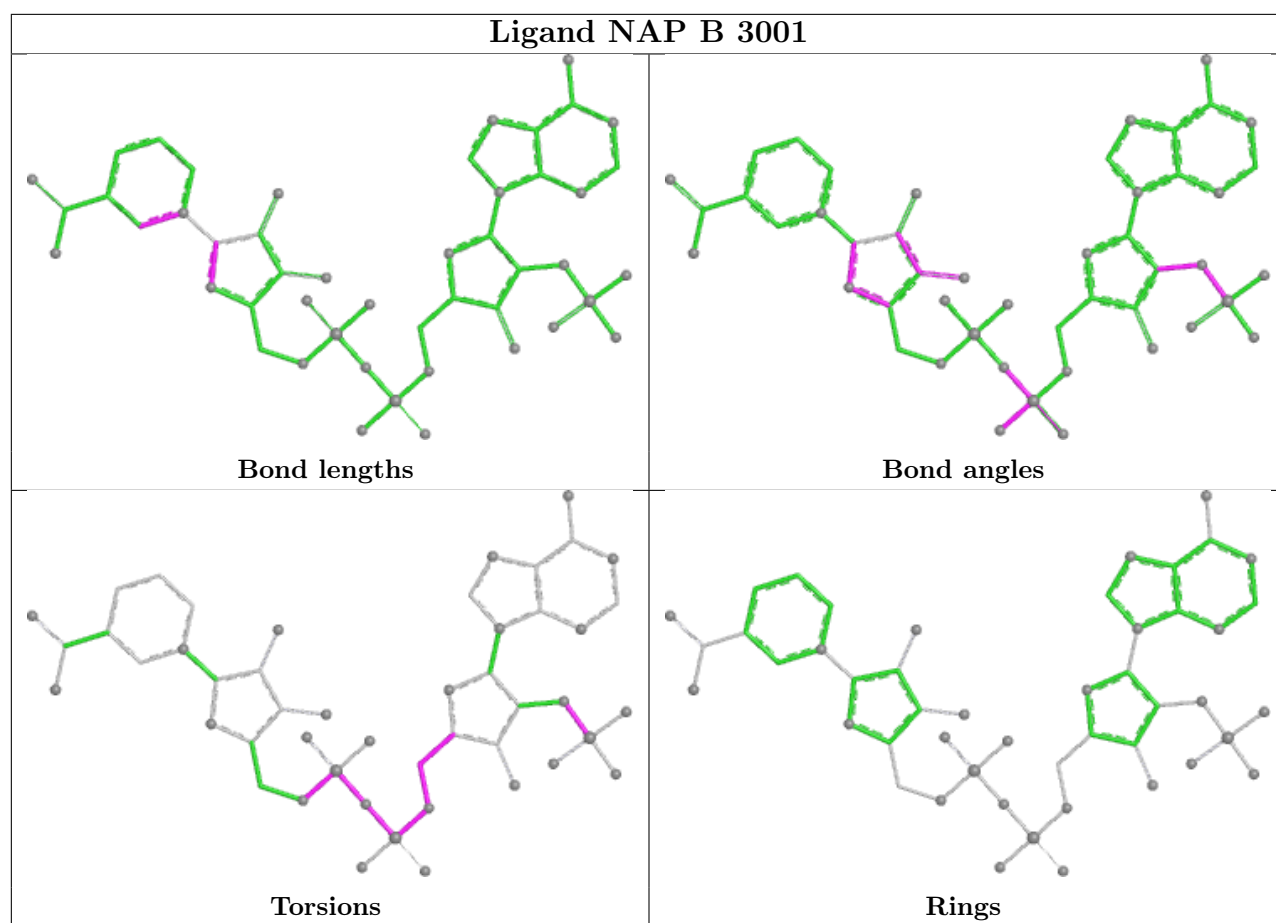
10 monomers are involved in 15 short contacts:

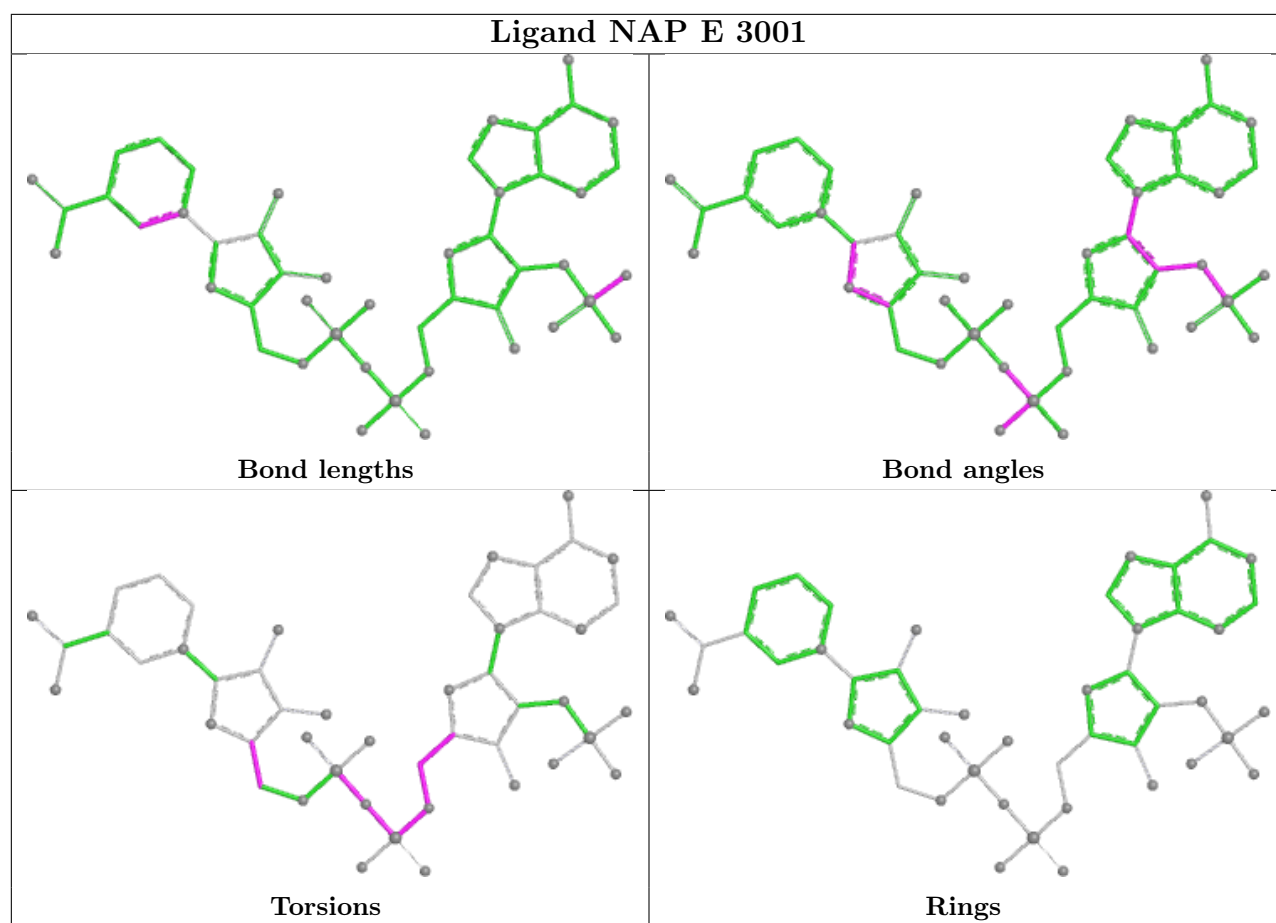
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	NAP	2	0
2	B	3001	NAP	2	0
2	E	3001	NAP	1	0
2	I	3001	NAP	1	0
2	L	3001	NAP	1	0
2	O	3001	NAP	1	0
2	F	3001	NAP	2	0
2	K	3001	NAP	2	0
2	C	3001	NAP	1	0
2	D	3001	NAP	2	0

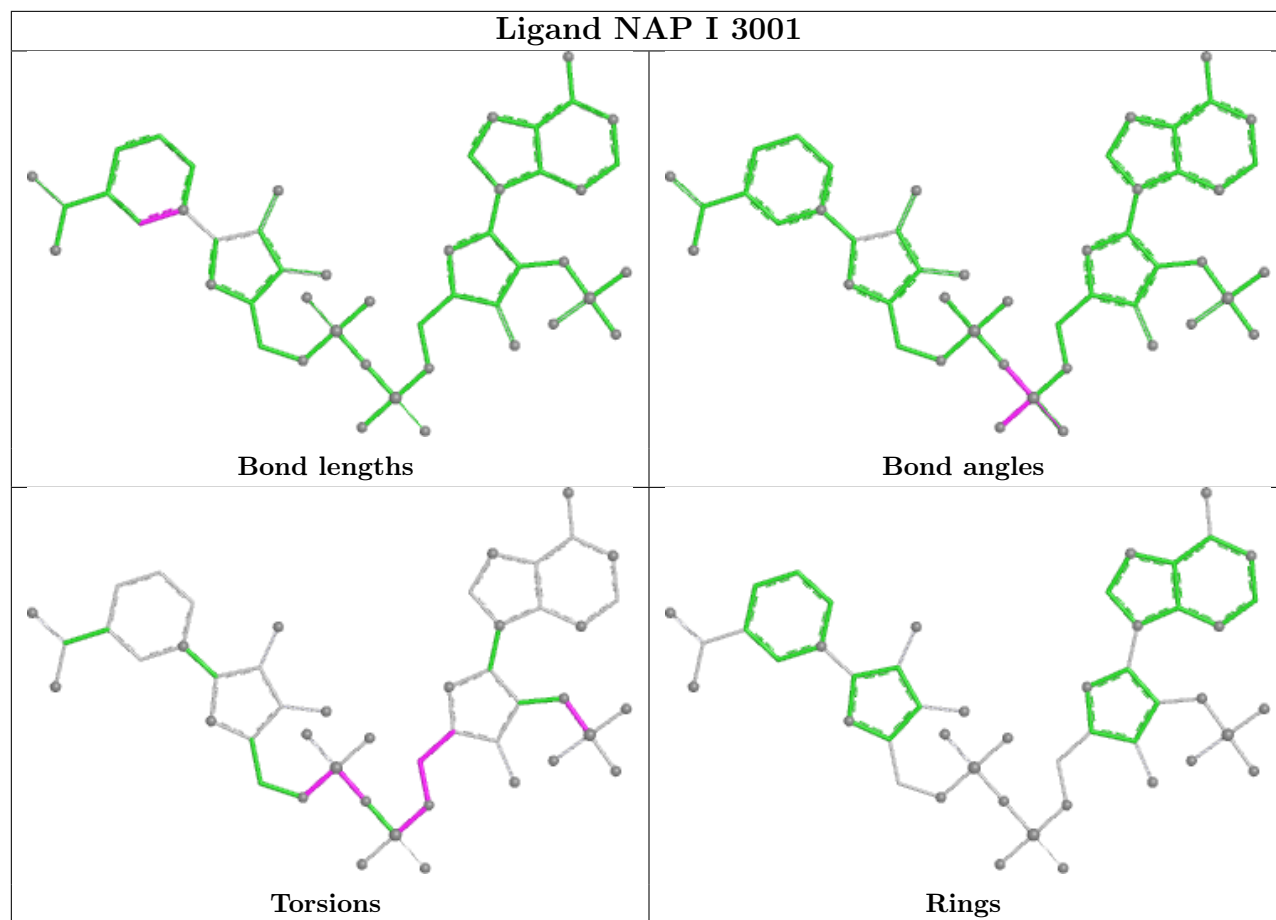
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



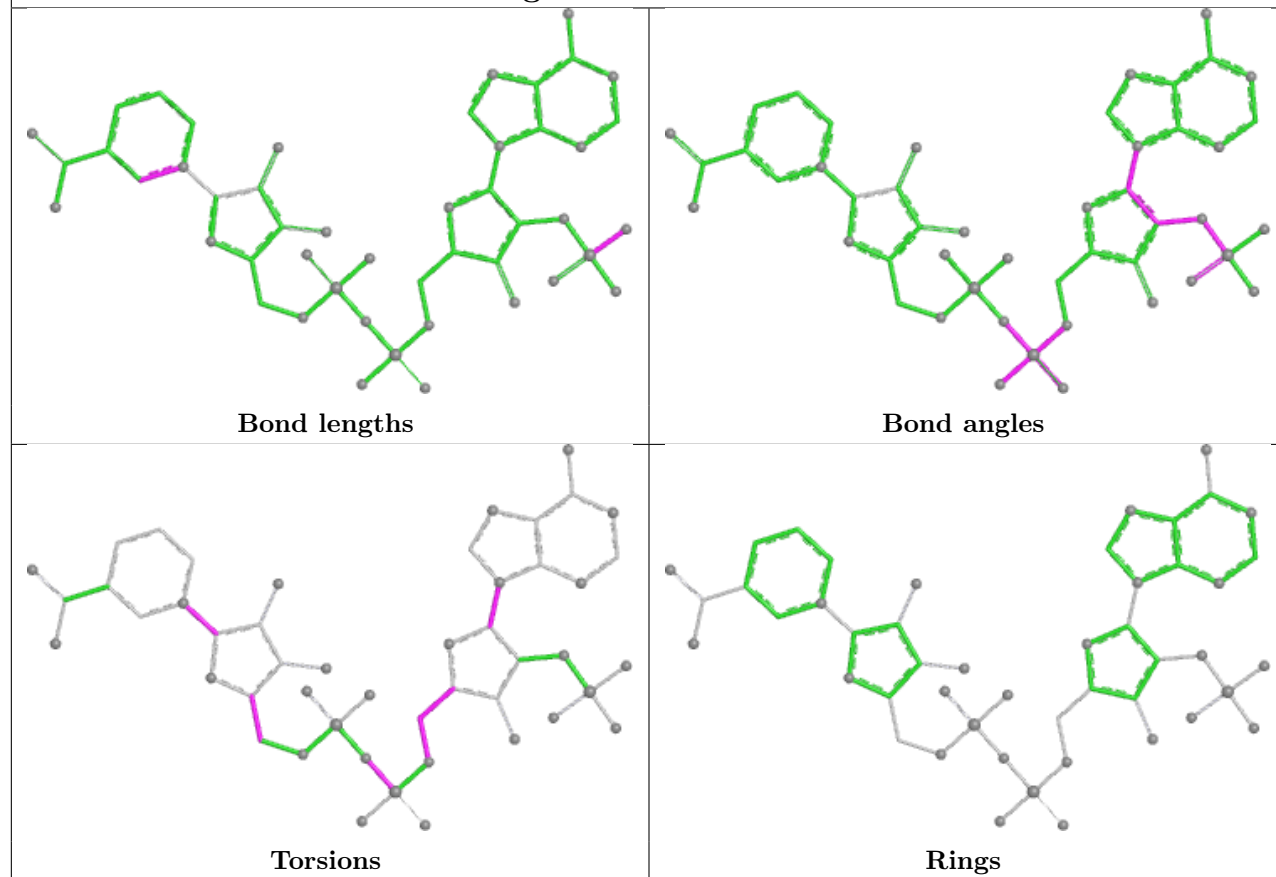




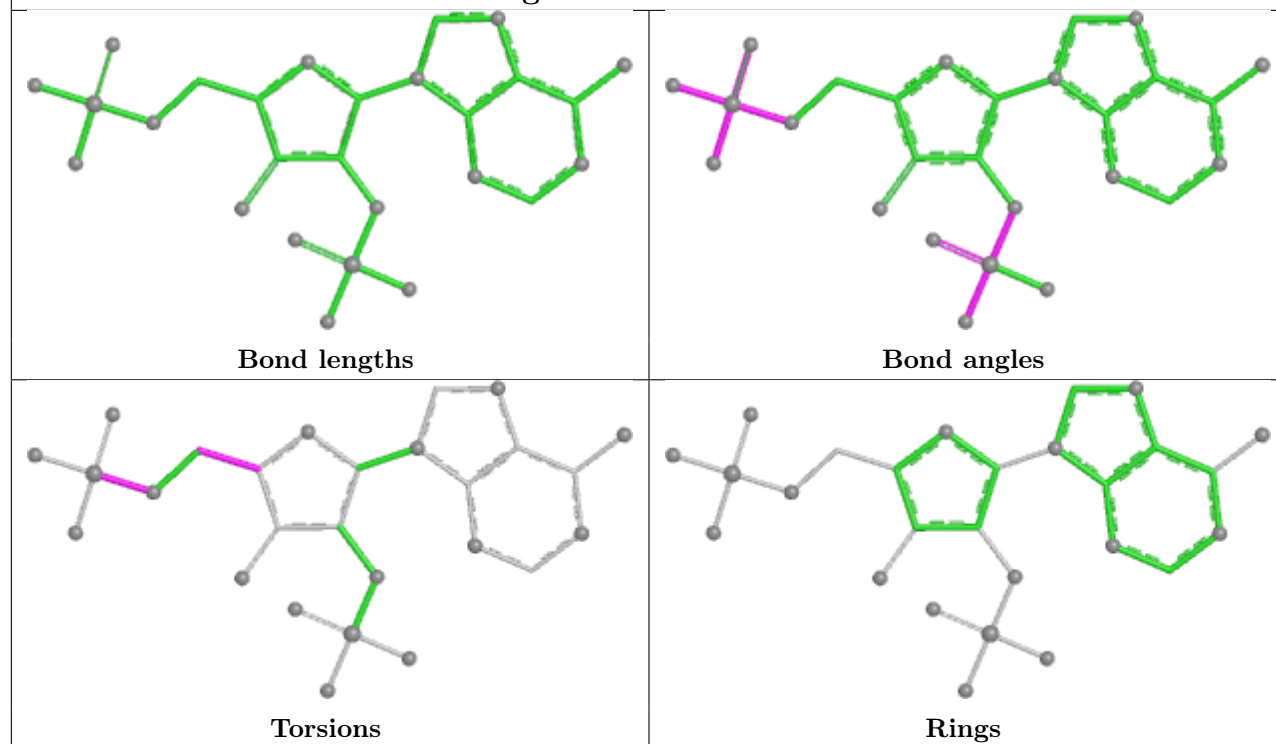


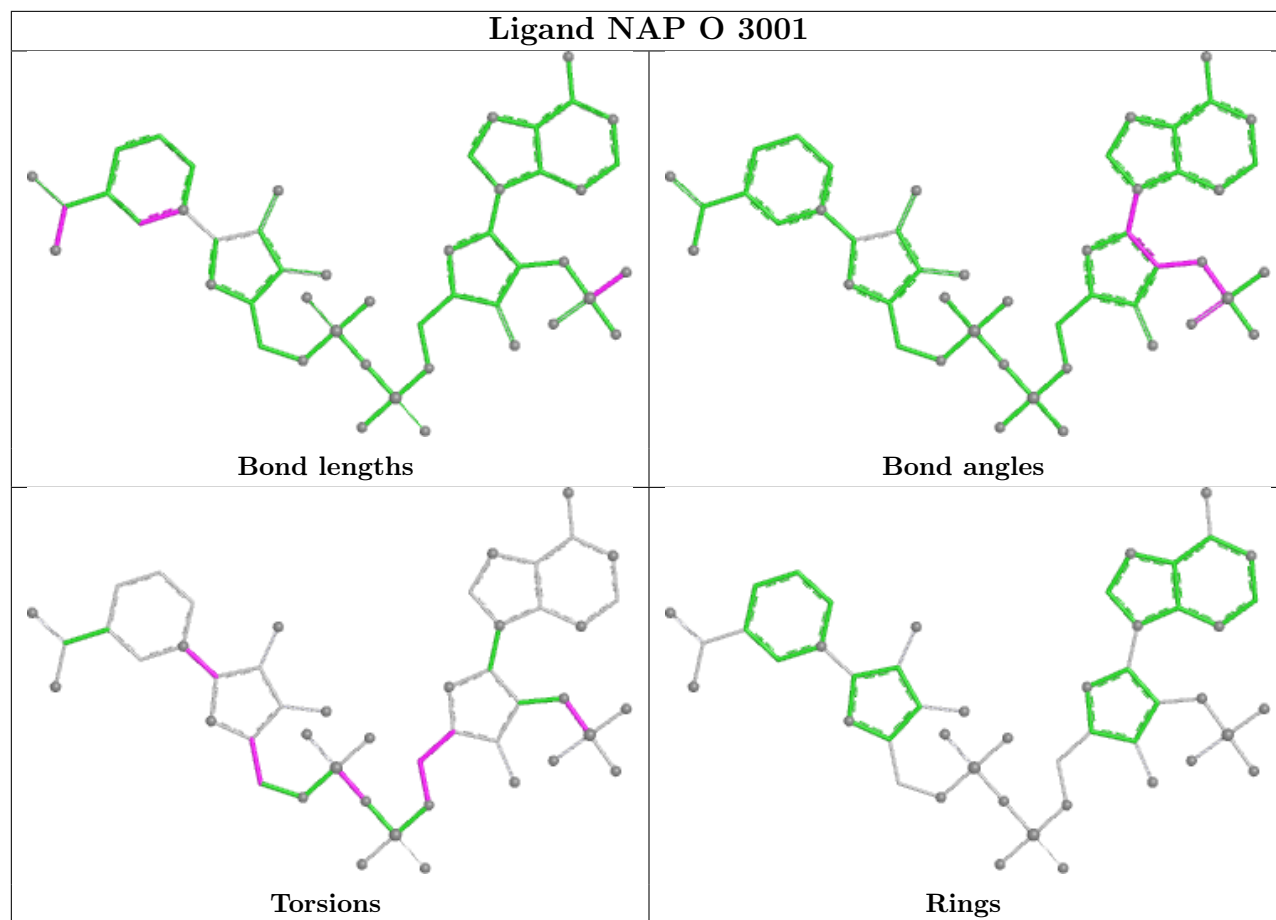


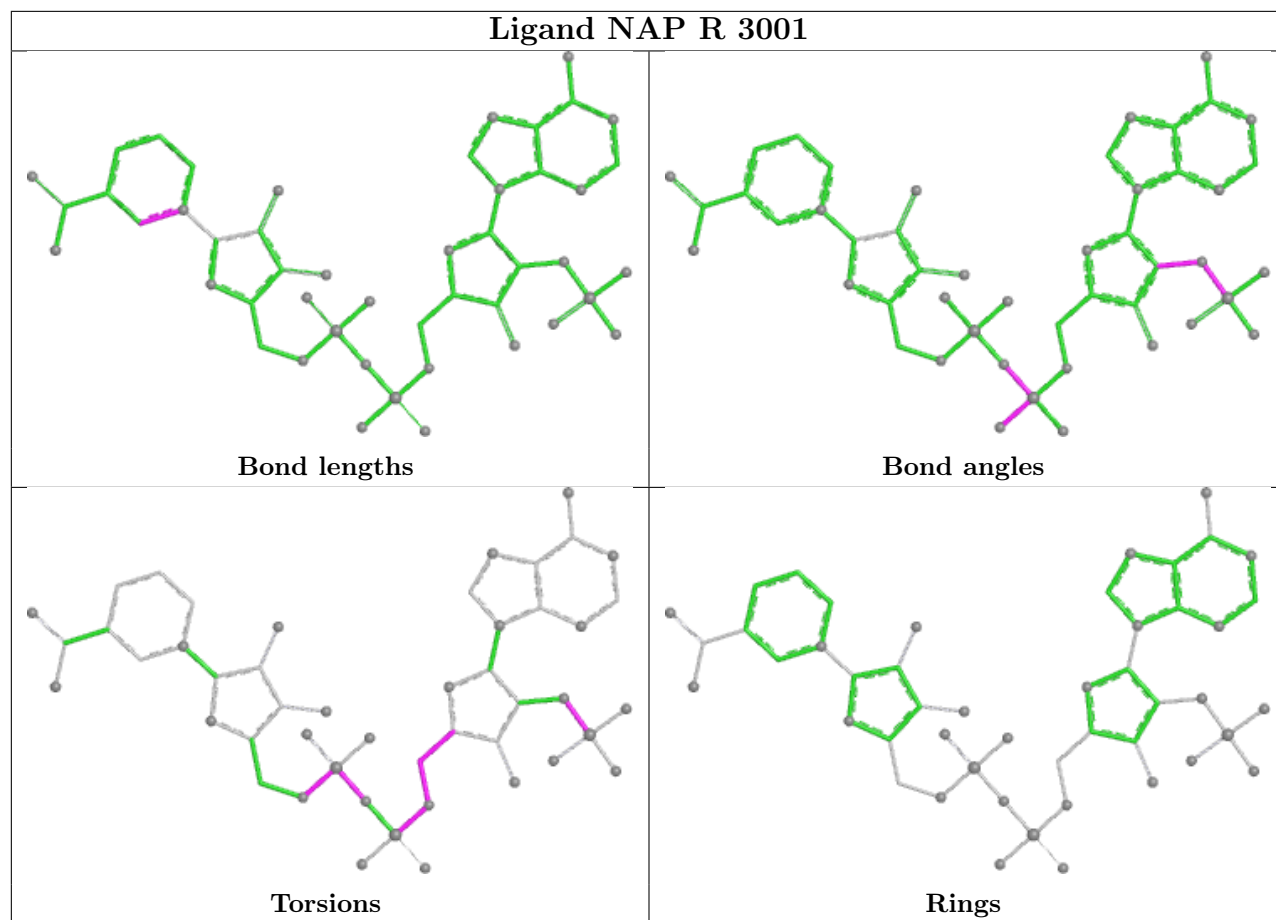
Ligand NAP L 3001

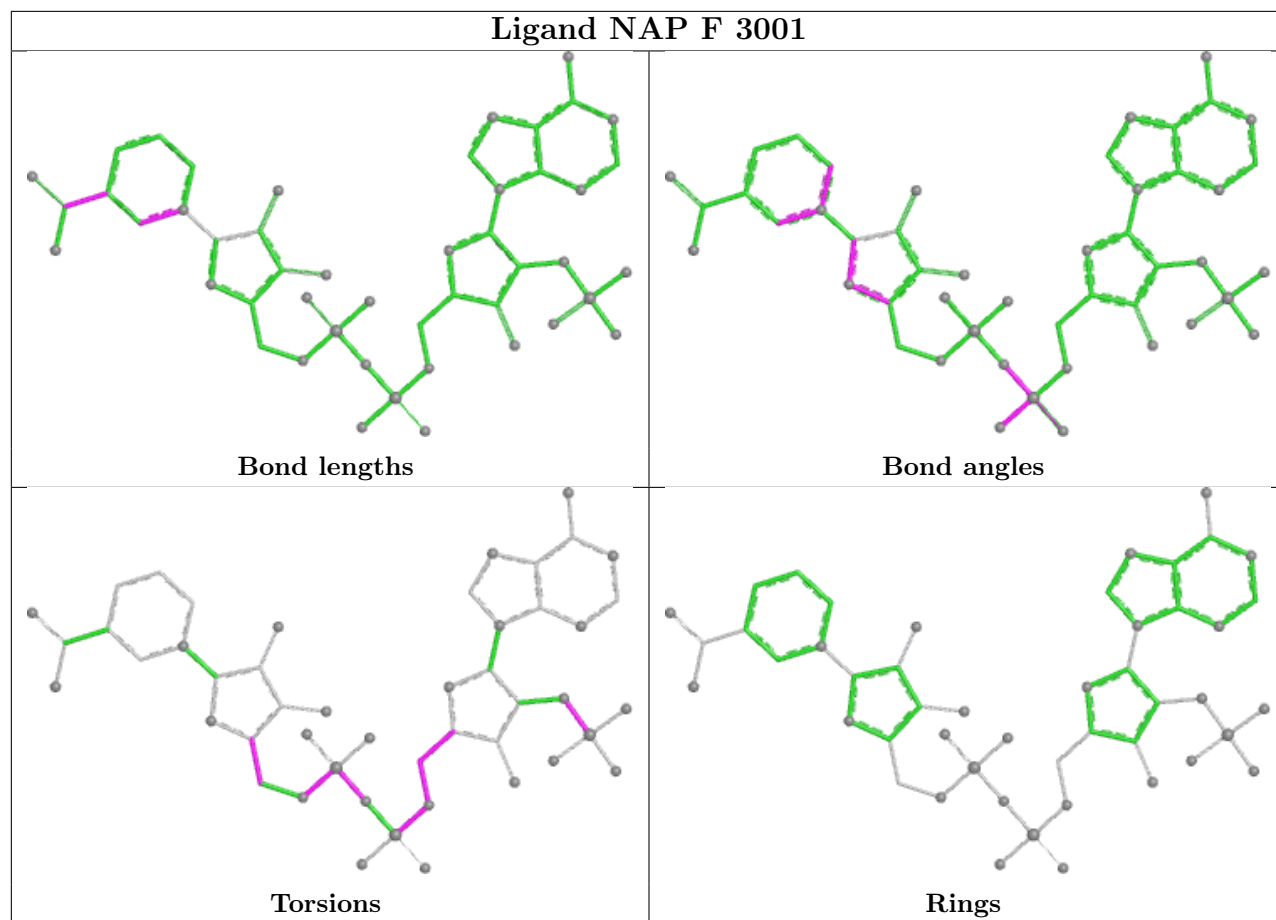


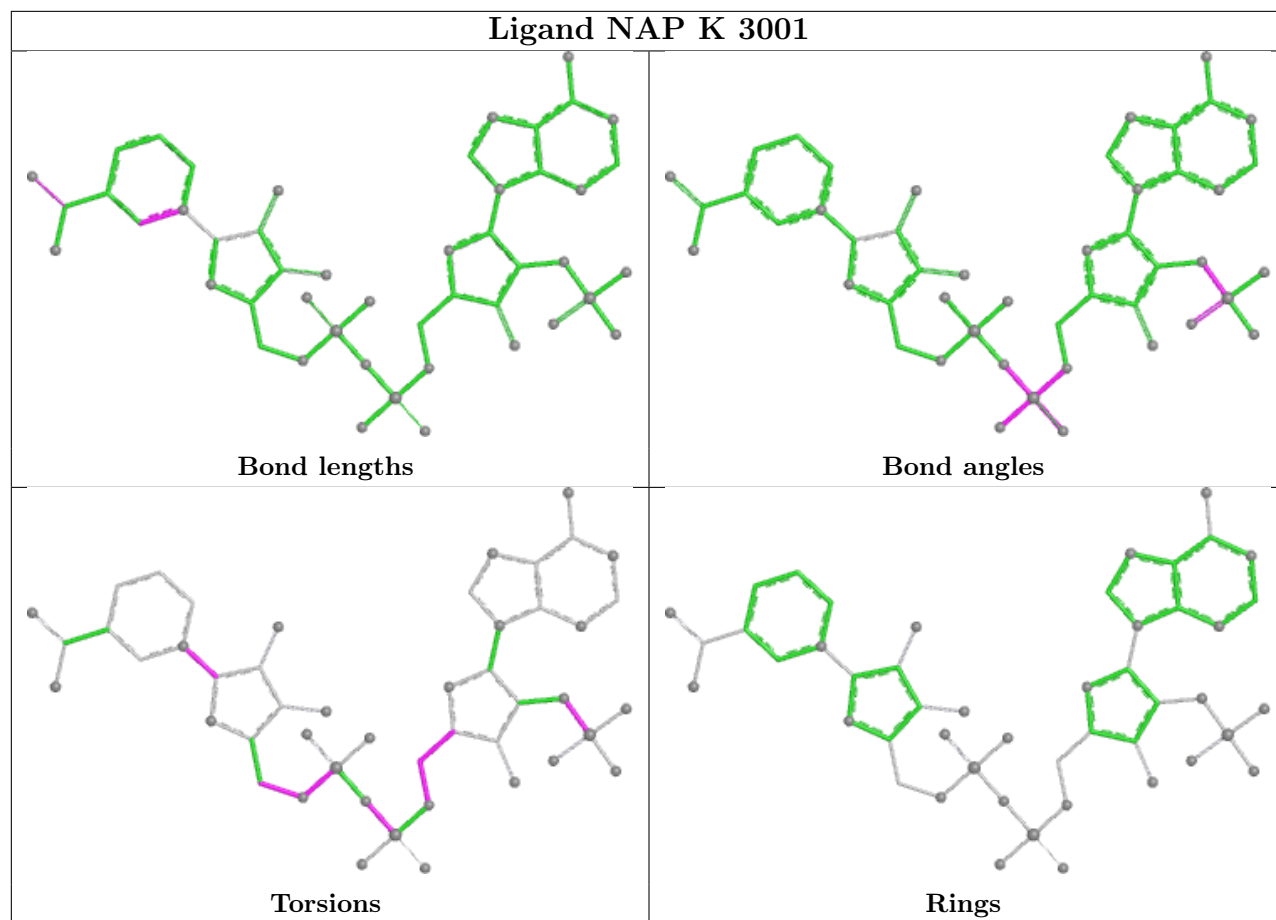
Ligand NAP F 3002

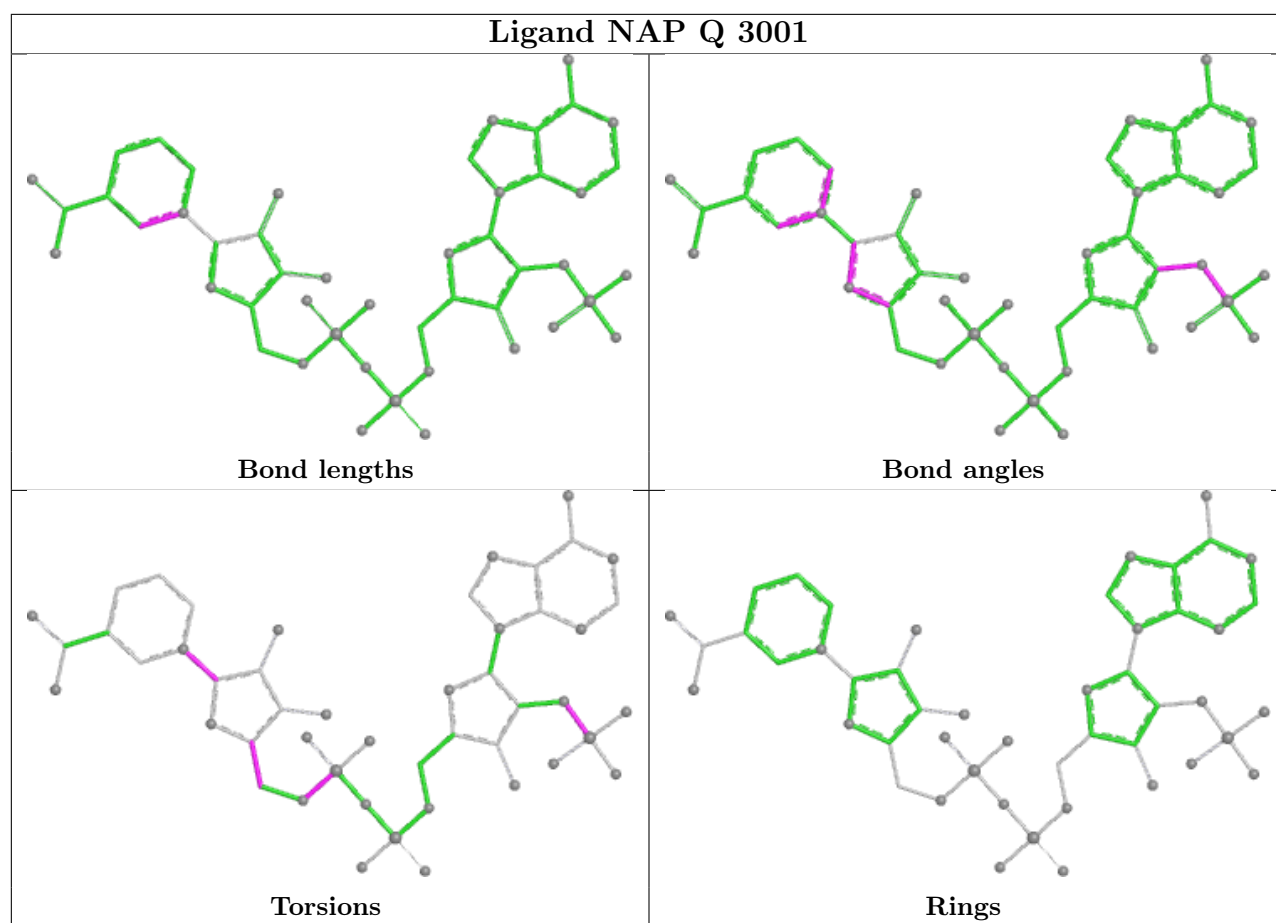




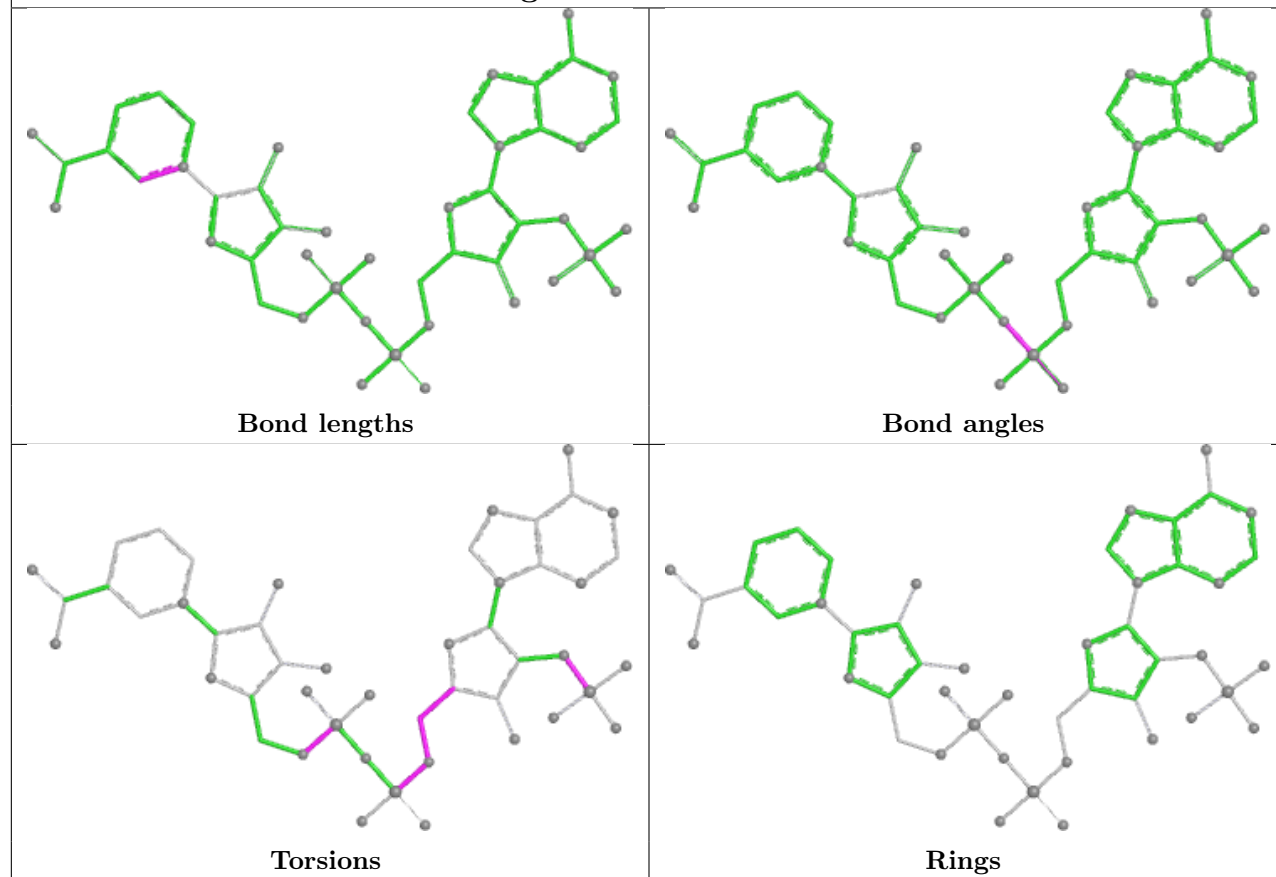




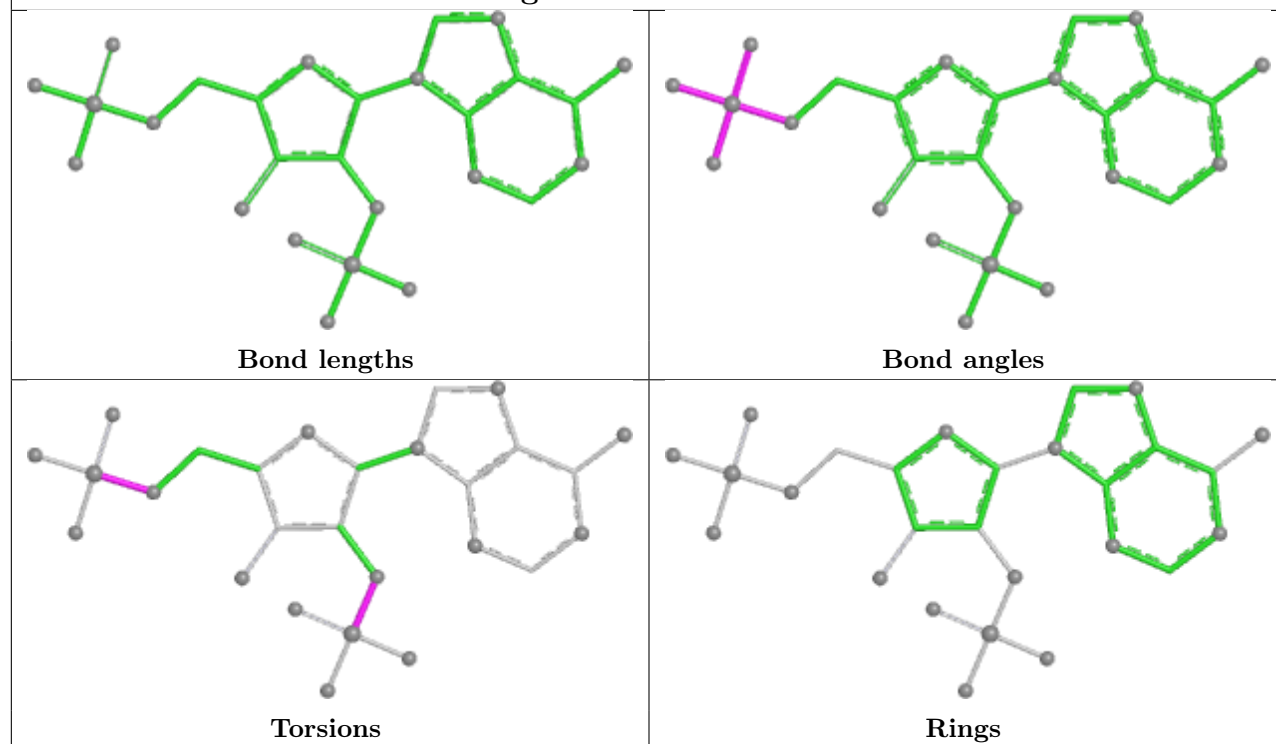




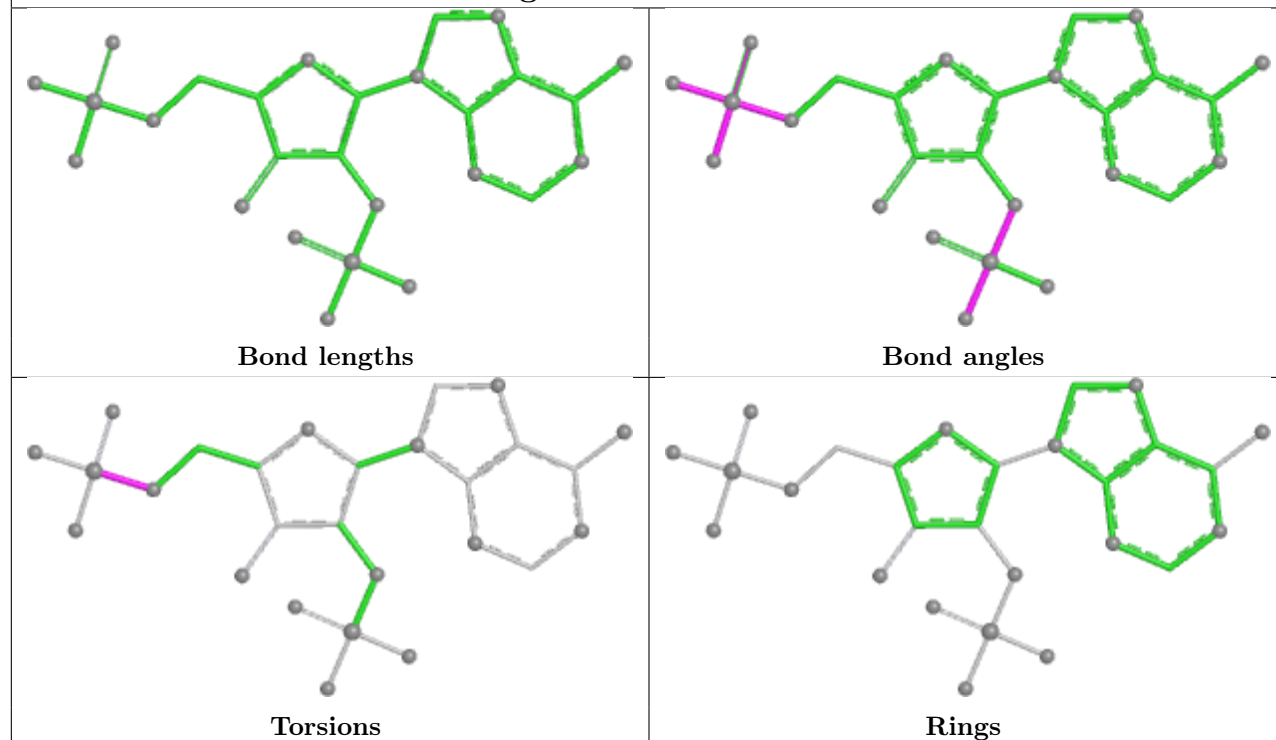
Ligand NAP C 3001



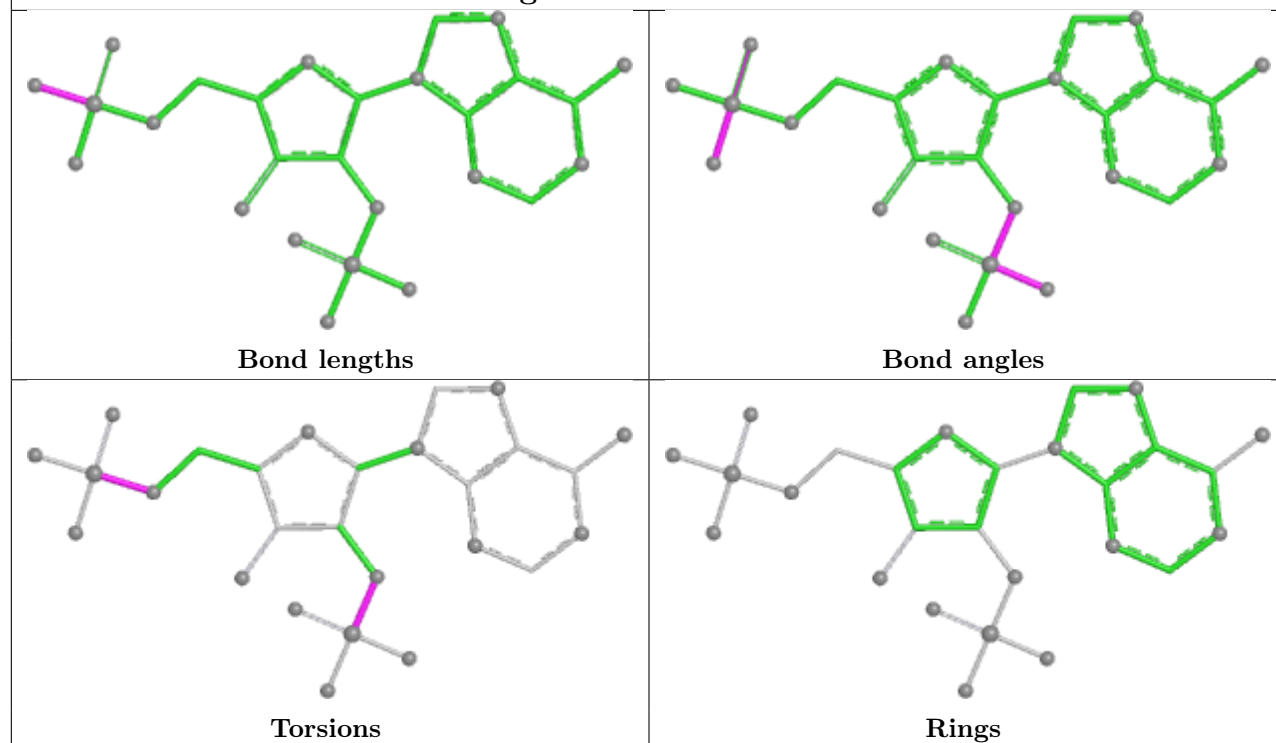
Ligand NAP B 3002



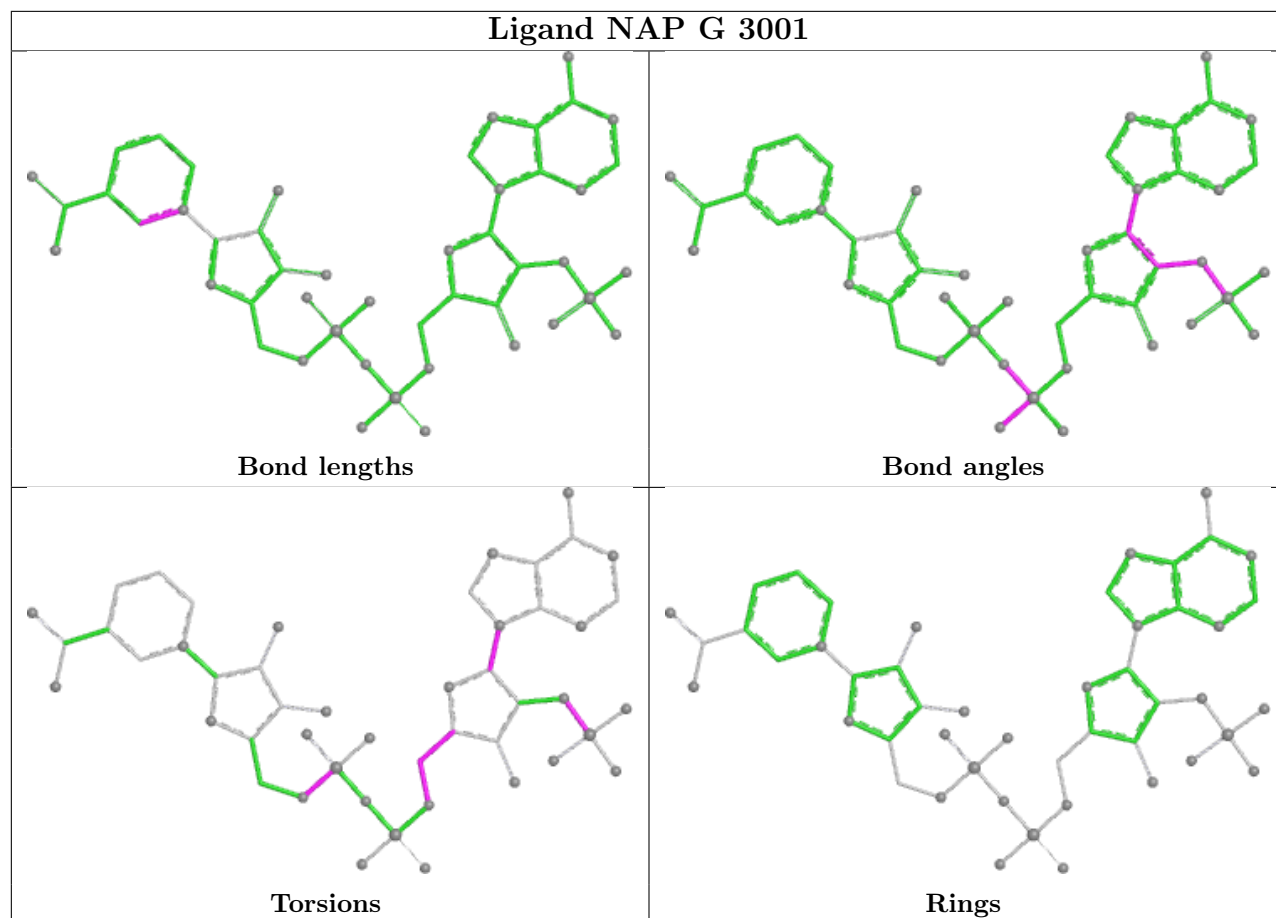
Ligand NAP H 3002



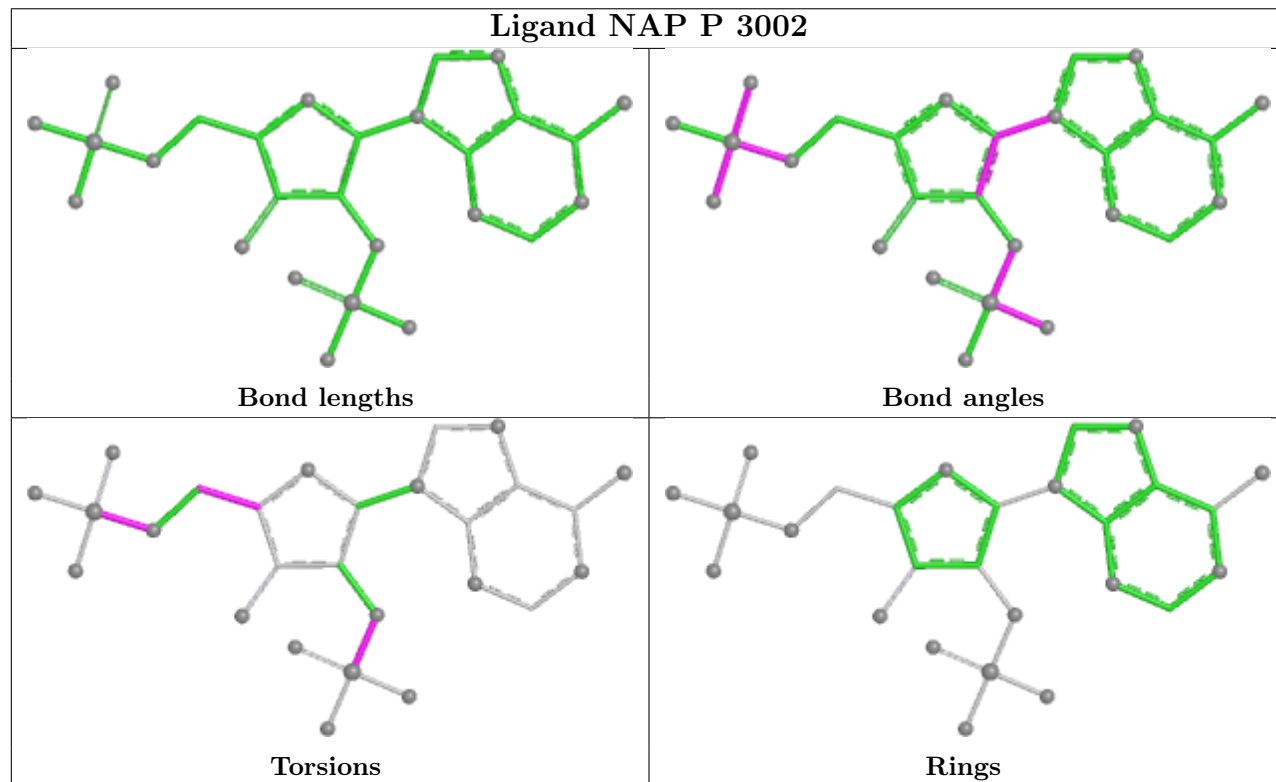
Ligand NAP N 3002



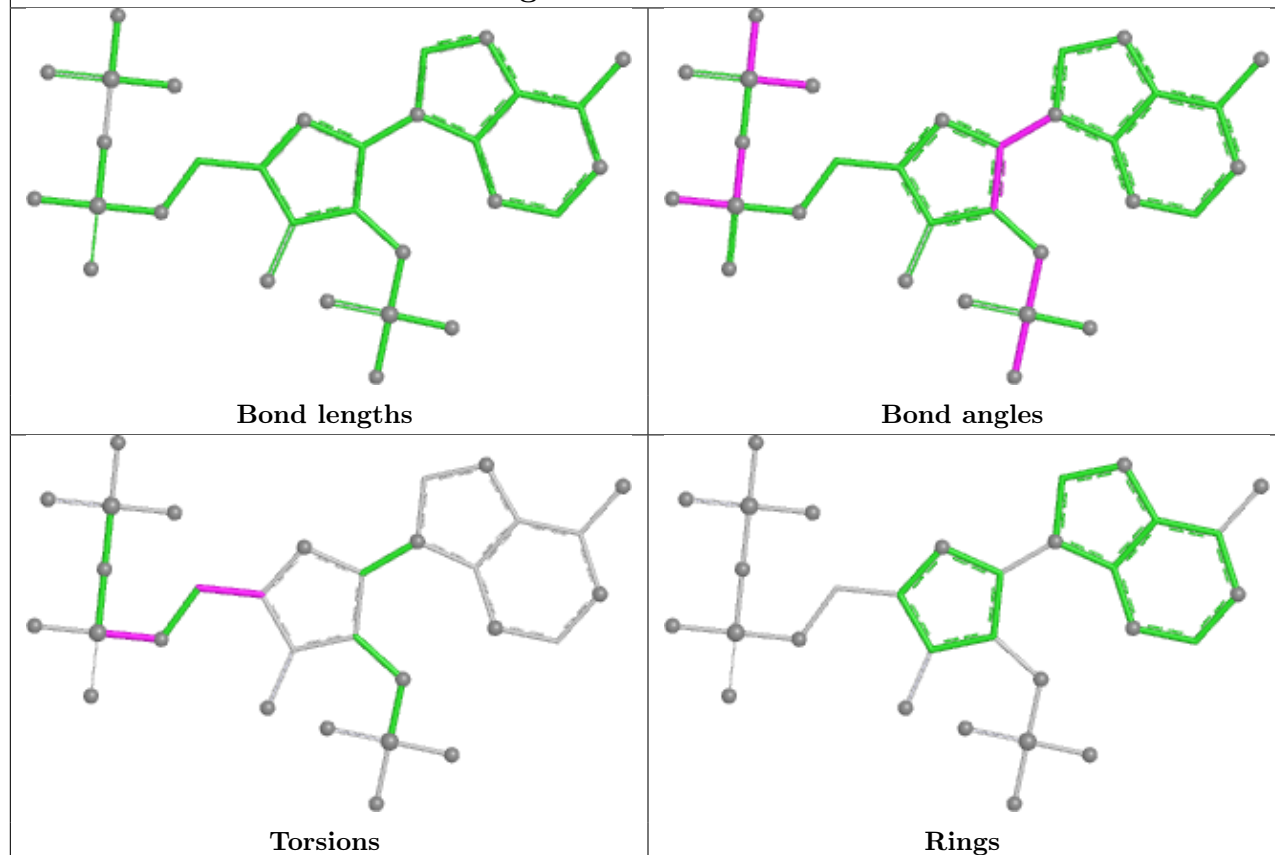
Ligand NAP G 3001



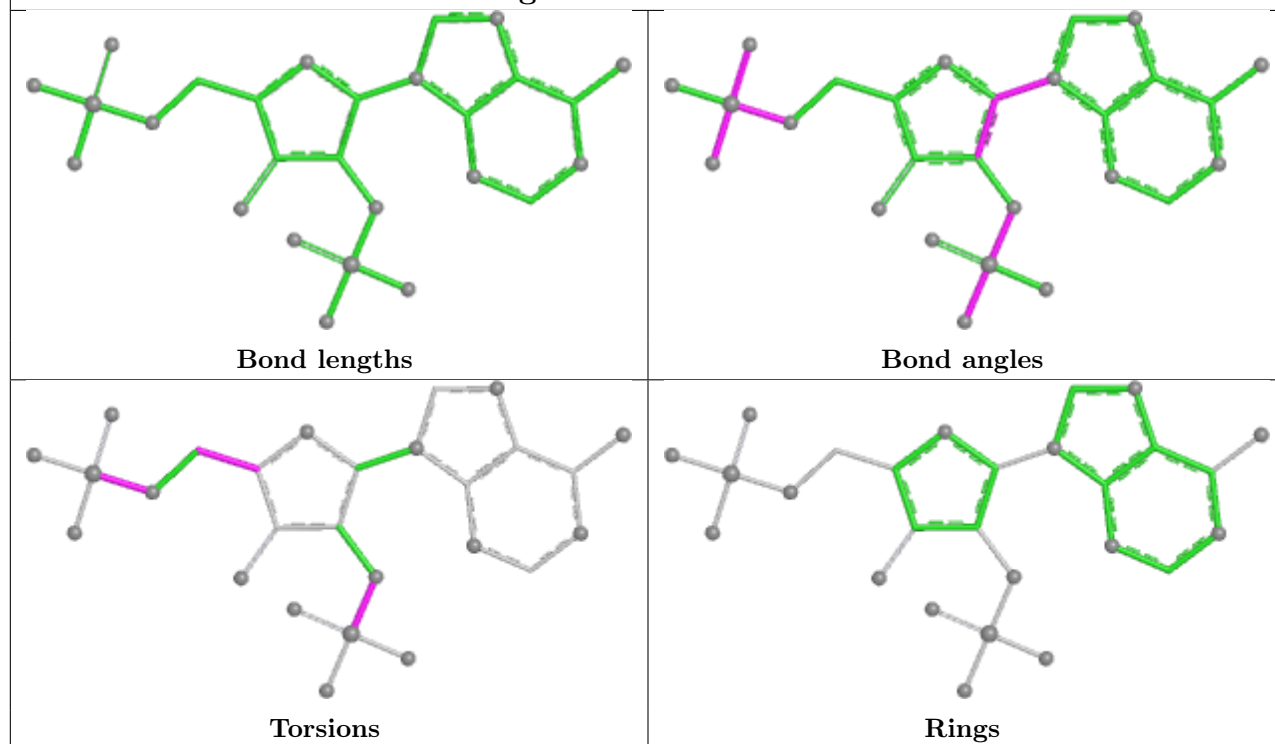
Ligand NAP P 3002



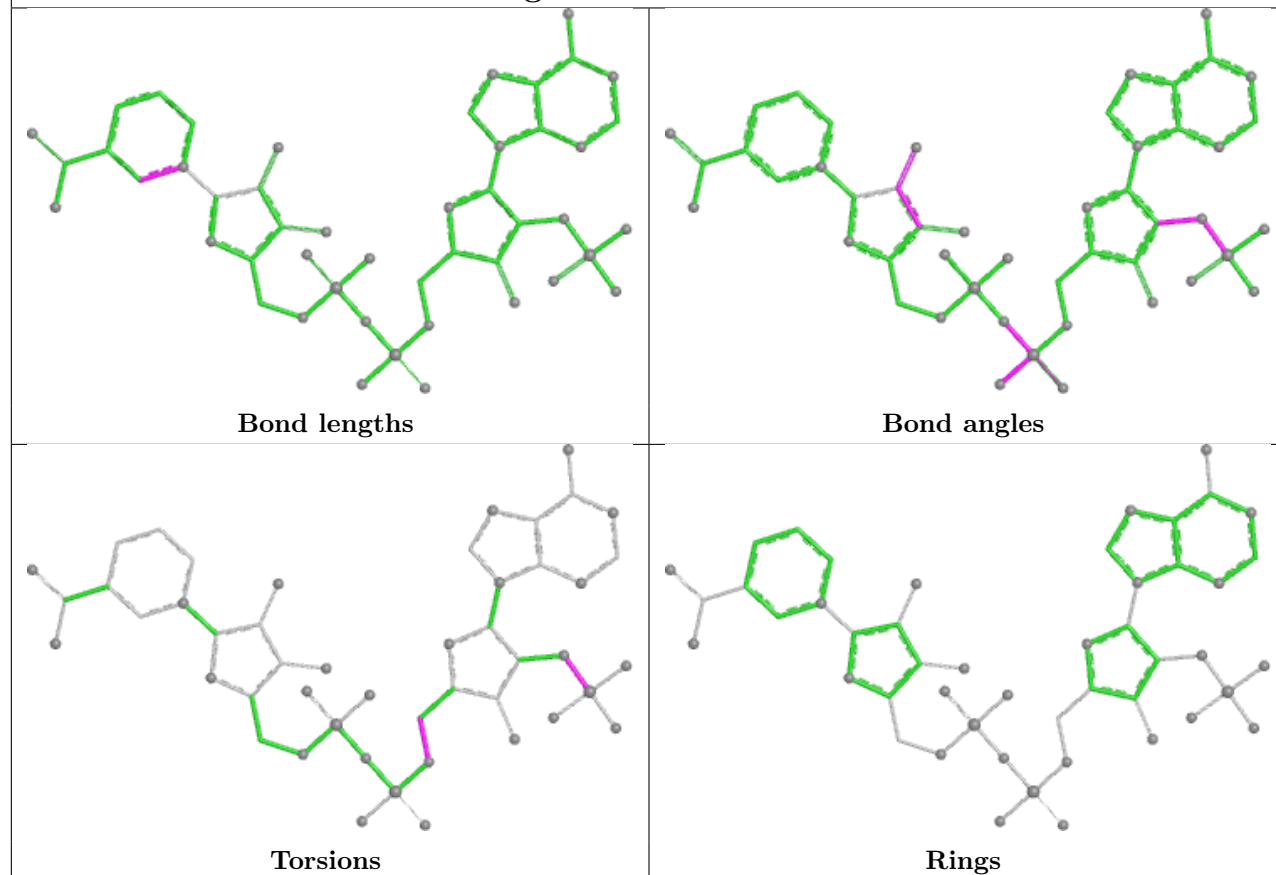
Ligand NAP C 3002



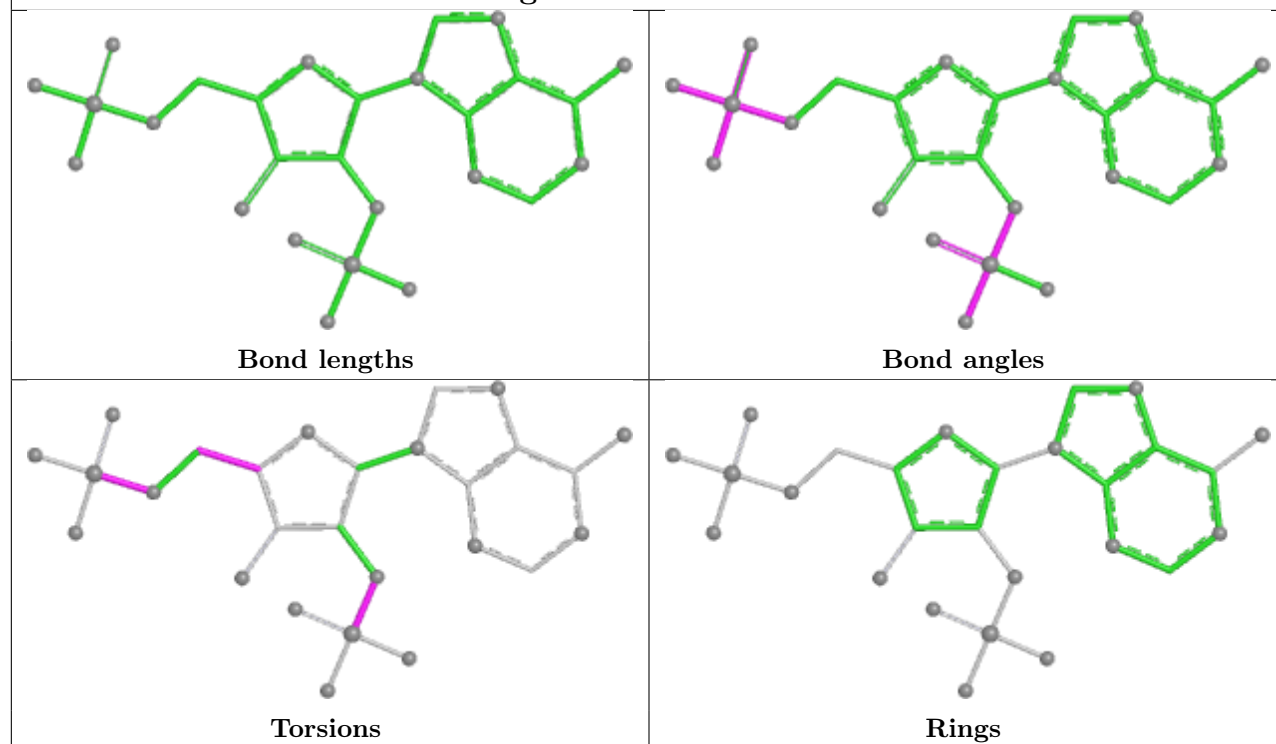
Ligand NAP D 3002

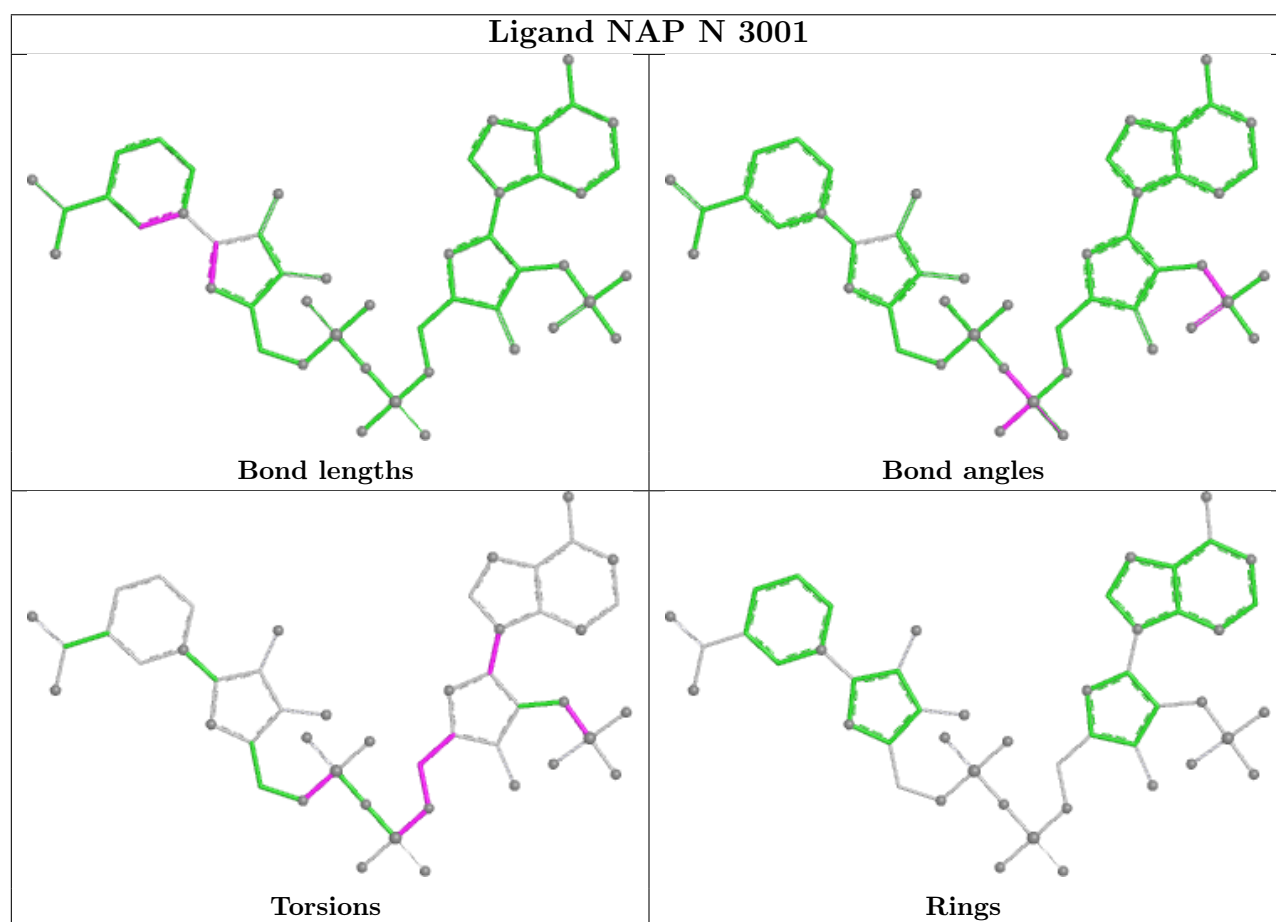
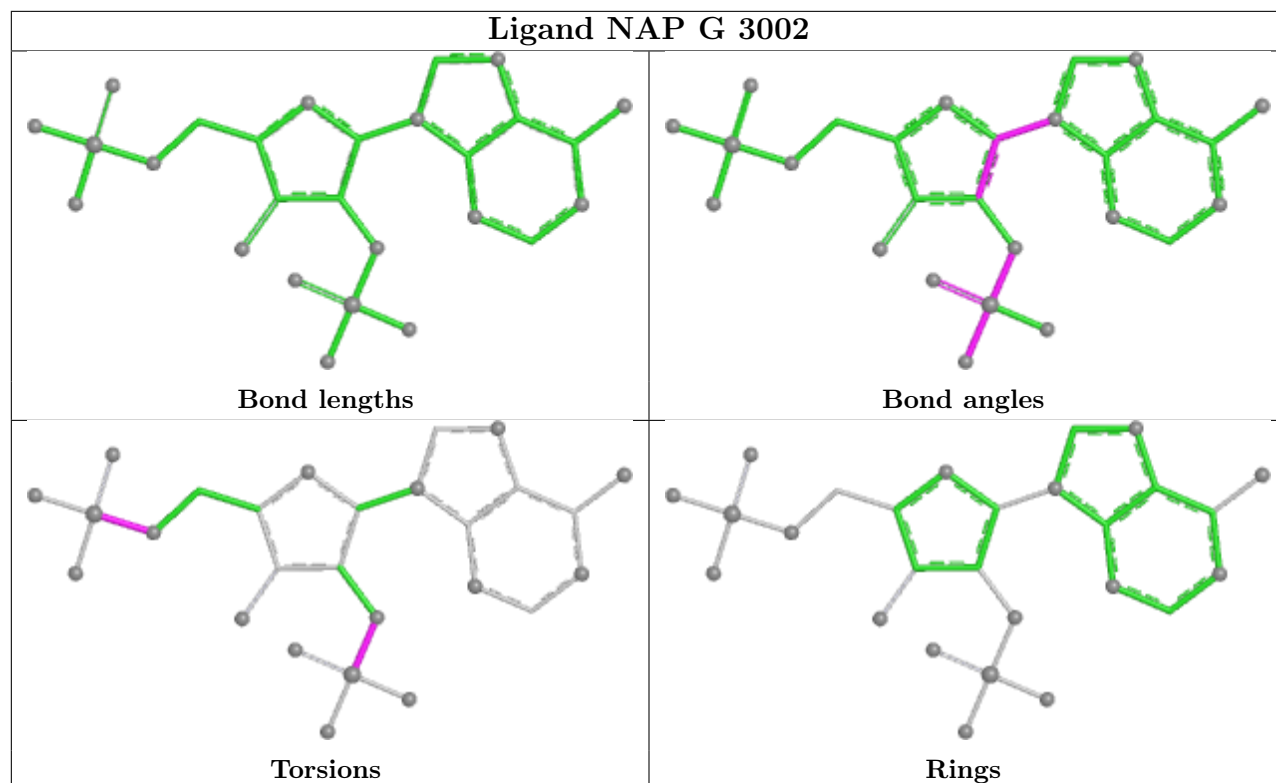


Ligand NAP J 3001

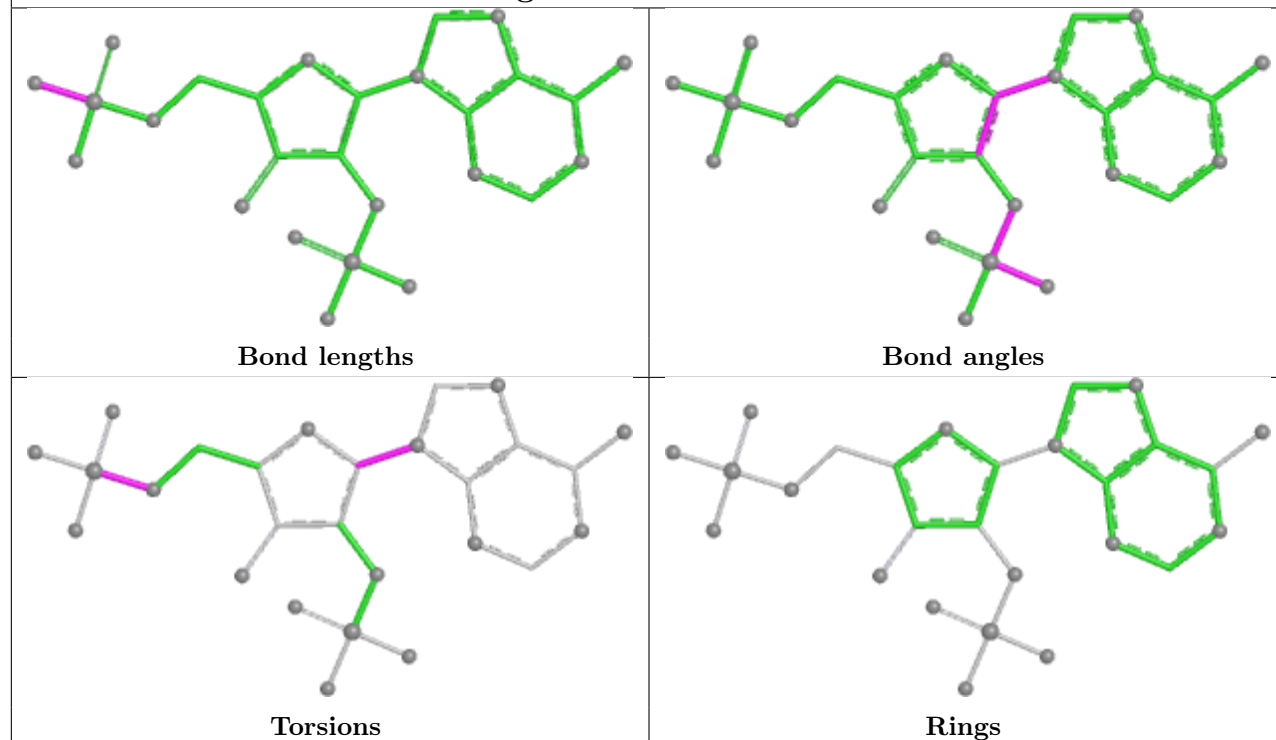


Ligand NAP K 3002

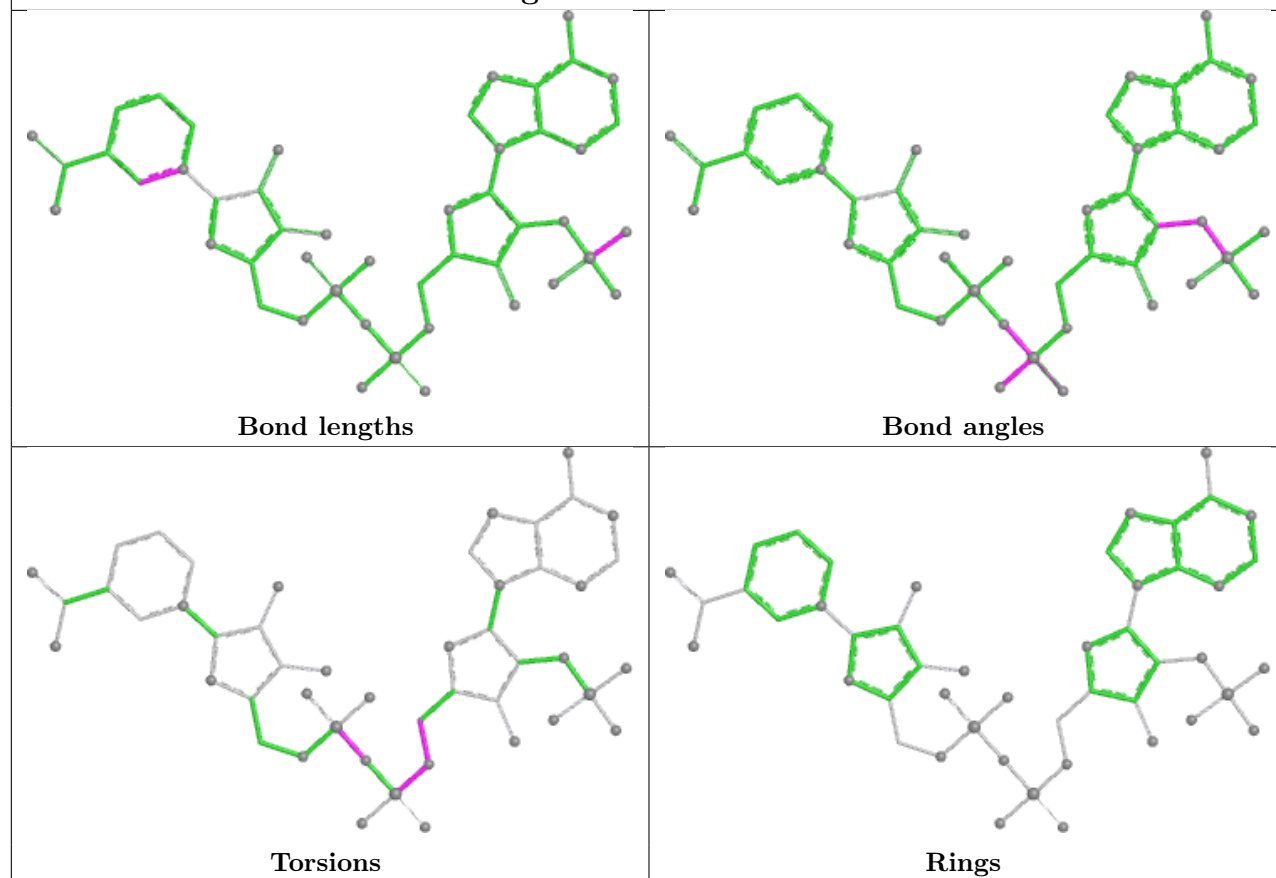




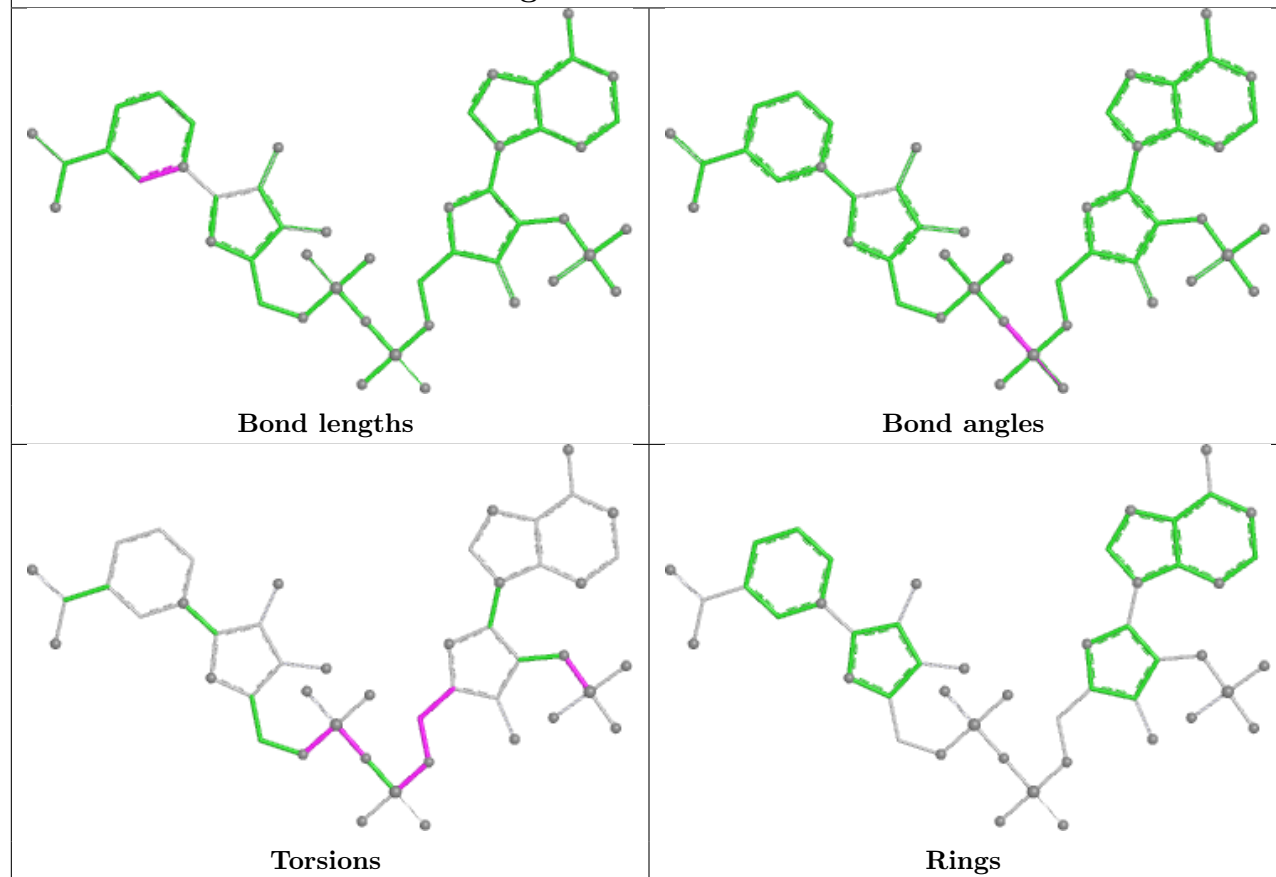
Ligand NAP M 3002



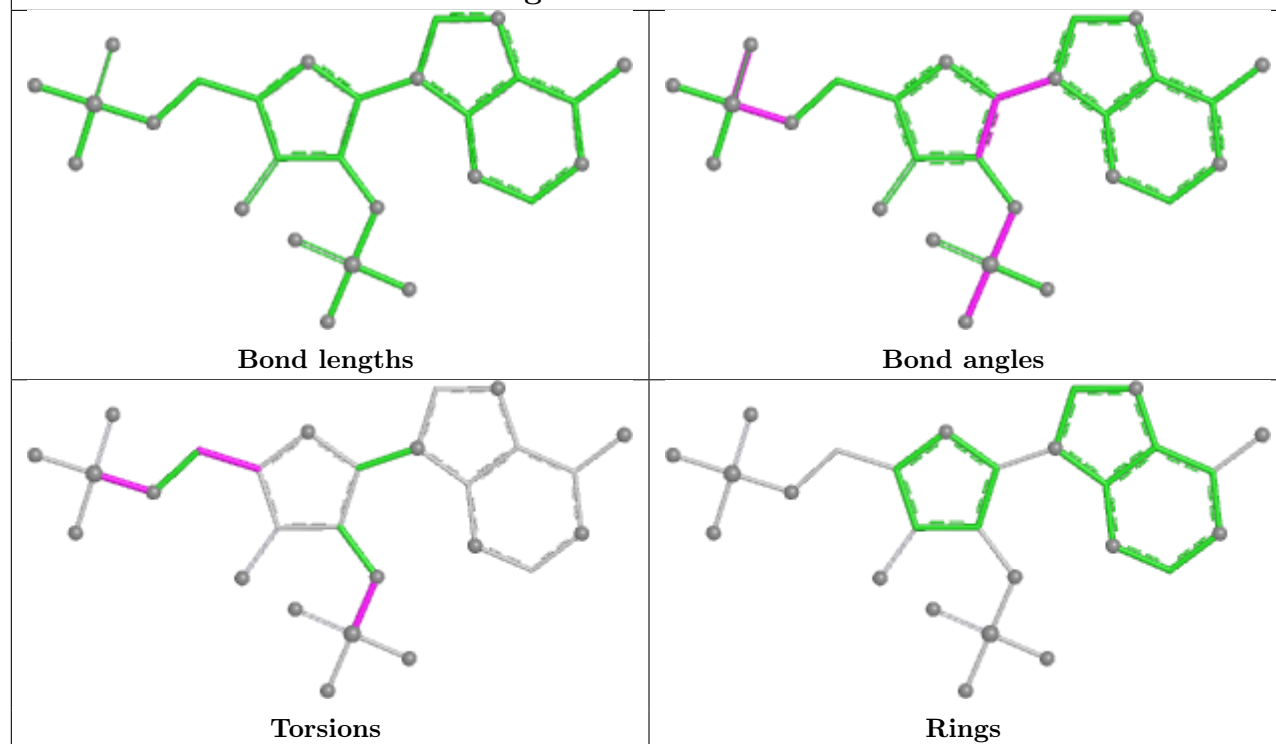
Ligand NAP P 3001



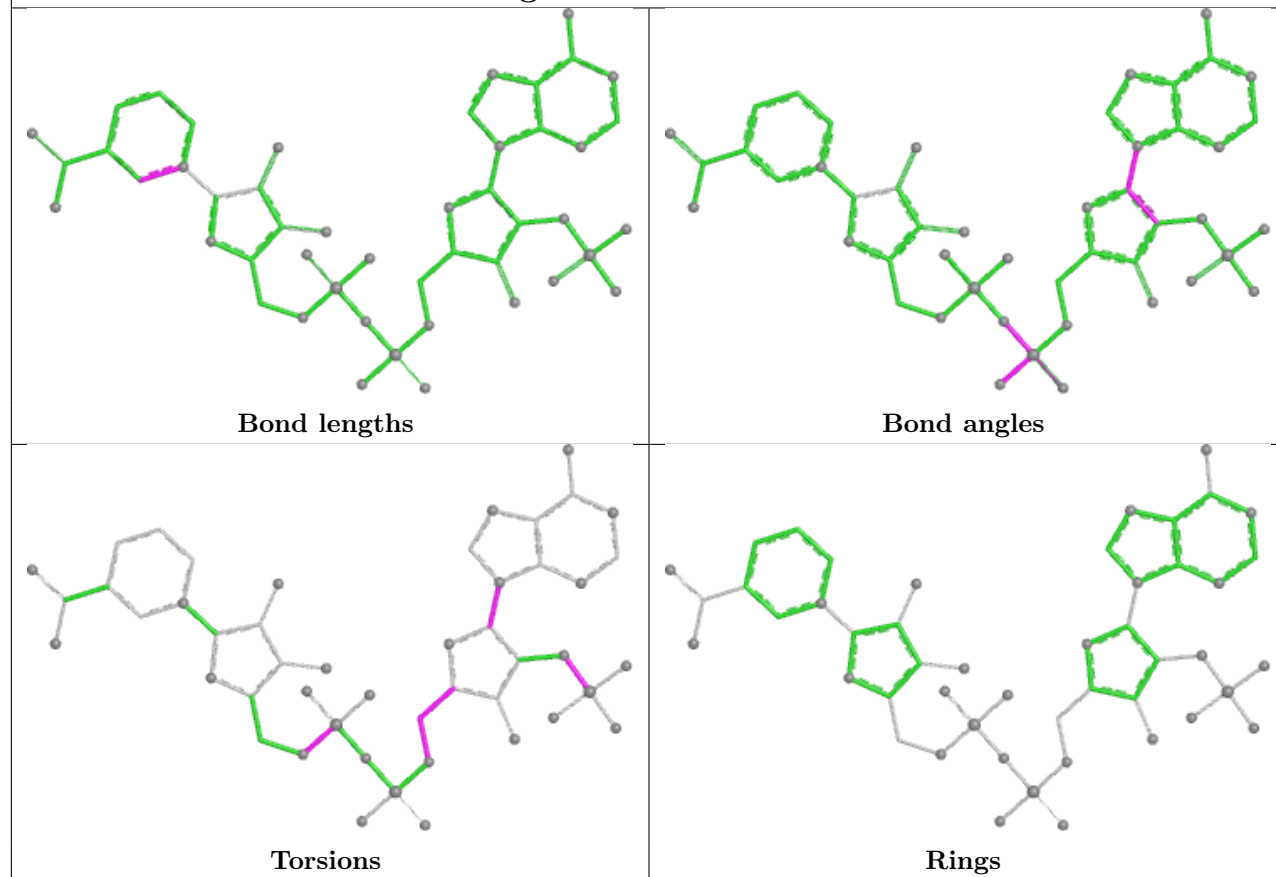
Ligand NAP D 3001



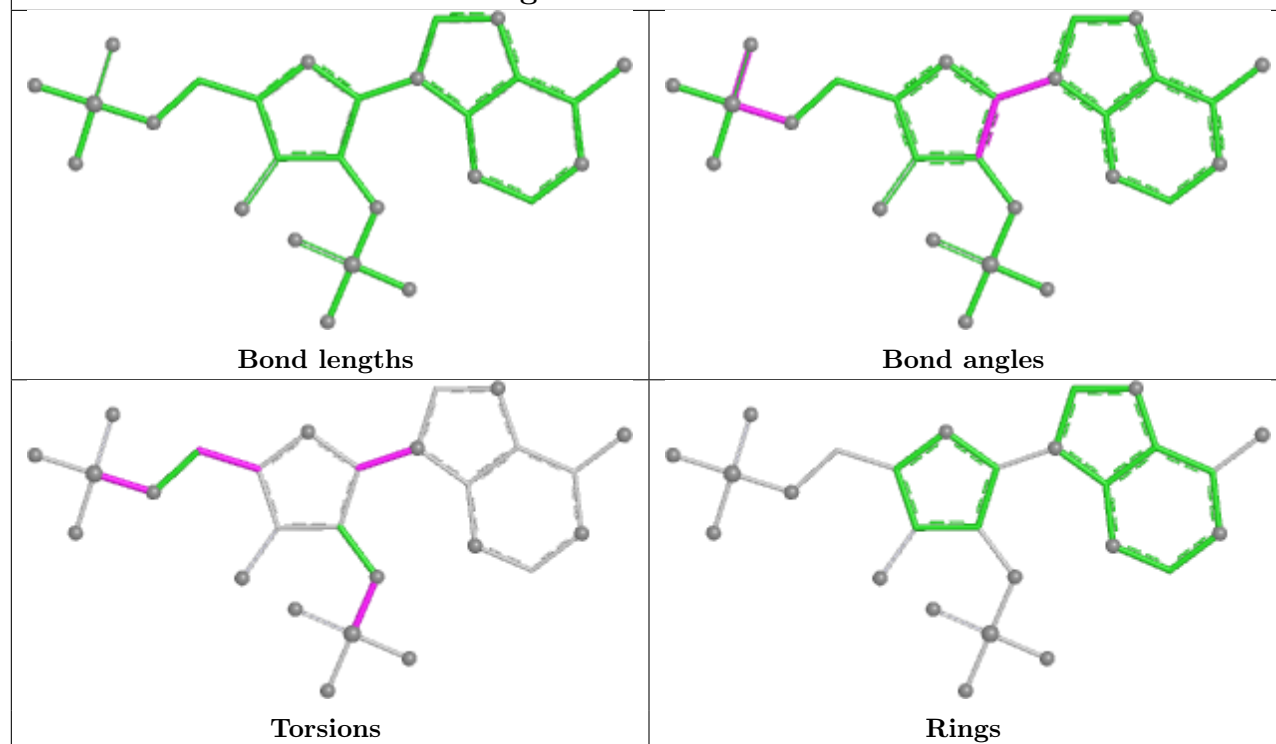
Ligand NAP J 3002



Ligand NAP H 3001



Ligand NAP A 3002



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1102/1140 (96%)	0.02	21 (1%) 66 44	84, 166, 264, 278	0
1	B	1102/1140 (96%)	0.03	18 (1%) 70 47	85, 136, 220, 241	0
1	C	1102/1140 (96%)	0.13	34 (3%) 51 34	88, 162, 233, 262	0
1	D	1102/1140 (96%)	0.06	28 (2%) 58 39	92, 172, 262, 282	0
1	E	1089/1140 (95%)	0.14	30 (2%) 55 36	127, 203, 264, 278	0
1	F	1093/1140 (95%)	0.13	28 (2%) 57 38	125, 193, 236, 258	0
1	G	1088/1140 (95%)	0.08	30 (2%) 55 36	108, 174, 224, 261	0
1	H	1097/1140 (96%)	0.04	21 (1%) 66 44	114, 180, 220, 255	0
1	I	655/1140 (57%)	-0.05	8 (1%) 76 54	94, 167, 220, 255	0
1	J	1089/1140 (95%)	0.03	18 (1%) 69 46	94, 165, 213, 252	0
1	K	1089/1140 (95%)	-0.01	9 (0%) 82 62	84, 137, 187, 223	0
1	L	897/1140 (78%)	0.12	32 (3%) 46 31	80, 144, 244, 263	0
1	M	1089/1140 (95%)	0.03	18 (1%) 69 46	112, 175, 240, 265	0
1	N	1089/1140 (95%)	0.04	27 (2%) 58 39	104, 157, 205, 255	0
1	O	633/1140 (55%)	-0.07	5 (0%) 82 62	83, 130, 183, 224	0
1	P	1089/1140 (95%)	0.06	24 (2%) 62 43	84, 150, 211, 247	0
1	Q	608/1140 (53%)	0.54	49 (8%) 18 16	179, 228, 264, 279	0
1	R	637/1140 (55%)	0.19	13 (2%) 65 43	156, 210, 246, 267	0
All	All	17650/20520 (86%)	0.08	413 (2%) 61 41	80, 169, 243, 282	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	1074	THR	9.8
1	Q	1073	PRO	7.0
1	L	1768	VAL	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1276	VAL	5.2
1	A	1275	ALA	5.2
1	D	1971	PHE	5.1
1	L	1879	ALA	5.1
1	N	948	CYS	5.0
1	E	906	SER	5.0
1	G	1108	ALA	4.9
1	Q	948	CYS	4.9
1	L	1871	ASP	4.8
1	F	1655	GLU	4.8
1	R	1683	LEU	4.8
1	Q	942	LEU	4.6
1	G	1301	VAL	4.5
1	E	1697	LEU	4.5
1	C	1777	GLY	4.5
1	C	1792	ILE	4.4
1	G	1347	LEU	4.3
1	E	1025	ALA	4.3
1	Q	946	ALA	4.3
1	F	1971	PHE	4.2
1	E	1221	ALA	4.1
1	L	1985	ALA	4.1
1	R	1669	LEU	4.0
1	M	1886	VAL	4.0
1	N	945	ALA	4.0
1	H	1971	PHE	4.0
1	R	1654	VAL	4.0
1	Q	1571	VAL	3.9
1	L	1784	MET	3.9
1	C	1274	VAL	3.9
1	H	1602	TRP	3.9
1	A	1324	VAL	3.9
1	A	1221	ALA	3.9
1	J	1669	LEU	3.8
1	G	1769	ILE	3.8
1	P	948	CYS	3.8
1	L	1838	ALA	3.8
1	C	1222	GLY	3.7
1	N	1907	ALA	3.7
1	Q	947	TYR	3.7
1	E	1729	ILE	3.7
1	Q	1102	CYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	1221	ALA	3.6
1	P	1221	ALA	3.6
1	L	1780	LEU	3.5
1	L	1882	LEU	3.5
1	E	1549	GLY	3.5
1	I	1106	VAL	3.5
1	E	1761	PHE	3.5
1	N	1781	ALA	3.5
1	A	1323	VAL	3.5
1	E	1074	THR	3.5
1	Q	943	PRO	3.5
1	L	962	THR	3.5
1	A	1274	VAL	3.5
1	L	1793	VAL	3.5
1	P	1769	ILE	3.4
1	F	1768	VAL	3.4
1	J	1971	PHE	3.4
1	C	948	CYS	3.4
1	K	1929	GLN	3.3
1	R	1681	VAL	3.3
1	J	1222	GLY	3.3
1	L	1971	PHE	3.3
1	M	1794	VAL	3.3
1	Q	1172	LEU	3.3
1	C	1603	GLY	3.3
1	R	1100	ASP	3.3
1	H	1222	GLY	3.3
1	Q	1029	ASP	3.2
1	G	1222	GLY	3.2
1	Q	1128	LEU	3.2
1	N	1782	GLU	3.2
1	N	1221	ALA	3.2
1	E	1274	VAL	3.2
1	M	1759	PRO	3.2
1	G	1308	ALA	3.2
1	G	1304	LEU	3.2
1	D	1761	PHE	3.1
1	F	1792	ILE	3.1
1	C	1983	GLY	3.1
1	B	885	ASP	3.1
1	G	1076	VAL	3.1
1	L	960	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1880	TRP	3.1
1	F	1506	GLY	3.1
1	L	1908	LEU	3.1
1	B	1842	GLY	3.1
1	E	1164	THR	3.1
1	J	1221	ALA	3.0
1	F	1222	GLY	3.0
1	G	1195	ILE	3.0
1	L	1967	GLY	3.0
1	F	1573	GLN	3.0
1	N	923	VAL	3.0
1	Q	899	SER	3.0
1	Q	944	GLY	3.0
1	Q	1103	PHE	3.0
1	C	1221	ALA	3.0
1	Q	1107	ILE	2.9
1	R	1655	GLU	2.9
1	B	1971	PHE	2.9
1	B	1540	GLY	2.9
1	D	1544	GLY	2.9
1	Q	950	MET	2.9
1	C	1276	VAL	2.9
1	P	1879	ALA	2.9
1	M	1311	LEU	2.9
1	C	1772	GLY	2.9
1	H	1076	VAL	2.9
1	J	1105	SER	2.9
1	F	1769	ILE	2.9
1	I	1660	ASP	2.9
1	D	1351	VAL	2.9
1	L	1825	ILE	2.9
1	L	1860	LEU	2.9
1	K	1323	VAL	2.9
1	M	1074	THR	2.9
1	A	1399	LEU	2.9
1	A	1322	TYR	2.9
1	E	943	PRO	2.9
1	I	1471	PRO	2.9
1	Q	1124	GLY	2.8
1	C	1193	LEU	2.8
1	K	1221	ALA	2.8
1	P	1971	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	1399	LEU	2.8
1	G	1773	LEU	2.8
1	P	1294	ALA	2.8
1	Q	1060	ALA	2.8
1	R	1103	PHE	2.8
1	A	1217	LEU	2.8
1	L	1818	ILE	2.8
1	D	1909	VAL	2.8
1	H	1781	ALA	2.8
1	L	1770	THR	2.8
1	M	1102	CYS	2.8
1	C	1780	LEU	2.8
1	G	1032	LEU	2.8
1	Q	998	VAL	2.8
1	D	1222	GLY	2.8
1	C	1275	ALA	2.8
1	P	1400	CYS	2.8
1	O	1683	LEU	2.8
1	P	1993	LEU	2.8
1	E	1539	VAL	2.8
1	O	1744	PRO	2.8
1	D	1533	GLU	2.8
1	L	1983	GLY	2.8
1	D	1193	LEU	2.7
1	A	1382	SER	2.7
1	H	1139	TYR	2.7
1	A	1222	GLY	2.7
1	C	1873	ALA	2.7
1	C	1972	GLU	2.7
1	N	1776	LEU	2.7
1	G	1278	VAL	2.7
1	M	948	CYS	2.7
1	D	2006	PHE	2.7
1	D	1826	ALA	2.7
1	D	1106	VAL	2.7
1	D	1683	LEU	2.7
1	I	948	CYS	2.7
1	K	1347	LEU	2.7
1	G	916	GLU	2.7
1	G	1109	HIS	2.7
1	Q	1142	SER	2.7
1	F	1575	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1219	ILE	2.7
1	B	1386	GLU	2.7
1	N	1603	GLY	2.6
1	Q	1588	ALA	2.6
1	F	1094	VAL	2.6
1	F	1681	VAL	2.6
1	Q	1075	VAL	2.6
1	N	1850	HIS	2.6
1	Q	1143	ARG	2.6
1	L	1781	ALA	2.6
1	O	1102	CYS	2.6
1	M	1883	HIS	2.6
1	Q	1104	GLN	2.6
1	E	1880	TRP	2.6
1	G	1930	TRP	2.6
1	Q	1513	TRP	2.6
1	Q	989	THR	2.6
1	D	1768	VAL	2.6
1	M	1195	ILE	2.6
1	J	1538	ALA	2.6
1	L	1031	LEU	2.6
1	J	1992	TRP	2.6
1	P	1655	GLU	2.6
1	F	1218	VAL	2.6
1	H	1902	PHE	2.6
1	B	1382	SER	2.6
1	E	1760	VAL	2.6
1	C	1602	TRP	2.5
1	R	1094	VAL	2.5
1	B	1304	LEU	2.5
1	P	1780	LEU	2.5
1	D	1377	GLN	2.5
1	F	1538	ALA	2.5
1	L	1567	ALA	2.5
1	N	1755	PRO	2.5
1	F	1107	ILE	2.5
1	F	1105	SER	2.5
1	C	1218	VAL	2.5
1	G	1793	VAL	2.5
1	K	1324	VAL	2.5
1	Q	968	LEU	2.5
1	D	1347	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1780	LEU	2.5
1	H	1908	LEU	2.5
1	L	1794	VAL	2.5
1	J	1230	ALA	2.5
1	D	1697	LEU	2.5
1	C	2006	PHE	2.5
1	G	1902	PHE	2.5
1	G	2002	PHE	2.5
1	L	1808	ILE	2.5
1	G	910	LEU	2.5
1	J	954	ALA	2.4
1	J	1800	PRO	2.4
1	Q	1423	LEU	2.4
1	G	1820	VAL	2.4
1	L	1883	HIS	2.4
1	N	1534	HIS	2.4
1	F	1698	LEU	2.4
1	P	1849	LEU	2.4
1	K	1102	CYS	2.4
1	F	1576	ILE	2.4
1	Q	1014	LEU	2.4
1	B	1222	GLY	2.4
1	A	1106	VAL	2.4
1	D	1311	LEU	2.4
1	N	1423	LEU	2.4
1	N	1780	LEU	2.4
1	H	1850	HIS	2.4
1	L	1850	HIS	2.4
1	H	1231	ALA	2.4
1	J	1851	ALA	2.4
1	A	1074	THR	2.4
1	M	1301	VAL	2.4
1	B	1363	ILE	2.4
1	A	1386	GLU	2.4
1	F	1161	ALA	2.4
1	N	950	MET	2.4
1	R	1640	GLN	2.4
1	N	1971	PHE	2.4
1	C	1698	LEU	2.4
1	F	1098	LEU	2.4
1	H	1849	LEU	2.4
1	N	1108	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	1021	GLU	2.4
1	Q	920	GLN	2.3
1	B	1530	GLY	2.3
1	E	1321	LEU	2.3
1	Q	1523	LEU	2.3
1	H	954	ALA	2.3
1	H	1226	GLU	2.3
1	P	1542	ALA	2.3
1	D	1103	PHE	2.3
1	E	1219	ILE	2.3
1	M	1276	VAL	2.3
1	H	1221	ALA	2.3
1	P	1781	ALA	2.3
1	P	1226	GLU	2.3
1	E	1217	LEU	2.3
1	R	942	LEU	2.3
1	C	1301	VAL	2.3
1	F	1102	CYS	2.3
1	N	947	TYR	2.3
1	J	1714	GLU	2.3
1	J	1780	LEU	2.3
1	D	1221	ALA	2.3
1	G	1033	ALA	2.3
1	Q	1144	ILE	2.3
1	N	1226	GLU	2.3
1	R	1660	ASP	2.3
1	D	1465	VAL	2.3
1	C	1599	LEU	2.3
1	G	1193	LEU	2.3
1	Q	1683	LEU	2.3
1	D	1277	ILE	2.3
1	F	1437	VAL	2.3
1	G	1276	VAL	2.3
1	J	1777	GLY	2.3
1	Q	1681	VAL	2.3
1	D	1498	HIS	2.2
1	G	1780	LEU	2.2
1	G	1849	LEU	2.2
1	N	1991	SER	2.2
1	E	1605	GLU	2.2
1	K	1222	GLY	2.2
1	C	1985	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1655	GLU	2.2
1	C	1794	VAL	2.2
1	K	1290	VAL	2.2
1	P	1214	GLY	2.2
1	Q	1013	VAL	2.2
1	Q	1061	GLY	2.2
1	R	908	VAL	2.2
1	Q	1158	LEU	2.2
1	A	885	ASP	2.2
1	B	1542	ALA	2.2
1	D	1034	ALA	2.2
1	M	2008	ALA	2.2
1	O	1407	ALA	2.2
1	C	974	LEU	2.2
1	E	942	LEU	2.2
1	E	1262	LEU	2.2
1	H	1193	LEU	2.2
1	Q	1120	LEU	2.2
1	Q	1174	LEU	2.2
1	C	1401	PRO	2.2
1	E	1649	PHE	2.2
1	N	1400	CYS	2.2
1	A	1321	LEU	2.2
1	C	1081	LEU	2.2
1	F	1566	SER	2.2
1	J	1220	LEU	2.2
1	C	1351	VAL	2.2
1	P	1487	VAL	2.2
1	L	1878	GLY	2.2
1	P	1222	GLY	2.2
1	I	1665	THR	2.2
1	A	1102	CYS	2.2
1	H	1632	LEU	2.2
1	R	1099	LEU	2.2
1	F	1868	VAL	2.2
1	A	1908	LEU	2.2
1	E	1024	ALA	2.1
1	H	1588	ALA	2.1
1	M	1304	LEU	2.2
1	F	1714	GLU	2.1
1	N	1655	GLU	2.1
1	C	1834	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	1347	LEU	2.1
1	B	1221	ALA	2.1
1	C	1905	ALA	2.1
1	L	1968	ALA	2.1
1	I	1640	GLN	2.1
1	Q	1113	GLN	2.1
1	F	1909	VAL	2.1
1	M	1076	VAL	2.1
1	N	1768	VAL	2.1
1	B	1506	GLY	2.1
1	H	918	LEU	2.1
1	B	1537	ALA	2.1
1	Q	994	ALA	2.1
1	G	1235	SER	2.1
1	F	1941	ILE	2.1
1	L	1769	ILE	2.1
1	P	1219	ILE	2.1
1	E	1233	VAL	2.1
1	Q	1122	PRO	2.1
1	J	1032	LEU	2.1
1	E	1762	ARG	2.1
1	C	1219	ILE	2.1
1	H	1459	ASN	2.1
1	P	1307	ILE	2.1
1	I	1103	PHE	2.1
1	Q	965	VAL	2.1
1	H	1777	GLY	2.1
1	B	1759	PRO	2.1
1	K	1821	GLU	2.1
1	M	1384	GLU	2.1
1	P	1384	GLU	2.1
1	E	1715	ILE	2.1
1	G	1804	SER	2.1
1	D	1982	ASN	2.1
1	O	1539	VAL	2.1
1	M	1541	LEU	2.1
1	P	1975	LEU	2.1
1	Q	918	LEU	2.1
1	E	1343	GLY	2.1
1	N	1222	GLY	2.1
1	A	1384	GLU	2.1
1	N	1143	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1307	ILE	2.1
1	F	1705	ILE	2.1
1	N	1230	ALA	2.1
1	A	1780	LEU	2.1
1	G	1120	LEU	2.1
1	P	1882	LEU	2.1
1	Q	1035	HIS	2.0
1	D	1759	PRO	2.0
1	N	1073	PRO	2.0
1	H	1852	ALA	2.0
1	I	1482	SER	2.0
1	P	945	ALA	2.0
1	C	1102	CYS	2.0
1	C	1683	LEU	2.0
1	E	1276	VAL	2.0
1	Q	1067	VAL	2.0
1	E	1883	HIS	2.0
1	B	1195	ILE	2.0
1	L	1530	GLY	2.0
1	P	1486	GLY	2.0
1	E	1759	PRO	2.0
1	J	1246	THR	2.0
1	B	1384	GLU	2.0
1	M	1513	TRP	2.0
1	D	1975	LEU	2.0
1	L	1141	LEU	2.0
1	Q	1667	LEU	2.0
1	L	1020	ALA	2.0
1	B	1218	VAL	2.0
1	D	1701	VAL	2.0
1	E	1278	VAL	2.0
1	J	1076	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

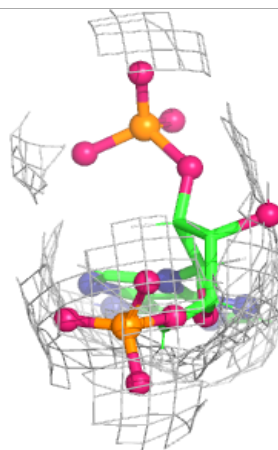
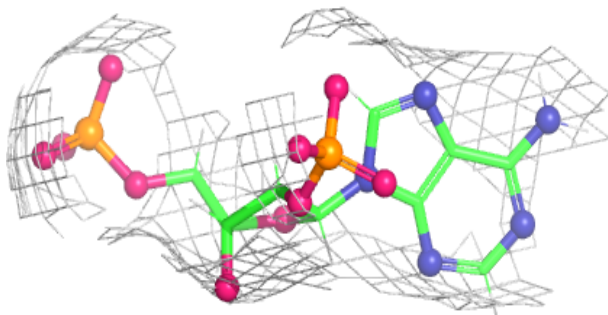
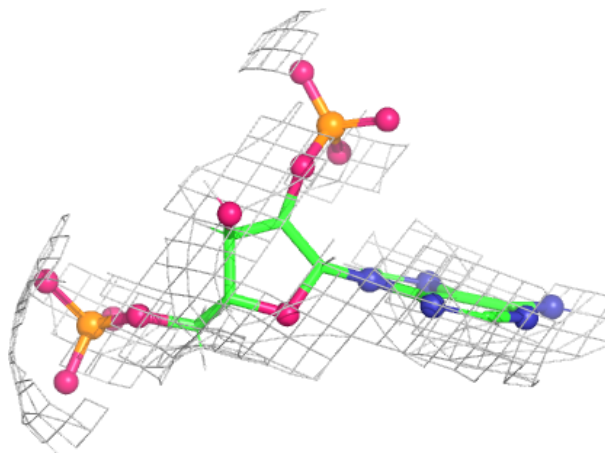
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	M	3002	27/48	0.58	0.10	233,235,240,240	0
2	NAP	Q	3001	48/48	0.71	0.15	222,225,232,235	0
2	NAP	A	3002	27/48	0.75	0.10	229,235,241,242	0
2	NAP	P	3002	27/48	0.79	0.09	191,203,209,210	0
2	NAP	G	3002	27/48	0.82	0.08	195,201,205,205	0
2	NAP	D	3002	27/48	0.84	0.08	193,197,199,199	0
2	NAP	R	3001	48/48	0.84	0.12	210,221,233,234	0
2	NAP	H	3002	27/48	0.85	0.07	179,187,190,190	0
2	NAP	J	3002	27/48	0.86	0.07	166,169,175,176	0
2	NAP	N	3002	27/48	0.87	0.08	156,165,181,182	0
2	NAP	H	3001	48/48	0.88	0.13	129,146,170,171	0
2	NAP	F	3001	48/48	0.88	0.13	165,176,183,184	0
2	NAP	F	3002	27/48	0.89	0.07	164,168,171,171	0
2	NAP	E	3001	48/48	0.89	0.11	181,193,197,198	0
2	NAP	K	3002	27/48	0.89	0.08	135,151,159,161	0
2	NAP	C	3002	31/48	0.89	0.07	141,162,203,205	0
2	NAP	B	3002	27/48	0.90	0.07	120,134,148,148	0
2	NAP	D	3001	48/48	0.92	0.11	114,124,138,139	0
2	NAP	C	3001	48/48	0.92	0.10	110,132,150,153	0
2	NAP	J	3001	48/48	0.92	0.11	115,126,149,153	0
2	NAP	N	3001	48/48	0.92	0.12	141,152,175,175	0
2	NAP	B	3001	48/48	0.93	0.10	103,111,127,129	0
2	NAP	P	3001	48/48	0.93	0.11	106,124,132,136	0
2	NAP	L	3001	48/48	0.93	0.09	110,118,130,134	0
2	NAP	I	3001	48/48	0.93	0.11	133,144,150,151	0
2	NAP	K	3001	48/48	0.93	0.11	109,123,141,145	0
2	NAP	A	3001	48/48	0.94	0.10	104,124,136,137	0
2	NAP	M	3001	48/48	0.94	0.09	132,144,158,161	0
2	NAP	G	3001	48/48	0.94	0.08	117,132,158,158	0
2	NAP	O	3001	48/48	0.95	0.09	101,113,135,138	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.

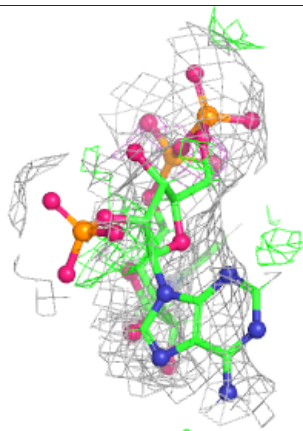
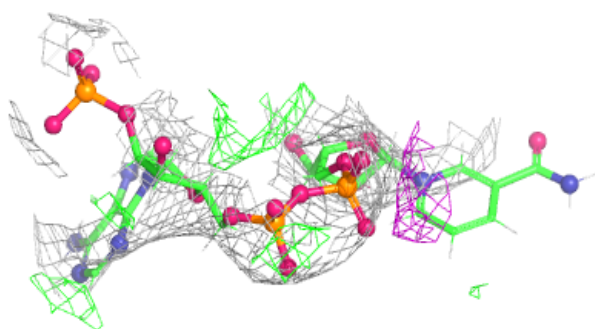
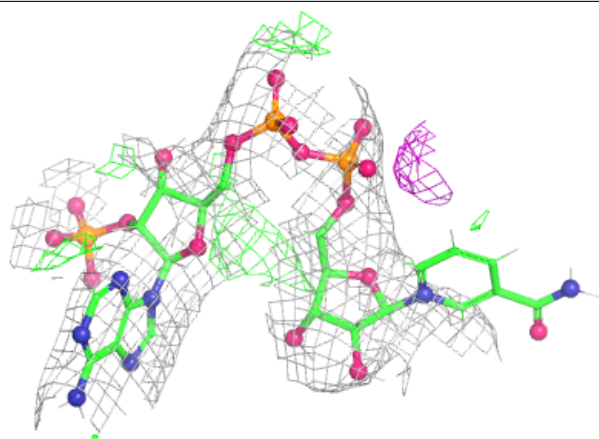
Electron density around NAP M 3002:

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

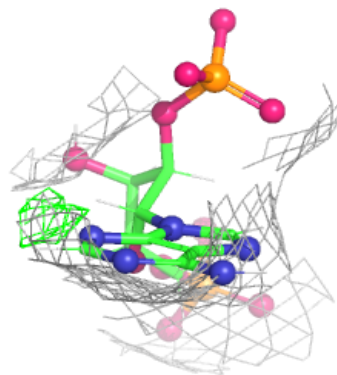
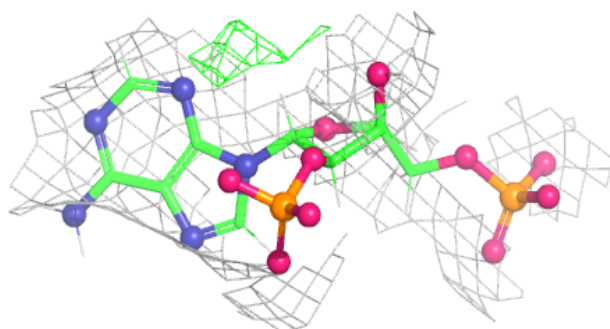
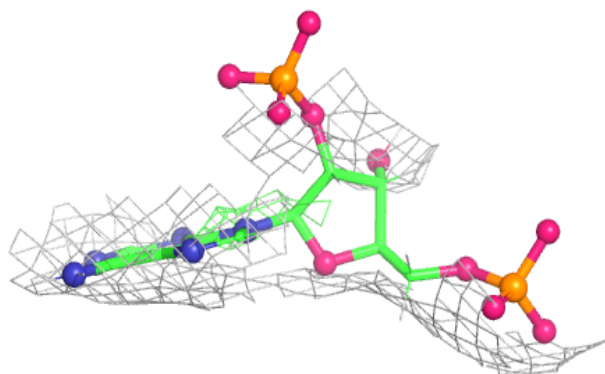


Electron density around NAP Q 3001:

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

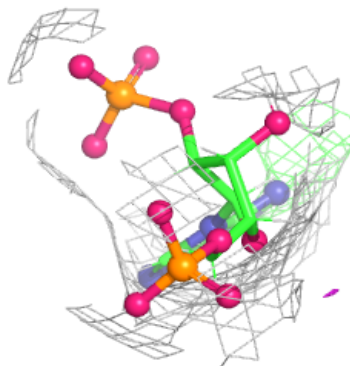
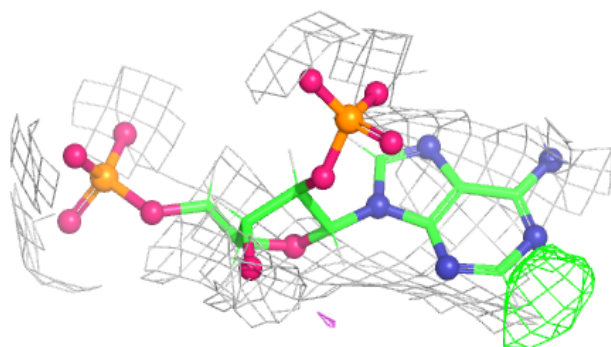
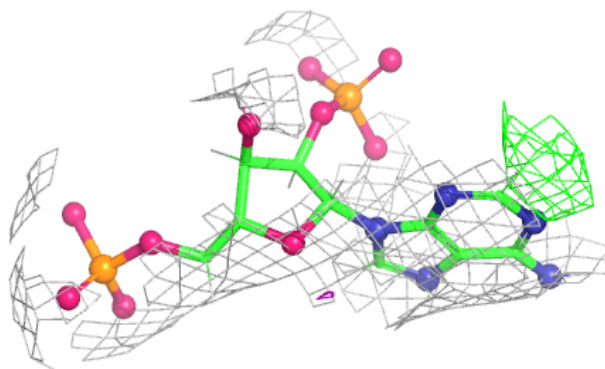
**Electron density around NAP A 3002:**

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

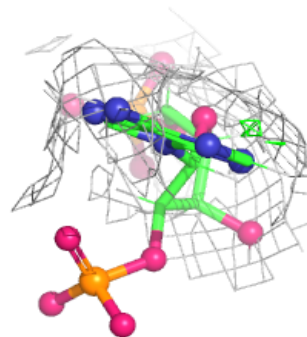
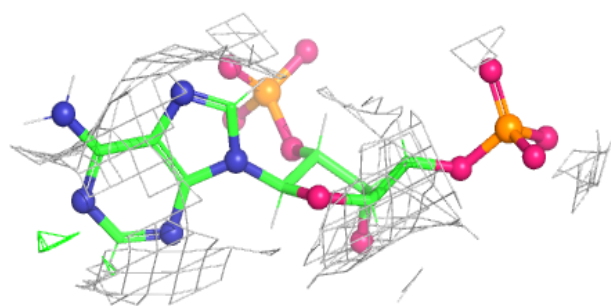
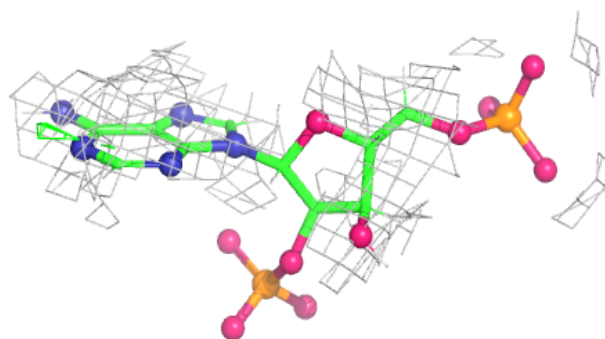


Electron density around NAP P 3002:

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

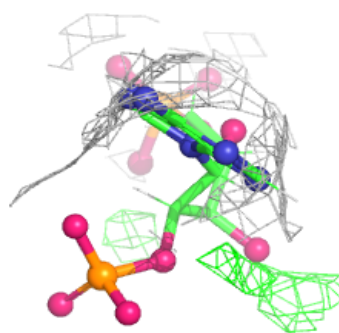
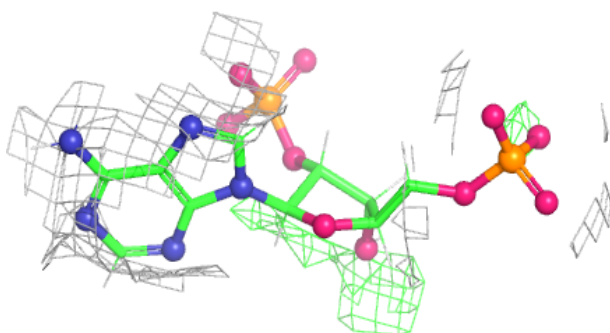
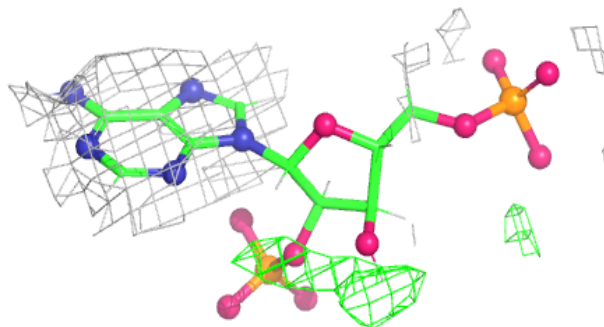
**Electron density around NAP G 3002:**

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

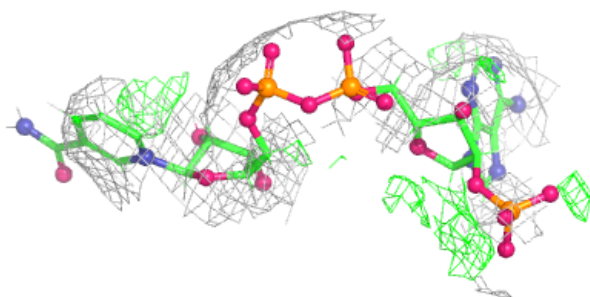
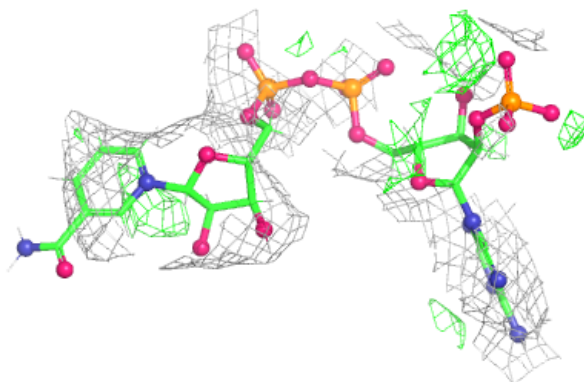


Electron density around NAP D 3002:

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

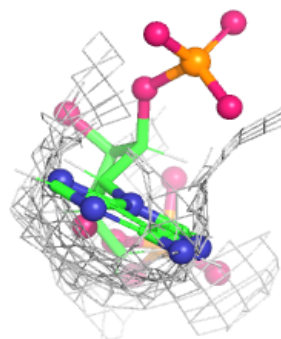
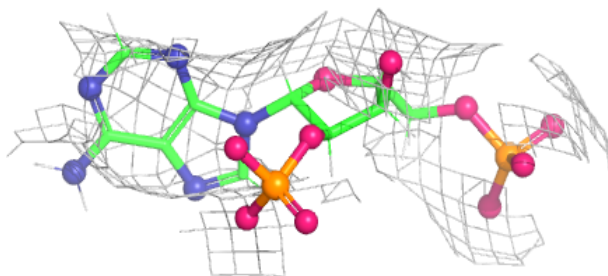
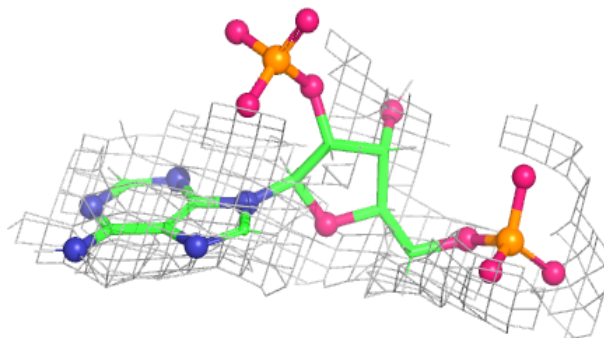
**Electron density around NAP R 3001:**

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

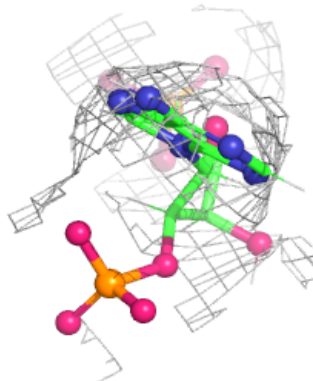
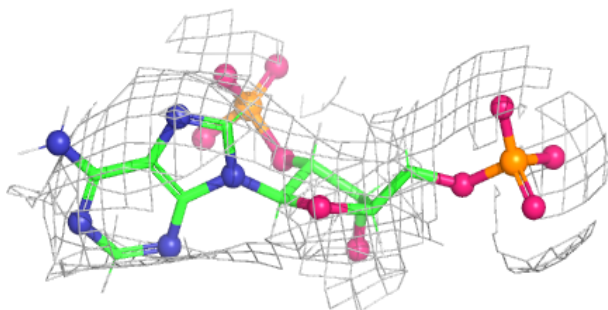
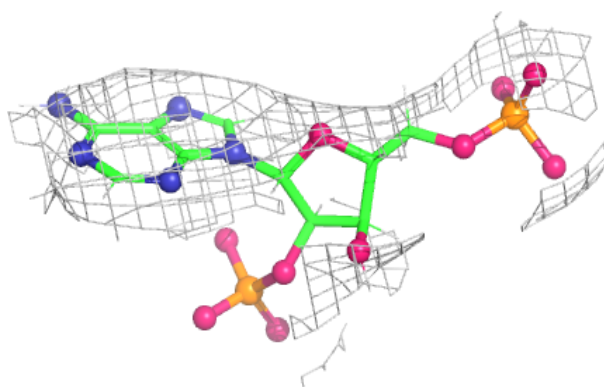


Electron density around NAP H 3002:

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

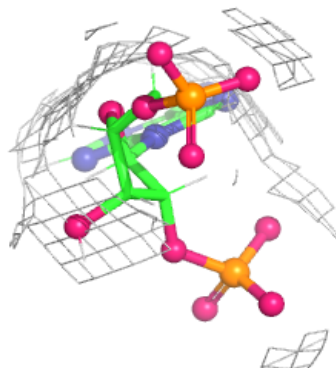
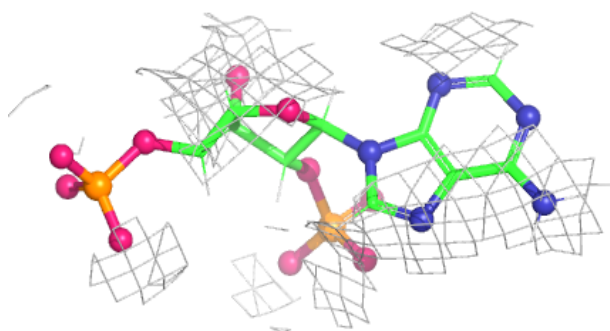
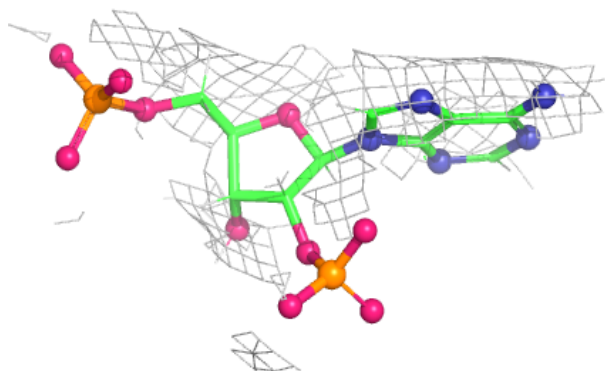
**Electron density around NAP J 3002:**

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

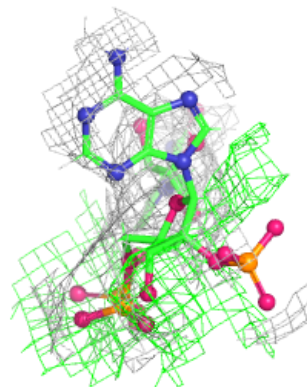
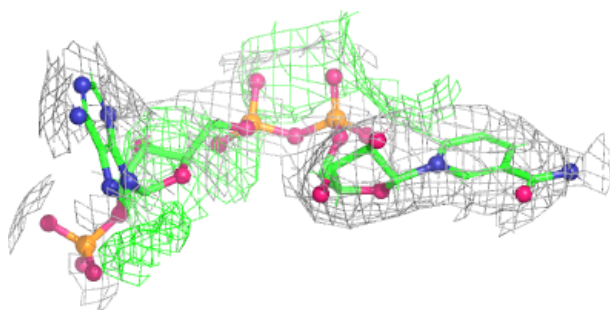
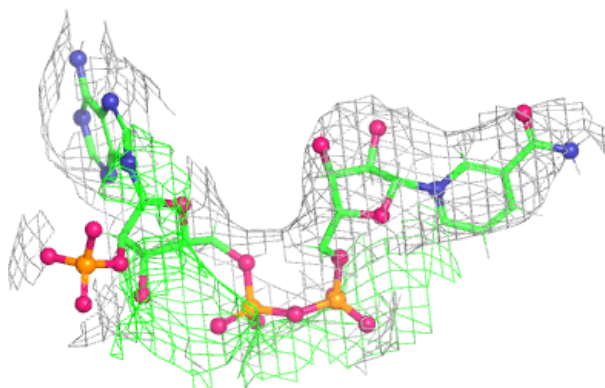


Electron density around NAP N 3002:

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

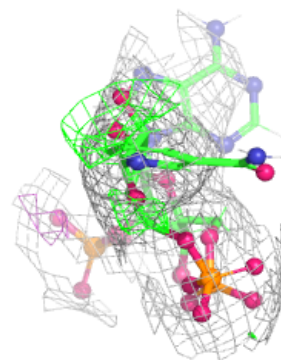
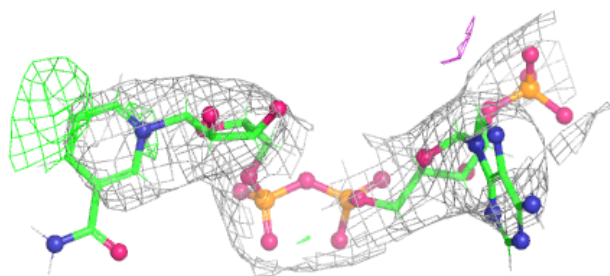
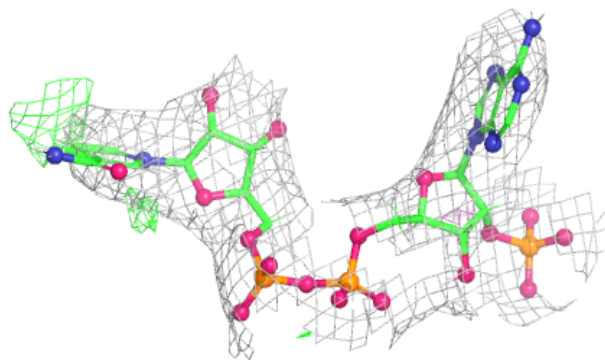
**Electron density around NAP H 3001:**

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

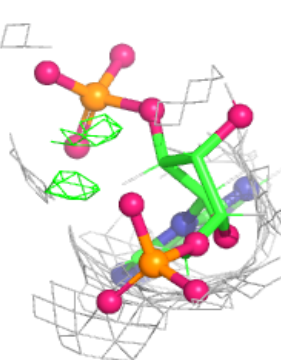
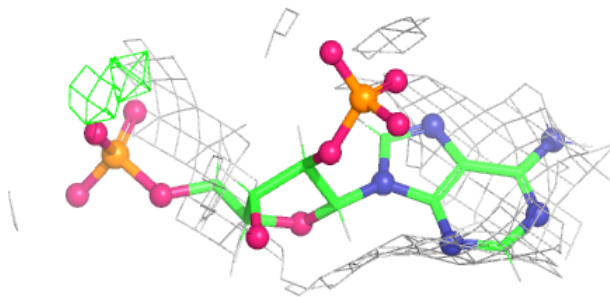
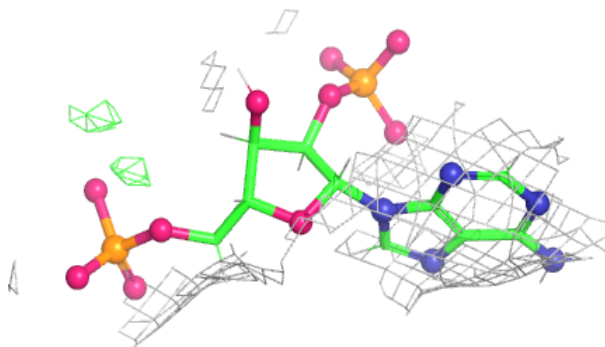


Electron density around NAP F 3001:

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

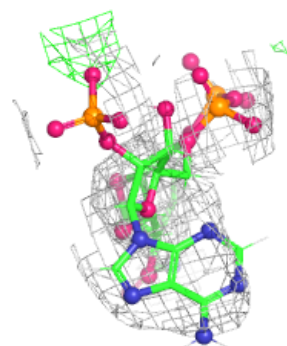
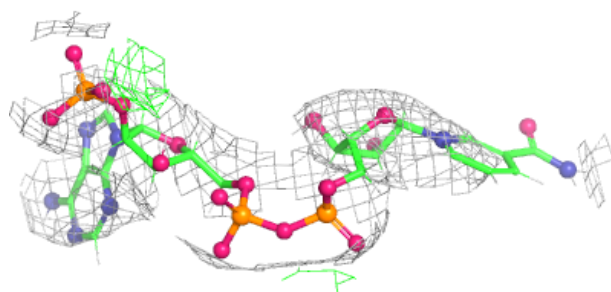
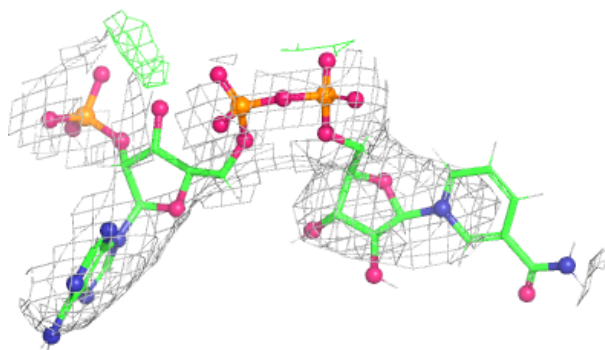
**Electron density around NAP F 3002:**

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

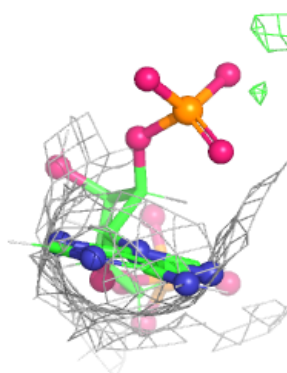
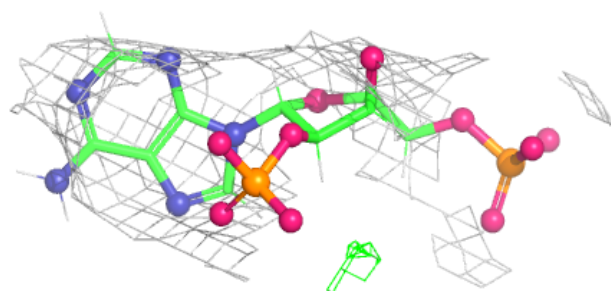
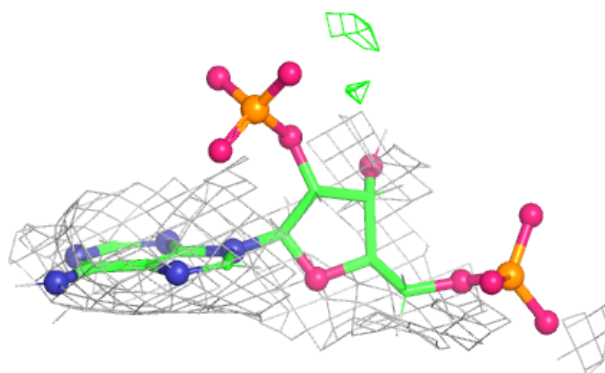


Electron density around NAP E 3001:

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

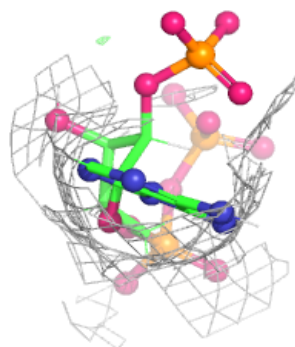
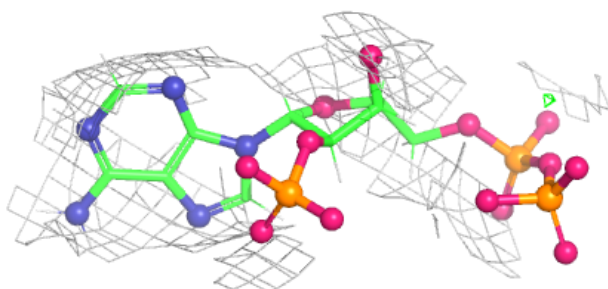
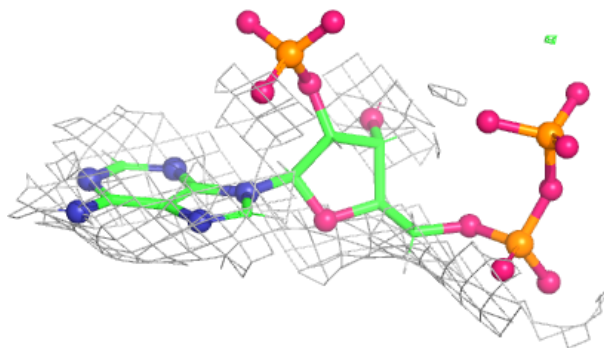
**Electron density around NAP K 3002:**

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

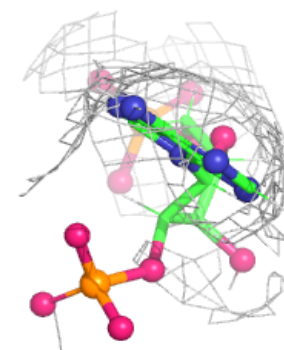
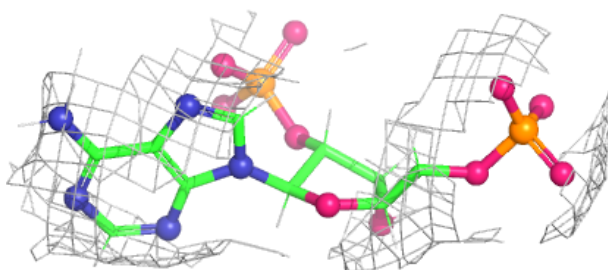
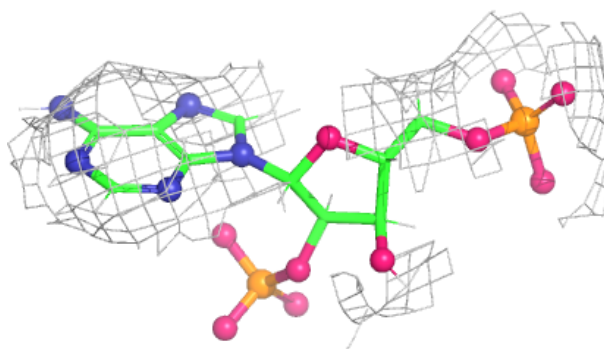


Electron density around NAP C 3002:

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

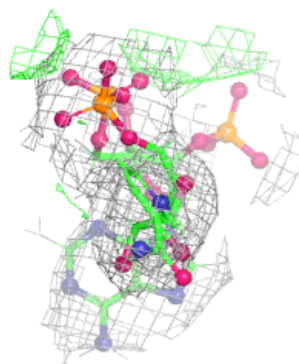
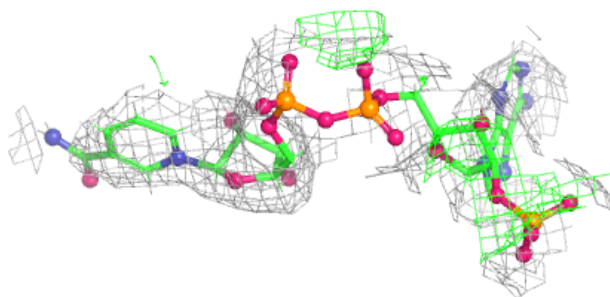
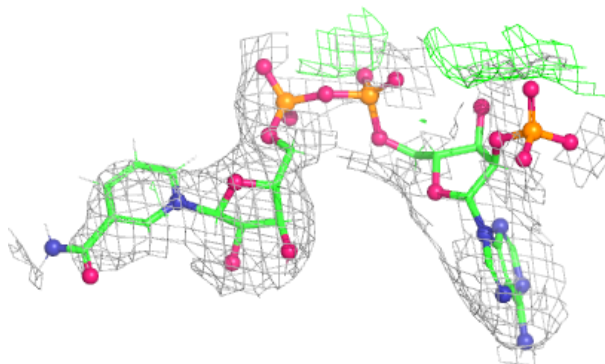
**Electron density around NAP B 3002:**

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

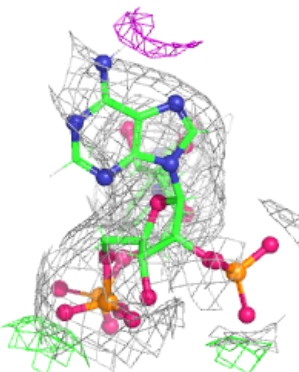
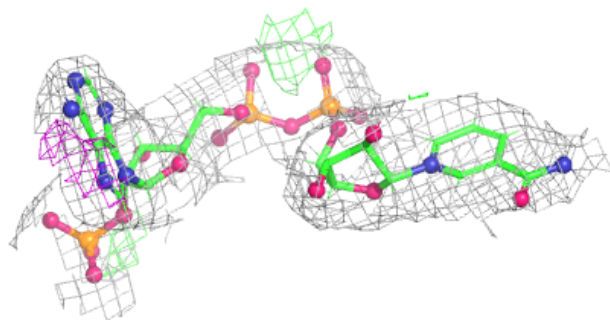
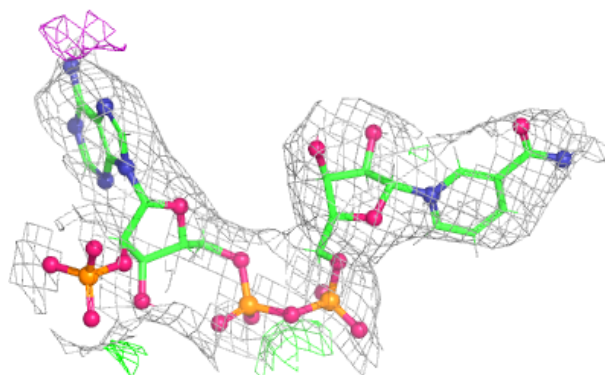


Electron density around NAP D 3001:

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

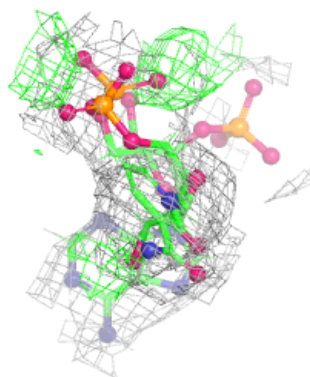
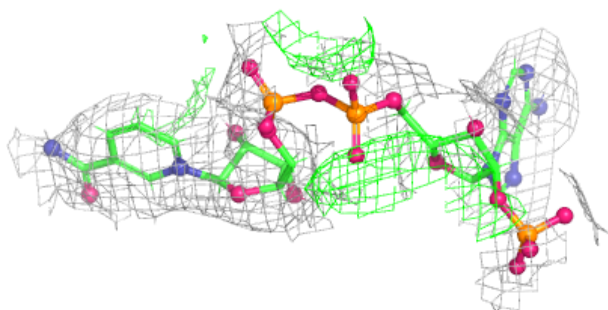
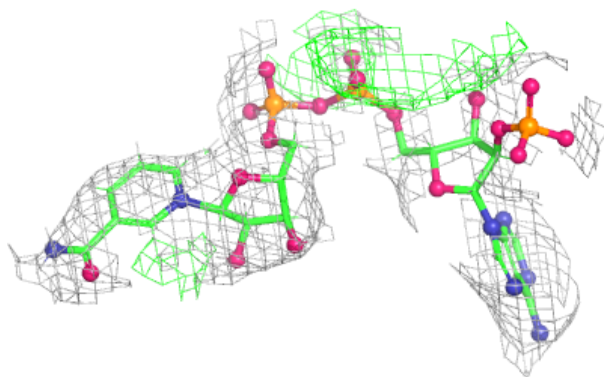
**Electron density around NAP C 3001:**

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

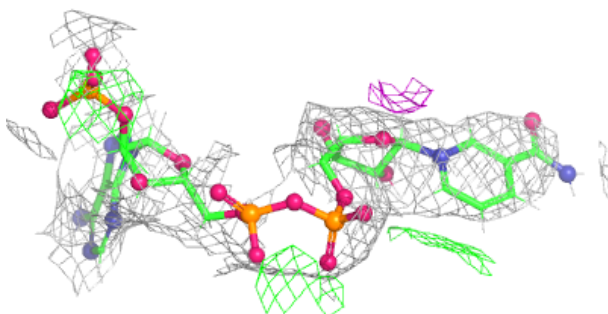
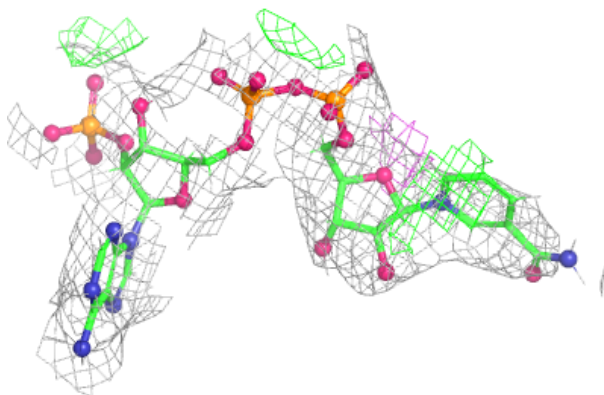


Electron density around NAP J 3001:

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

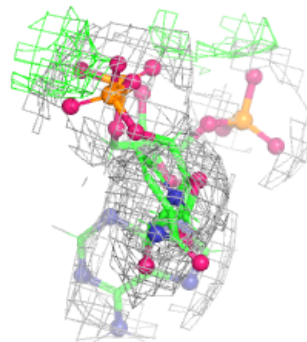
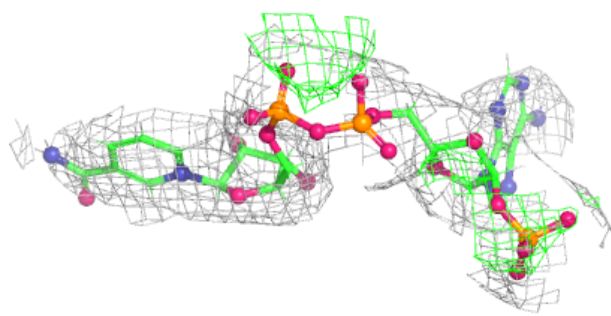
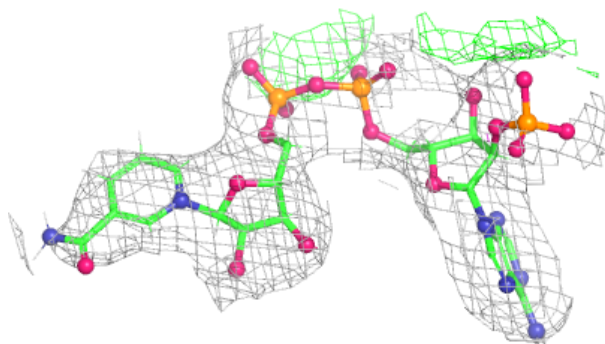
**Electron density around NAP N 3001:**

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

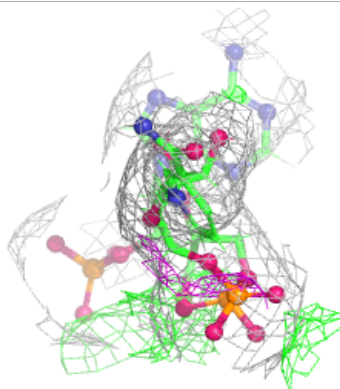
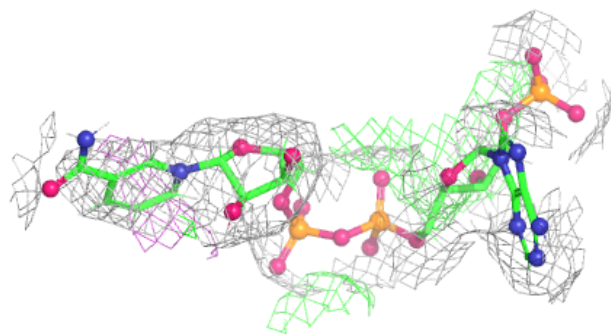
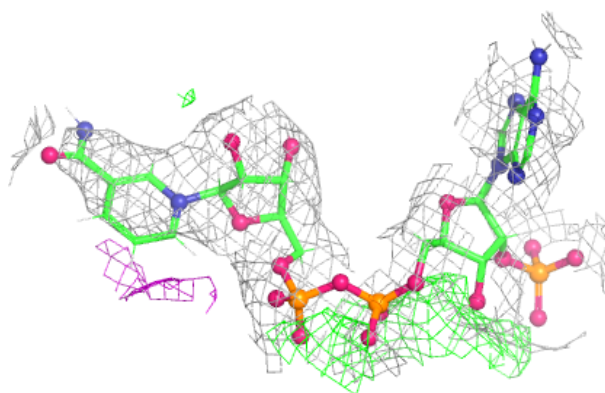


Electron density around NAP B 3001:

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

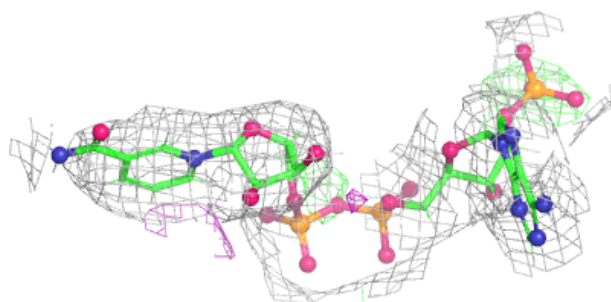
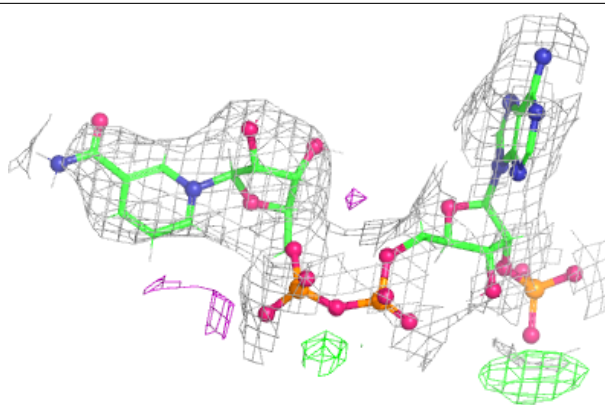
**Electron density around NAP P 3001:**

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

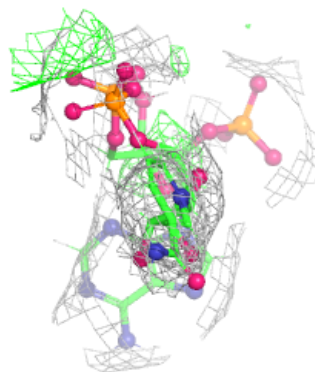
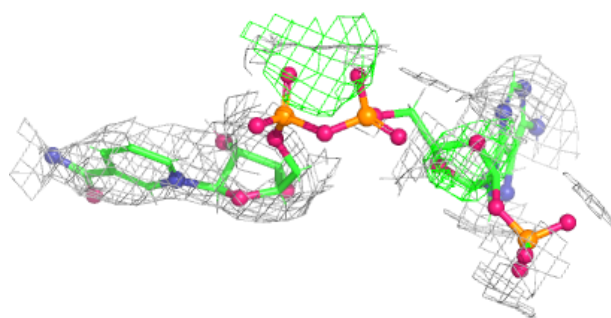
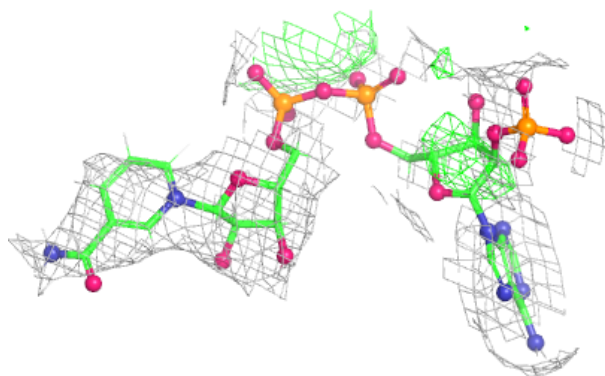


Electron density around NAP L 3001:

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

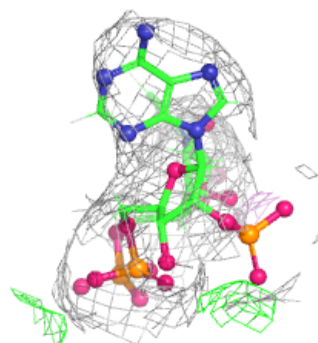
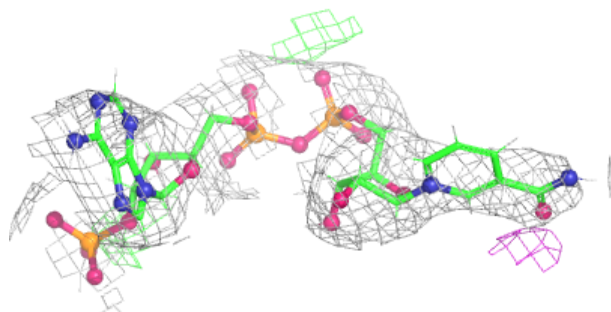
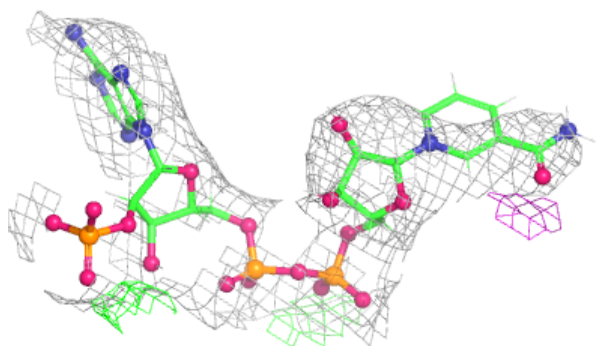
**Electron density around NAP I 3001:**

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

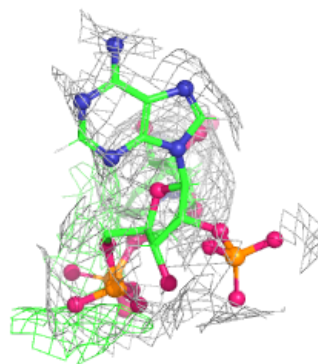
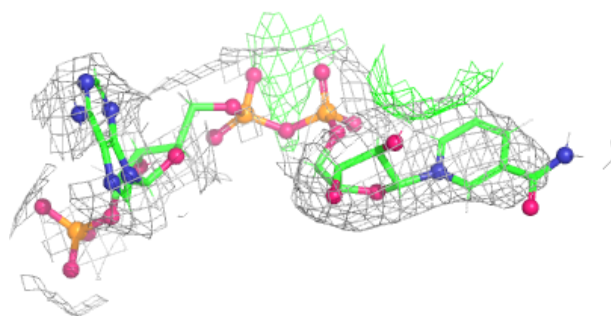
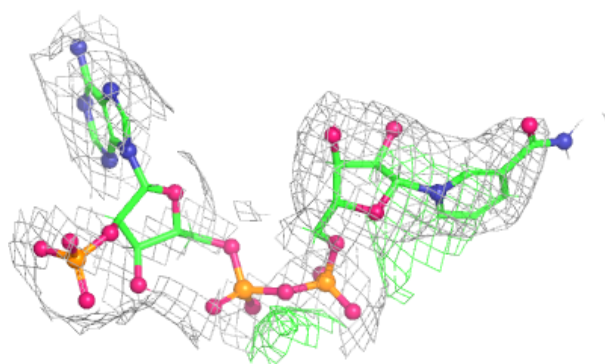


Electron density around NAP K 3001:

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

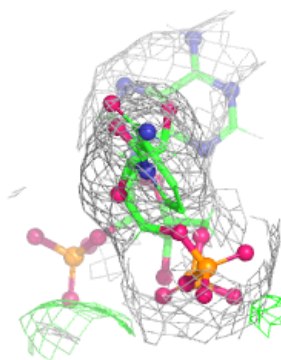
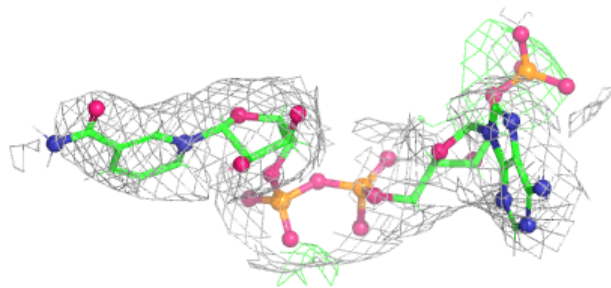
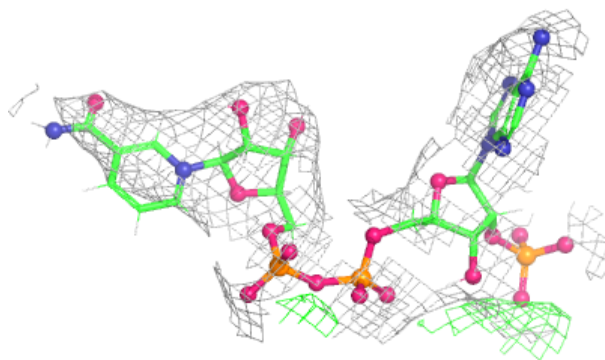
**Electron density around NAP A 3001:**

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

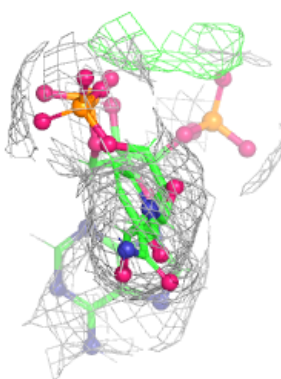
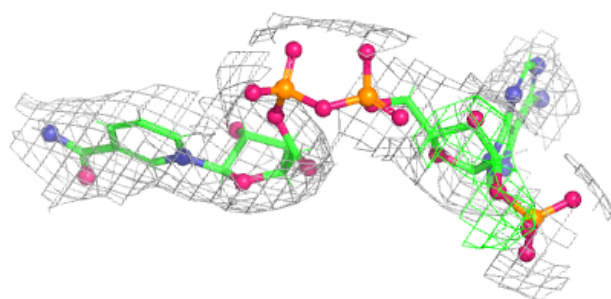
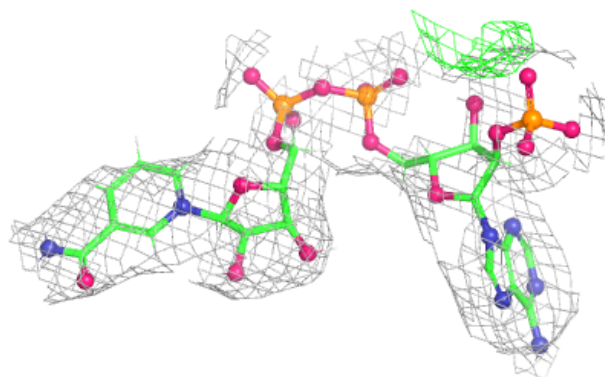


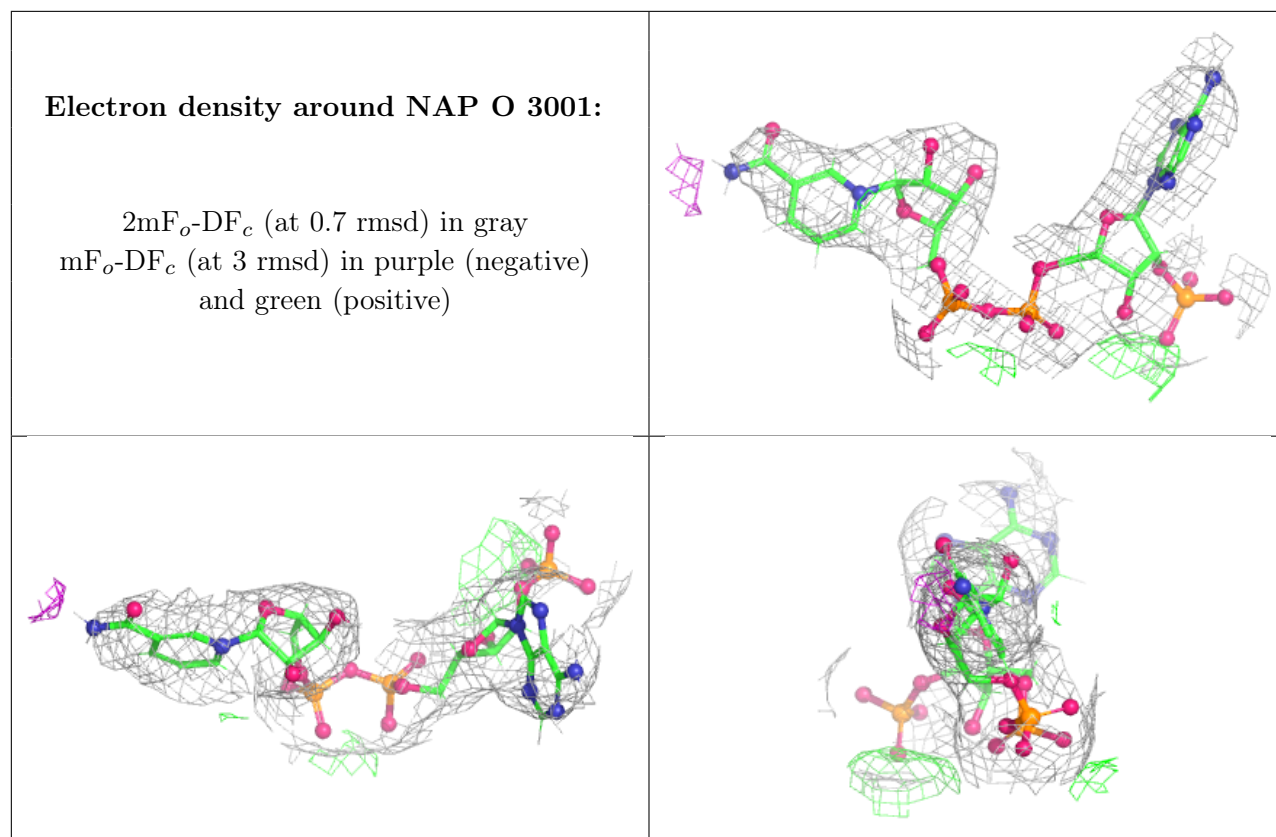
Electron density around NAP M 3001:

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

**Electron density around NAP G 3001:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.